



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 11:48 AM EDT

PDB ID : 2MLS  
BMRB ID : 7089  
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Beta-face  
Authors : Koppiseti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.  
Deposited on : 2014-03-04

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.

The types of validation reports are described at

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

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

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)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

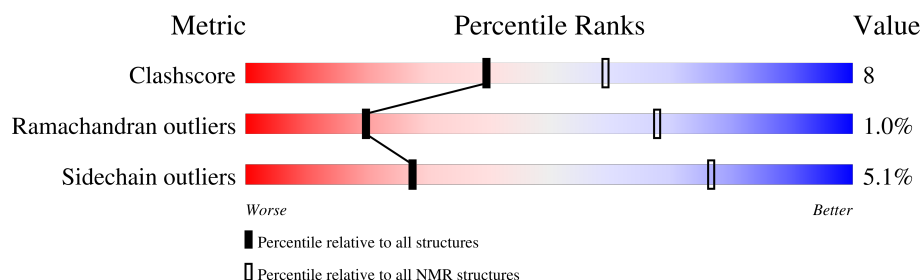
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 82%.

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	164	 81% 16% ..

## 2 Ensemble composition and analysis

This entry contains 14 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:101-A:262 (162)	0.69	8

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 5 single-model clusters were found.

Cluster number	Models
1	5, 8, 10, 13
2	11, 12, 14
3	1, 2
Single-model clusters	3; 4; 6; 7; 9

### 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2508	824	1221	225	234	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	GLU	engineered mutation	UNP P39900

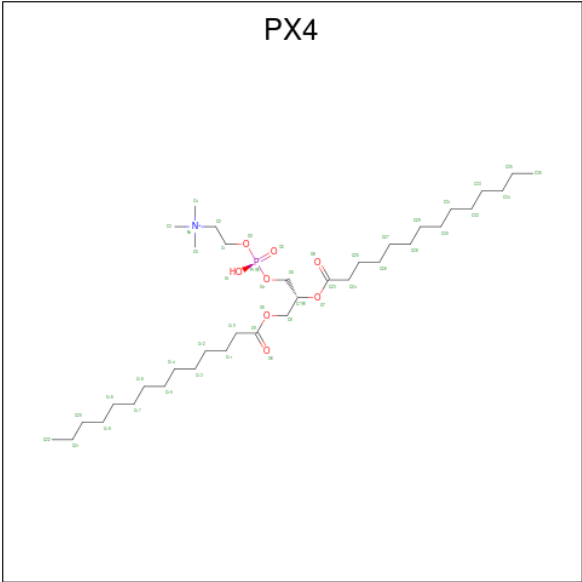
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	3	Total	Ca
			3	3

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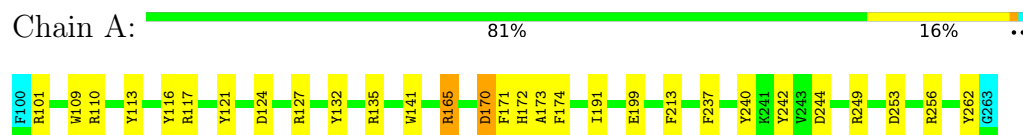
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	A	1	46	36	1	8	1
4	A	1	46	36	1	8	1
4	A	1	46	36	1	8	1
4	A	1	46	36	1	8	1
4	A	1	46	36	1	8	1
4	A	1	46	36	1	8	1

## 4 Residue-property plots

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

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

- Molecule 1: Macrophage metalloelastase

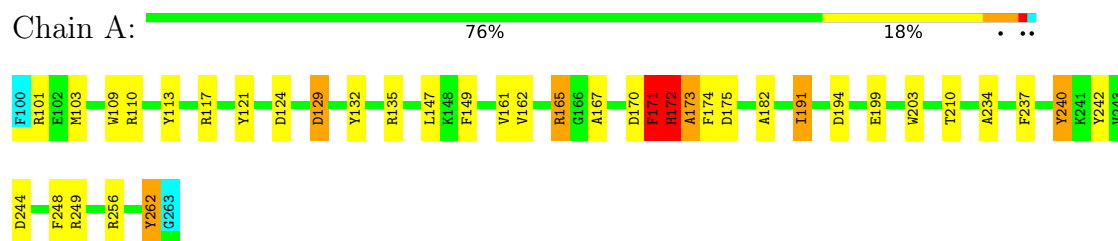


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

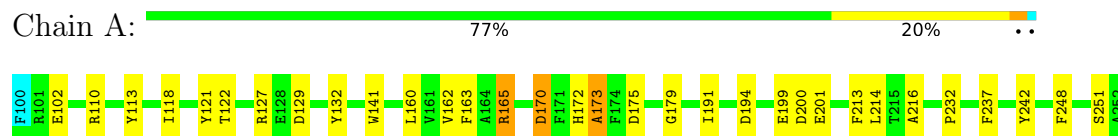
#### 4.2.1 Score per residue for model 1

- Molecule 1: Macrophage metalloelastase



#### 4.2.2 Score per residue for model 2

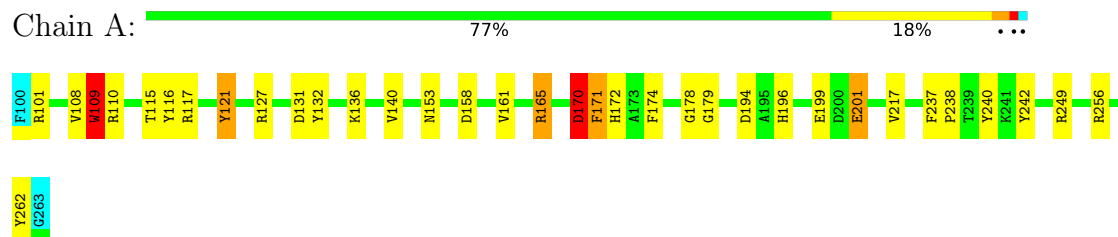
- Molecule 1: Macrophage metalloelastase





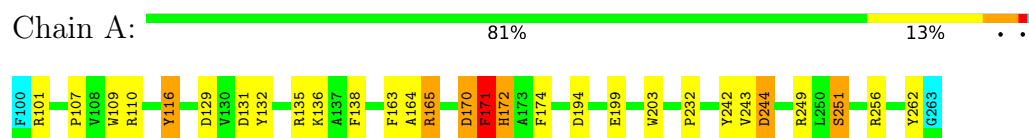
### 4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



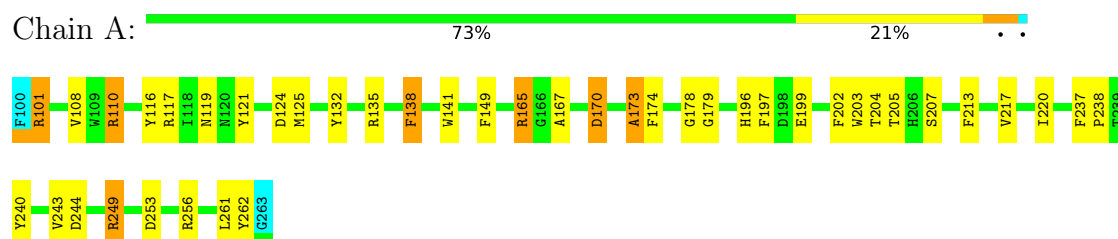
### 4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase



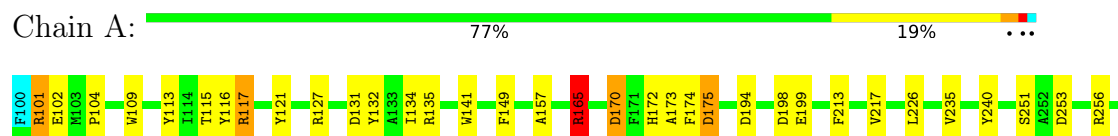
### 4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase



### 4.2.6 Score per residue for model 6

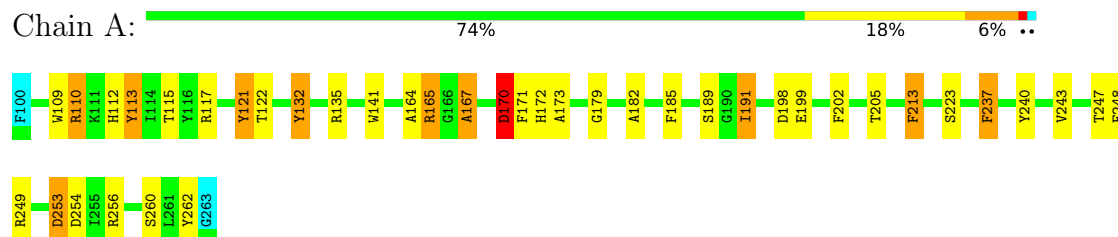
- Molecule 1: Macrophage metalloelastase





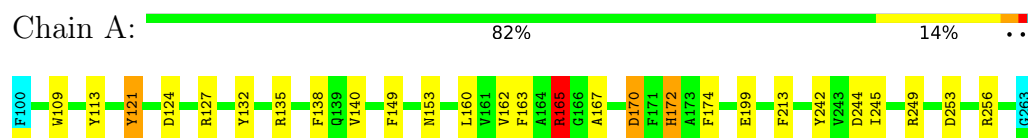
#### 4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



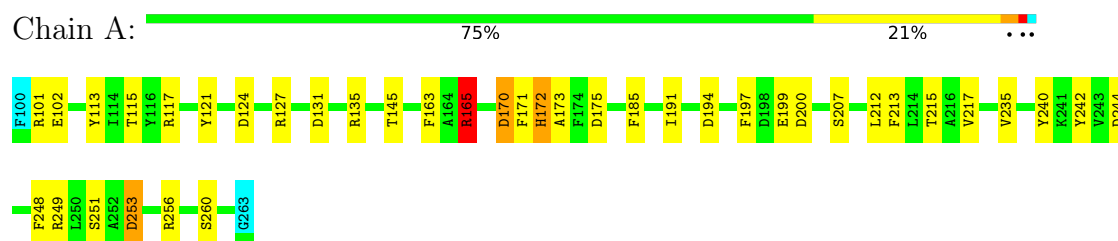
#### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Macrophage metalloelastase



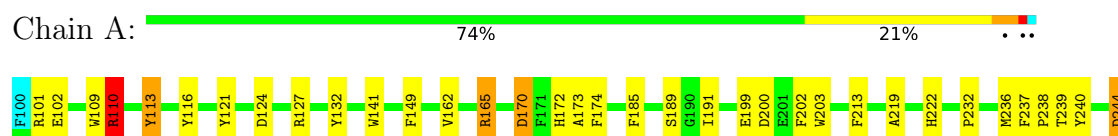
#### 4.2.9 Score per residue for model 9

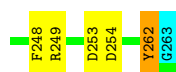
- Molecule 1: Macrophage metalloelastase



#### 4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase

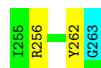
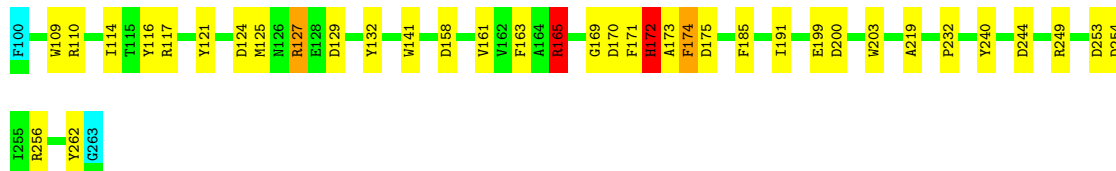




#### 4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase

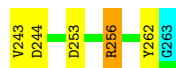
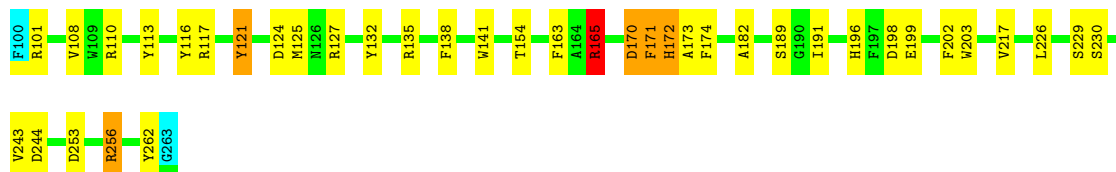
Chain A: 76% 20% ..



#### 4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase

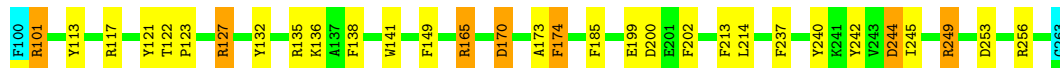
Chain A: 75% 20% ..



#### 4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase

Chain A: 80% 15% ..



#### 4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase

Chain A: 79% 16% ..



## 5 Refinement protocol and experimental data overview

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

Of the 14 calculated structures, 14 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
GROMACS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

## 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	0.57±0.00	0±0/1311 ( 0.0± 0.0%)	2.03±0.06	38±6/1779 ( 2.2± 0.4%)
All	All	0.57	0/18354 ( 0.0%)	2.03	537/24906 ( 2.2%)

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	4.9±2.3
All	All	0	68

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	110	ARG	NE-CZ-NH1	19.82	130.21	120.30	10	5
1	A	170	ASP	CB-CG-OD1	16.29	132.96	118.30	7	14
1	A	256	ARG	NE-CZ-NH1	16.04	128.32	120.30	5	9
1	A	101	ARG	NE-CZ-NH1	-15.89	112.36	120.30	6	7
1	A	197	PHE	CB-CG-CD1	15.56	131.69	120.80	5	3
1	A	197	PHE	CB-CG-CD2	-15.03	110.28	120.80	5	1
1	A	113	TYR	CB-CG-CD1	-13.32	113.01	121.00	12	3
1	A	262	TYR	CB-CG-CD1	-13.06	113.16	121.00	1	5
1	A	127	ARG	NE-CZ-NH1	13.03	126.81	120.30	13	6
1	A	165	ARG	NE-CZ-NH2	-12.96	113.82	120.30	11	6
1	A	121	TYR	CB-CG-CD1	-12.83	113.30	121.00	12	6
1	A	121	TYR	CB-CG-CD2	-12.73	113.36	121.00	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	249	ARG	NE-CZ-NH2	-12.54	114.03	120.30	11	6
1	A	262	TYR	CB-CG-CD2	-12.52	113.49	121.00	14	5
1	A	101	ARG	NE-CZ-NH2	-12.21	114.20	120.30	12	7
1	A	165	ARG	NE-CZ-NH1	12.20	126.40	120.30	8	10
1	A	127	ARG	NE-CZ-NH2	-12.02	114.29	120.30	12	8
1	A	198	ASP	CB-CG-OD1	11.77	128.90	118.30	7	1
1	A	194	ASP	CB-CG-OD2	11.54	128.69	118.30	3	5
1	A	171	PHE	CB-CG-CD1	-11.41	112.81	120.80	7	2
1	A	124	ASP	CB-CG-OD1	11.08	128.27	118.30	1	5
1	A	256	ARG	NE-CZ-NH2	-10.71	114.94	120.30	6	6
1	A	171	PHE	CB-CG-CD2	-10.53	113.43	120.80	4	4
1	A	135	ARG	NE-CZ-NH1	10.40	125.50	120.30	12	4
1	A	149	PHE	CB-CG-CD1	10.19	127.94	120.80	13	4
1	A	170	ASP	CB-CG-OD2	10.17	127.45	118.30	1	2
1	A	110	ARG	NE-CZ-NH2	-10.04	115.28	120.30	4	9
1	A	129	ASP	CB-CG-OD1	9.94	127.24	118.30	4	2
1	A	249	ARG	NE-CZ-NH1	9.44	125.02	120.30	8	8
1	A	248	PHE	CB-CG-CD2	-9.41	114.22	120.80	10	1
1	A	175	ASP	CB-CG-OD2	9.36	126.72	118.30	2	4
1	A	117	ARG	NE-CZ-NH1	9.30	124.95	120.30	7	6
1	A	240	TYR	CB-CG-CD1	-9.16	115.50	121.00	6	5
1	A	185	PHE	CB-CG-CD1	9.11	127.18	120.80	7	3
1	A	132	TYR	CB-CG-CD2	9.07	126.44	121.00	1	6
1	A	165	ARG	NH1-CZ-NH2	-9.03	109.46	119.40	8	2
1	A	135	ARG	NE-CZ-NH2	-9.00	115.80	120.30	9	4
1	A	194	ASP	CB-CG-OD1	8.99	126.39	118.30	2	3
1	A	213	PHE	CB-CG-CD1	-8.99	114.51	120.80	2	4
1	A	244	ASP	CB-CG-OD1	-8.78	110.40	118.30	14	6
1	A	244	ASP	CB-CG-OD2	8.69	126.12	118.30	4	4
1	A	170	ASP	OD1-CG-OD2	-8.68	106.81	123.30	6	13
1	A	132	TYR	CB-CG-CD1	-8.66	115.80	121.00	1	7
1	A	163	PHE	CB-CG-CD1	-8.56	114.81	120.80	8	1
1	A	237	PHE	CB-CG-CD1	-8.52	114.84	120.80	5	6
1	A	254	ASP	CB-CG-OD1	8.40	125.86	118.30	7	3
1	A	149	PHE	CB-CG-CD2	-8.40	114.92	120.80	13	2
1	A	141	TRP	CD1-NE1-CE2	8.27	116.45	109.00	7	5
1	A	113	TYR	CB-CG-CD2	-8.13	116.12	121.00	2	3
1	A	253	ASP	CB-CG-OD2	8.13	125.62	118.30	5	7
1	A	164	ALA	CB-CA-C	8.11	122.26	110.10	7	3
1	A	189	SER	N-CA-CB	-8.04	98.45	110.50	12	3
1	A	108	VAL	CA-CB-CG2	8.01	122.91	110.90	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	161	VAL	CA-CB-CG1	7.86	122.69	110.90	3	2
1	A	117	ARG	NE-CZ-NH2	7.82	124.21	120.30	11	4
1	A	262	TYR	CG-CD1-CE1	-7.73	115.11	121.30	14	3
1	A	202	PHE	CB-CG-CD2	-7.63	115.46	120.80	12	2
1	A	173	ALA	N-CA-CB	7.62	120.77	110.10	5	2
1	A	131	ASP	CB-CG-OD1	7.58	125.12	118.30	9	4
1	A	116	TYR	CB-CG-CD2	-7.58	116.45	121.00	5	2
1	A	200	ASP	CB-CG-OD1	7.54	125.09	118.30	10	2
1	A	157	ALA	N-CA-CB	-7.53	99.56	110.10	6	1
1	A	248	PHE	CB-CG-CD1	-7.51	115.54	120.80	2	2
1	A	163	PHE	CB-CG-CD2	7.51	126.06	120.80	2	5
1	A	222	HIS	CA-CB-CG	7.49	126.33	113.60	10	1
1	A	124	ASP	CB-CG-OD2	7.48	125.03	118.30	14	2
1	A	115	THR	CA-CB-CG2	7.47	122.86	112.40	3	2
1	A	141	TRP	CH2-CZ2-CE2	7.44	124.84	117.40	2	3
1	A	185	PHE	CB-CG-CD2	-7.43	115.60	120.80	9	3
1	A	240	TYR	CB-CG-CD2	-7.39	116.56	121.00	10	4
1	A	122	THR	CA-CB-CG2	7.36	122.70	112.40	13	3
1	A	242	TYR	CZ-CE2-CD2	-7.31	113.22	119.80	1	1
1	A	127	ARG	CD-NE-CZ	7.27	133.77	123.60	3	3
1	A	135	ARG	CD-NE-CZ	7.23	133.72	123.60	6	2
1	A	109	TRP	CA-CB-CG	7.20	127.37	113.70	3	2
1	A	219	ALA	N-CA-CB	7.19	120.17	110.10	11	1
1	A	182	ALA	N-CA-CB	7.17	120.14	110.10	12	2
1	A	140	VAL	CA-CB-CG1	7.14	121.61	110.90	3	1
1	A	220	ILE	CA-CB-CG2	7.09	125.09	110.90	5	1
1	A	253	ASP	CB-CG-OD1	-7.08	111.93	118.30	8	1
1	A	175	ASP	CB-CG-OD1	7.06	124.65	118.30	6	2
1	A	113	TYR	CG-CD1-CE1	-7.05	115.66	121.30	12	1
1	A	158	ASP	CB-CG-OD2	-6.99	112.01	118.30	3	1
1	A	116	TYR	CB-CG-CD1	-6.99	116.81	121.00	10	2
1	A	173	ALA	CB-CA-C	6.92	120.48	110.10	1	1
1	A	110	ARG	NH1-CZ-NH2	6.89	126.98	119.40	1	2
1	A	198	ASP	CB-CG-OD2	-6.84	112.15	118.30	12	3
1	A	124	ASP	OD1-CG-OD2	-6.83	110.32	123.30	14	1
1	A	138	PHE	CB-CG-CD1	6.79	125.56	120.80	12	3
1	A	262	TYR	CD1-CE1-CZ	6.76	125.88	119.80	2	1
1	A	121	TYR	CG-CD1-CE1	-6.74	115.91	121.30	11	2
1	A	141	TRP	CD1-CG-CD2	-6.74	100.91	106.30	2	1
1	A	254	ASP	CB-CG-OD2	-6.73	112.24	118.30	11	1
1	A	194	ASP	OD1-CG-OD2	-6.71	110.56	123.30	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	109	TRP	CE2-CD2-CG	6.69	112.66	107.30	4	1
1	A	167	ALA	CB-CA-C	6.69	120.14	110.10	7	1
1	A	232	PRO	N-CD-CG	6.68	113.23	103.20	2	1
1	A	109	TRP	NE1-CE2-CD2	-6.67	100.63	107.30	4	1
1	A	101	ARG	NH1-CZ-NH2	-6.67	112.06	119.40	4	1
1	A	256	ARG	CD-NE-CZ	6.61	132.86	123.60	14	3
1	A	174	PHE	CB-CG-CD2	-6.61	116.17	120.80	11	3
1	A	127	ARG	NH1-CZ-NH2	-6.60	112.14	119.40	13	1
1	A	242	TYR	CB-CG-CD2	-6.58	117.05	121.00	9	4
1	A	113	TYR	CG-CD2-CE2	-6.57	116.04	121.30	8	1
1	A	138	PHE	CB-CG-CD2	-6.57	116.20	120.80	12	1
1	A	101	ARG	CD-NE-CZ	6.56	132.78	123.60	14	2
1	A	232	PRO	N-CA-CB	6.49	111.08	103.30	10	4
1	A	162	VAL	CA-CB-CG2	6.47	120.61	110.90	10	1
1	A	125	MET	CA-CB-CG	6.43	124.22	113.30	11	2
1	A	178	GLY	C-N-CA	6.38	135.69	122.30	5	2
1	A	238	PRO	N-CA-CB	6.37	110.94	103.30	5	2
1	A	165	ARG	CD-NE-CZ	6.37	132.51	123.60	9	2
1	A	172	HIS	CA-CB-CG	6.34	124.37	113.60	11	3
1	A	215	THR	CA-CB-CG2	6.33	121.27	112.40	9	1
1	A	109	TRP	CD1-NE1-CE2	6.31	114.68	109.00	8	3
1	A	235	VAL	O-C-N	-6.30	112.62	122.70	6	1
1	A	104	PRO	N-CD-CG	6.30	112.65	103.20	14	2
1	A	247	THR	CA-CB-CG2	6.29	121.21	112.40	7	2
1	A	167	ALA	N-CA-CB	6.29	118.90	110.10	1	2
1	A	141	TRP	NE1-CE2-CZ2	6.29	137.31	130.40	12	1
1	A	213	PHE	CB-CG-CD2	-6.26	116.41	120.80	13	5
1	A	214	LEU	CB-CG-CD2	6.22	121.57	111.00	2	1
1	A	132	TYR	CA-CB-CG	6.15	125.09	113.40	4	2
1	A	248	PHE	C-N-CA	6.13	137.02	121.70	9	2
1	A	196	HIS	CA-CB-CG	6.07	123.92	113.60	5	2
1	A	243	VAL	CA-CB-CG2	6.05	119.98	110.90	4	2
1	A	116	TYR	CG-CD1-CE1	-6.05	116.46	121.30	6	1
1	A	200	ASP	CB-CG-OD2	6.04	123.74	118.30	14	3
1	A	109	TRP	NE1-CE2-CZ2	6.04	137.04	130.40	11	2
1	A	170	ASP	N-CA-CB	6.03	121.45	110.60	3	1
1	A	240	TYR	CZ-CE2-CD2	6.01	125.21	119.80	9	2
1	A	249	ARG	CD-NE-CZ	6.01	132.02	123.60	13	1
1	A	113	TYR	C-N-CA	5.98	136.65	121.70	10	2
1	A	175	ASP	OD1-CG-OD2	-5.97	111.96	123.30	6	1
1	A	153	ASN	O-C-N	-5.94	113.20	122.70	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	162	VAL	CB-CA-C	5.94	122.68	111.40	1	1
1	A	243	VAL	CG1-CB-CG2	-5.91	101.44	110.90	5	2
1	A	191	ILE	CA-CB-CG2	5.91	122.72	110.90	9	1
1	A	110	ARG	CD-NE-CZ	5.89	131.84	123.60	1	2
1	A	242	TYR	CG-CD1-CE1	-5.89	116.59	121.30	1	1
1	A	217	VAL	CA-CB-CG1	5.88	119.73	110.90	5	4
1	A	141	TRP	CZ3-CH2-CZ2	-5.87	114.56	121.60	2	1
1	A	158	ASP	C-N-CA	5.86	136.36	121.70	11	1
1	A	219	ALA	CB-CA-C	-5.84	101.34	110.10	11	1
1	A	237	PHE	CB-CG-CD2	5.83	124.88	120.80	1	1
1	A	124	ASP	CB-CA-C	-5.80	98.79	110.40	14	2
1	A	234	ALA	N-CA-CB	-5.80	101.98	110.10	1	1
1	A	138	PHE	CG-CD2-CE2	-5.78	114.44	120.80	5	1
1	A	217	VAL	CA-CB-CG2	5.78	119.56	110.90	9	1
1	A	147	LEU	CB-CG-CD2	-5.77	101.20	111.00	1	1
1	A	230	SER	CB-CA-C	5.75	121.03	110.10	12	1
1	A	161	VAL	CA-CB-CG2	5.75	119.53	110.90	11	1
1	A	207	SER	C-N-CA	5.74	134.36	122.30	9	1
1	A	141	TRP	NE1-CE2-CD2	-5.74	101.56	107.30	5	4
1	A	108	VAL	CB-CA-C	5.72	122.27	111.40	3	1
1	A	251	SER	N-CA-CB	-5.70	101.94	110.50	4	3
1	A	102	GLU	OE1-CD-OE2	-5.68	116.49	123.30	9	2
1	A	131	ASP	CB-CG-OD2	5.68	123.41	118.30	4	1
1	A	141	TRP	CG-CD1-NE1	-5.66	104.44	110.10	7	3
1	A	145	THR	CA-CB-CG2	5.64	120.30	112.40	9	1
1	A	240	TYR	CG-CD2-CE2	-5.63	116.80	121.30	9	1
1	A	226	LEU	CB-CG-CD2	5.61	120.53	111.00	12	1
1	A	114	ILE	CA-CB-CG1	5.59	121.62	111.00	11	1
1	A	170	ASP	CB-CA-C	5.56	121.51	110.40	7	2
1	A	260	SER	CA-C-O	-5.54	108.47	120.10	6	1
1	A	175	ASP	CA-CB-CG	5.53	125.57	113.40	14	1
1	A	203	TRP	CD1-NE1-CE2	5.53	113.97	109.00	1	2
1	A	115	THR	CA-CB-OG1	5.52	120.59	109.00	7	1
1	A	165	ARG	N-CA-CB	5.51	120.52	110.60	10	1
1	A	121	TYR	CZ-CE2-CD2	5.51	124.75	119.80	2	1
1	A	202	PHE	CB-CA-C	5.50	121.39	110.40	10	1
1	A	262	TYR	N-CA-CB	5.49	120.48	110.60	4	1
1	A	210	THR	OG1-CB-CG2	-5.49	97.38	110.00	1	1
1	A	226	LEU	C-N-CA	5.48	133.80	122.30	6	1
1	A	116	TYR	CB-CA-C	5.47	121.34	110.40	12	1
1	A	117	ARG	NH1-CZ-NH2	5.44	125.39	119.40	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	163	PHE	O-C-N	-5.44	114.00	122.70	2	1
1	A	171	PHE	N-CA-CB	5.43	120.38	110.60	1	1
1	A	216	ALA	CB-CA-C	-5.43	101.95	110.10	2	1
1	A	170	ASP	C-N-CA	5.43	135.28	121.70	5	2
1	A	203	TRP	CZ3-CH2-CZ2	-5.42	115.09	121.60	12	1
1	A	171	PHE	O-C-N	-5.42	114.03	122.70	12	1
1	A	140	VAL	CA-CB-CG2	5.41	119.02	110.90	14	1
1	A	132	TYR	CZ-CE2-CD2	5.41	124.67	119.80	2	1
1	A	134	ILE	CA-CB-CG1	5.40	121.26	111.00	6	1
1	A	260	SER	N-CA-CB	-5.40	102.41	110.50	9	1
1	A	121	TYR	C-N-CA	5.39	135.18	121.70	7	1
1	A	202	PHE	CG-CD1-CE1	-5.39	114.87	120.80	7	1
1	A	239	THR	N-CA-CB	-5.39	100.06	110.30	10	1
1	A	163	PHE	N-CA-CB	-5.35	100.96	110.60	11	1
1	A	201	GLU	OE1-CD-OE2	-5.35	116.88	123.30	3	1
1	A	141	TRP	CD2-CE3-CZ3	5.34	125.75	118.80	13	1
1	A	125	MET	CB-CA-C	5.34	121.08	110.40	5	1
1	A	129	ASP	CB-CG-OD2	5.32	123.09	118.30	1	1
1	A	101	ARG	CB-CA-C	-5.30	99.80	110.40	9	1
1	A	245	ILE	CB-CA-C	5.28	122.16	111.60	13	1
1	A	102	GLU	O-C-N	-5.26	114.29	122.70	10	1
1	A	118	ILE	CA-CB-CG2	5.24	121.39	110.90	2	1
1	A	259	GLN	N-CA-CB	-5.24	101.17	110.60	14	1
1	A	154	THR	C-N-CA	5.23	133.28	122.30	12	1
1	A	205	THR	CA-CB-CG2	5.22	119.70	112.40	7	1
1	A	240	TYR	CG-CD1-CE1	-5.21	117.13	121.30	7	1
1	A	153	ASN	CB-CA-C	5.19	120.79	110.40	3	1
1	A	238	PRO	N-CD-CG	5.19	110.98	103.20	5	1
1	A	207	SER	N-CA-CB	-5.18	102.72	110.50	5	1
1	A	207	SER	CA-CB-OG	5.16	125.13	111.20	5	1
1	A	262	TYR	CZ-CE2-CD2	-5.15	115.16	119.80	14	1
1	A	203	TRP	CD2-CE3-CZ3	5.13	125.47	118.80	4	1
1	A	203	TRP	CH2-CZ2-CE2	5.12	122.52	117.40	4	2
1	A	204	THR	CA-CB-CG2	5.12	119.57	112.40	5	1
1	A	240	TYR	CD1-CE1-CZ	-5.12	115.19	119.80	5	1
1	A	121	TYR	CG-CD2-CE2	-5.11	117.21	121.30	1	1
1	A	229	SER	N-CA-CB	-5.10	102.85	110.50	12	1
1	A	124	ASP	CA-CB-CG	5.10	124.62	113.40	11	1
1	A	205	THR	C-N-CA	5.09	134.43	121.70	5	1
1	A	112	HIS	N-CA-CB	-5.09	101.44	110.60	7	1
1	A	235	VAL	CA-CB-CG1	5.08	118.53	110.90	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	160	LEU	CB-CG-CD1	5.08	119.64	111.00	2	1
1	A	132	TYR	CG-CD2-CE2	-5.08	117.24	121.30	2	1
1	A	191	ILE	CB-CA-C	5.08	121.76	111.60	7	1
1	A	203	TRP	NE1-CE2-CD2	-5.08	102.22	107.30	5	1
1	A	136	LYS	N-CA-CB	-5.07	101.47	110.60	3	1
1	A	116	TYR	CZ-CE2-CD2	-5.07	115.24	119.80	4	1
1	A	245	ILE	CA-CB-CG1	5.06	120.61	111.00	8	1
1	A	214	LEU	CB-CG-CD1	5.05	119.59	111.00	13	1
1	A	101	ARG	C-N-CA	5.04	134.31	121.70	14	1
1	A	103	MET	N-CA-CB	-5.04	101.52	110.60	1	1
1	A	169	GLY	C-N-CA	5.04	134.29	121.70	11	1
1	A	172	HIS	N-CA-CB	-5.03	101.55	110.60	12	1
1	A	253	ASP	O-C-N	-5.02	114.67	122.70	5	1
1	A	115	THR	N-CA-CB	-5.01	100.78	110.30	9	1
1	A	170	ASP	O-C-N	-5.01	114.69	122.70	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	174	PHE	Peptide,Sidechain	11
1	A	121	TYR	Sidechain	6
1	A	262	TYR	Sidechain	5
1	A	171	PHE	Sidechain	4
1	A	132	TYR	Sidechain,Mainchain	4
1	A	242	TYR	Sidechain	3
1	A	113	TYR	Sidechain	3
1	A	117	ARG	Sidechain	2
1	A	249	ARG	Peptide,Sidechain	2
1	A	101	ARG	Sidechain	2
1	A	110	ARG	Sidechain	2
1	A	135	ARG	Sidechain	2
1	A	172	HIS	Sidechain	2
1	A	127	ARG	Sidechain,Mainchain	2
1	A	256	ARG	Sidechain	2
1	A	182	ALA	Peptide	1
1	A	240	TYR	Sidechain	1
1	A	191	ILE	Peptide	1
1	A	116	TYR	Sidechain	1
1	A	167	ALA	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	165	ARG	Sidechain	1
1	A	175	ASP	Sidechain	1
1	A	213	PHE	Sidechain	1
1	A	237	PHE	Sidechain	1
1	A	248	PHE	Sidechain	1
1	A	149	PHE	Sidechain	1
1	A	219	ALA	Mainchain	1
1	A	196	HIS	Sidechain	1
1	A	185	PHE	Sidechain	1
1	A	138	PHE	Sidechain	1
1	A	251	SER	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	1271	1207	1207	2±1
4	A	5750	0	9000	132±12
All	All	98364	16898	142898	1849

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:423:PX4:H16	4:A:424:PX4:H24	1.02	1.23	7	1
4:A:347:PX4:H56	4:A:355:PX4:H25	0.99	1.33	11	1
4:A:321:PX4:H51	4:A:354:PX4:H34	0.93	1.41	10	1
4:A:306:PX4:H23	4:A:360:PX4:H44	0.91	1.42	1	1
4:A:408:PX4:H15	4:A:409:PX4:H2	0.90	1.44	10	2
4:A:361:PX4:H68	4:A:369:PX4:H36	0.84	1.49	12	1
4:A:404:PX4:H34	4:A:412:PX4:H37	0.84	1.49	11	1
4:A:347:PX4:H37	4:A:348:PX4:H64	0.84	1.49	8	1
4:A:313:PX4:H26	4:A:366:PX4:H22	0.84	1.47	13	1
4:A:308:PX4:H30	4:A:308:PX4:H67	0.83	1.50	3	1
4:A:422:PX4:H17	4:A:425:PX4:H56	0.83	1.48	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PX4:H53	4:A:422:PX4:H28	0.83	1.50	4	1
4:A:350:PX4:H30	4:A:350:PX4:H59	0.83	1.49	14	1
4:A:389:PX4:H15	4:A:398:PX4:H15	0.83	1.49	12	2
4:A:399:PX4:H62	4:A:407:PX4:H36	0.82	1.49	2	1
4:A:314:PX4:H39	4:A:362:PX4:H16	0.82	1.48	4	4
4:A:396:PX4:H57	4:A:398:PX4:H28	0.82	1.49	4	1
4:A:313:PX4:H47	4:A:328:PX4:H16	0.81	1.50	12	4
4:A:312:PX4:H51	4:A:359:PX4:H46	0.81	1.51	2	1
4:A:396:PX4:H19	4:A:397:PX4:H22	0.81	1.50	12	1
4:A:345:PX4:H22	4:A:353:PX4:H17	0.80	1.54	11	1
4:A:315:PX4:H52	4:A:323:PX4:H49	0.80	1.54	7	1
4:A:313:PX4:H27	4:A:359:PX4:H25	0.80	1.53	6	1
4:A:353:PX4:H50	4:A:354:PX4:H61	0.79	1.52	4	1
4:A:388:PX4:H49	4:A:397:PX4:H60	0.79	1.52	7	1
4:A:317:PX4:H55	4:A:342:PX4:H19	0.79	1.55	4	1
4:A:345:PX4:H20	4:A:345:PX4:H54	0.78	1.54	10	1
4:A:368:PX4:H37	4:A:418:PX4:H29	0.78	1.56	2	1
4:A:375:PX4:H49	4:A:429:PX4:H19	0.77	1.54	8	1
4:A:338:PX4:H35	4:A:343:PX4:H58	0.77	1.55	11	1
4:A:338:PX4:H49	4:A:355:PX4:H16	0.77	1.54	10	1
4:A:323:PX4:H60	4:A:368:PX4:H42	0.76	1.57	11	1
4:A:325:PX4:H22	4:A:341:PX4:H56	0.76	1.55	4	1
4:A:405:PX4:H25	4:A:423:PX4:H70	0.76	1.58	12	1
4:A:310:PX4:H50	4:A:311:PX4:H46	0.76	1.57	2	1
4:A:387:PX4:H65	4:A:402:PX4:H25	0.76	1.58	3	1
4:A:406:PX4:H37	4:A:422:PX4:H30	0.76	1.58	3	1
4:A:383:PX4:H35	4:A:390:PX4:H39	0.76	1.58	6	1
4:A:400:PX4:H30	4:A:417:PX4:H28	0.75	1.56	8	1
4:A:307:PX4:H48	4:A:314:PX4:H22	0.75	1.57	2	1
4:A:381:PX4:H51	4:A:397:PX4:H47	0.75	1.57	8	1
4:A:340:PX4:H60	4:A:341:PX4:H24	0.75	1.57	12	1
4:A:345:PX4:H61	4:A:345:PX4:H28	0.75	1.55	7	1
4:A:321:PX4:H62	4:A:425:PX4:H41	0.75	1.59	14	1
4:A:389:PX4:H37	4:A:397:PX4:H41	0.75	1.59	14	1
4:A:378:PX4:H49	4:A:410:PX4:H17	0.75	1.59	12	1
4:A:323:PX4:H42	4:A:333:PX4:H68	0.74	1.58	13	1
4:A:374:PX4:H24	4:A:427:PX4:H19	0.74	1.58	6	1
4:A:310:PX4:H57	4:A:364:PX4:H27	0.74	1.57	1	1
4:A:388:PX4:H24	4:A:396:PX4:H47	0.74	1.58	14	1
4:A:385:PX4:H45	4:A:394:PX4:H65	0.74	1.59	9	1
4:A:307:PX4:H46	4:A:314:PX4:H19	0.74	1.58	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H16	4:A:345:PX4:H52	0.74	1.59	10	1
4:A:373:PX4:H32	4:A:381:PX4:H47	0.74	1.58	14	1
4:A:412:PX4:H56	4:A:419:PX4:H25	0.73	1.59	14	1
4:A:358:PX4:H32	4:A:358:PX4:H52	0.73	1.58	7	1
4:A:391:PX4:H39	4:A:405:PX4:H69	0.73	1.61	9	1
4:A:406:PX4:H31	4:A:424:PX4:H37	0.73	1.58	4	1
4:A:322:PX4:H49	4:A:361:PX4:H51	0.73	1.61	3	1
4:A:422:PX4:H26	4:A:425:PX4:H63	0.73	1.58	2	1
4:A:367:PX4:H50	4:A:412:PX4:H18	0.73	1.60	4	1
4:A:327:PX4:H72	4:A:328:PX4:H33	0.73	1.60	9	1
4:A:420:PX4:H42	4:A:427:PX4:H38	0.72	1.61	6	1
4:A:367:PX4:H21	4:A:428:PX4:H18	0.72	1.60	1	1
4:A:368:PX4:H51	4:A:424:PX4:H58	0.72	1.58	3	1
4:A:317:PX4:H39	4:A:363:PX4:H62	0.72	1.61	10	1
4:A:334:PX4:H36	4:A:334:PX4:H69	0.72	1.62	4	1
4:A:400:PX4:H39	4:A:401:PX4:H72	0.72	1.61	4	1
4:A:346:PX4:H49	4:A:362:PX4:H50	0.71	1.62	5	3
4:A:415:PX4:H49	4:A:422:PX4:H24	0.71	1.59	4	1
4:A:327:PX4:H39	4:A:327:PX4:H65	0.71	1.62	6	1
4:A:409:PX4:H68	4:A:422:PX4:H68	0.71	1.63	1	1
4:A:318:PX4:H17	4:A:327:PX4:H48	0.71	1.61	2	1
4:A:328:PX4:H17	4:A:360:PX4:H45	0.71	1.61	5	1
4:A:403:PX4:H12	4:A:404:PX4:H16	0.71	1.63	7	1
4:A:397:PX4:H27	4:A:398:PX4:H58	0.71	1.62	2	1
4:A:412:PX4:H35	4:A:419:PX4:H51	0.71	1.63	4	1
4:A:400:PX4:H5	4:A:408:PX4:H49	0.71	1.61	1	1
4:A:335:PX4:H23	4:A:343:PX4:H26	0.71	1.60	5	1
4:A:331:PX4:H49	4:A:331:PX4:H21	0.71	1.61	3	1
4:A:419:PX4:H64	4:A:427:PX4:H58	0.71	1.63	10	1
4:A:328:PX4:H56	4:A:329:PX4:H58	0.70	1.62	2	1
4:A:398:PX4:H24	4:A:407:PX4:H46	0.70	1.63	8	1
4:A:369:PX4:H17	4:A:425:PX4:H22	0.70	1.60	6	1
4:A:390:PX4:H14	4:A:399:PX4:H20	0.70	1.60	11	1
4:A:317:PX4:H48	4:A:324:PX4:H19	0.70	1.63	8	1
4:A:380:PX4:H48	4:A:402:PX4:H25	0.70	1.62	11	1
4:A:423:PX4:H48	4:A:424:PX4:H24	0.70	1.60	12	1
4:A:374:PX4:H41	4:A:412:PX4:H31	0.70	1.63	7	1
4:A:409:PX4:H16	4:A:416:PX4:H53	0.70	1.63	8	1
4:A:313:PX4:H21	4:A:360:PX4:H17	0.70	1.64	10	1
4:A:308:PX4:H58	4:A:311:PX4:H54	0.70	1.61	1	1
4:A:329:PX4:H55	4:A:333:PX4:H45	0.70	1.63	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H37	4:A:419:PX4:H21	0.70	1.62	2	2
4:A:361:PX4:H25	4:A:362:PX4:H31	0.70	1.64	14	2
4:A:317:PX4:H52	4:A:324:PX4:H54	0.70	1.64	11	1
4:A:317:PX4:H17	4:A:324:PX4:H53	0.70	1.64	2	1
4:A:338:PX4:O8	4:A:348:PX4:H4	0.69	1.87	9	2
4:A:311:PX4:H58	4:A:363:PX4:H44	0.69	1.61	14	1
4:A:372:PX4:H51	4:A:384:PX4:H51	0.69	1.63	12	1
4:A:353:PX4:H72	4:A:354:PX4:H29	0.69	1.62	7	1
4:A:410:PX4:H49	4:A:426:PX4:H19	0.69	1.63	8	1
4:A:307:PX4:H4	4:A:361:PX4:H17	0.69	1.64	7	2
4:A:368:PX4:H34	4:A:429:PX4:H67	0.69	1.65	5	1
4:A:326:PX4:H25	4:A:341:PX4:H62	0.69	1.64	6	1
4:A:350:PX4:H45	4:A:363:PX4:H56	0.69	1.62	1	1
4:A:398:PX4:H30	4:A:407:PX4:H54	0.69	1.63	10	1
4:A:418:PX4:H26	4:A:425:PX4:H24	0.69	1.65	4	1
4:A:360:PX4:H50	4:A:366:PX4:H18	0.69	1.65	8	1
4:A:353:PX4:H70	4:A:413:PX4:H43	0.69	1.63	4	1
4:A:322:PX4:H28	4:A:323:PX4:H25	0.69	1.65	14	1
4:A:350:PX4:H72	4:A:365:PX4:H35	0.68	1.65	1	1
4:A:343:PX4:H64	4:A:347:PX4:H27	0.68	1.62	2	1
4:A:391:PX4:H24	4:A:393:PX4:H58	0.68	1.65	13	1
4:A:392:PX4:H52	4:A:393:PX4:H54	0.68	1.64	4	1
4:A:367:PX4:H55	4:A:430:PX4:H22	0.68	1.63	6	2
4:A:377:PX4:H13	4:A:377:PX4:H15	0.68	1.65	8	1
4:A:335:PX4:H16	4:A:344:PX4:H20	0.68	1.64	14	1
4:A:340:PX4:H30	4:A:347:PX4:H72	0.68	1.64	5	1
4:A:360:PX4:H68	4:A:419:PX4:H67	0.68	1.65	2	1
4:A:323:PX4:H14	4:A:333:PX4:H47	0.68	1.64	10	1
4:A:405:PX4:H41	4:A:414:PX4:H42	0.68	1.64	14	1
4:A:332:PX4:H28	4:A:340:PX4:H31	0.68	1.66	2	1
4:A:314:PX4:H38	4:A:355:PX4:H8	0.68	1.64	8	1
4:A:385:PX4:H23	4:A:393:PX4:H22	0.68	1.64	3	1
4:A:346:PX4:H40	4:A:355:PX4:H68	0.68	1.64	6	1
4:A:345:PX4:H34	4:A:353:PX4:H46	0.68	1.64	14	1
4:A:370:PX4:H42	4:A:403:PX4:H33	0.67	1.64	5	1
4:A:316:PX4:H47	4:A:319:PX4:H46	0.67	1.67	6	1
4:A:313:PX4:H26	4:A:366:PX4:H21	0.67	1.64	7	1
4:A:308:PX4:H47	4:A:310:PX4:H60	0.67	1.65	14	1
4:A:315:PX4:H52	4:A:316:PX4:H23	0.67	1.65	14	1
4:A:306:PX4:H57	4:A:423:PX4:H42	0.67	1.65	4	1
4:A:405:PX4:H17	4:A:414:PX4:H19	0.67	1.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:409:PX4:H55	4:A:415:PX4:H27	0.66	1.67	1	1
4:A:353:PX4:H69	4:A:362:PX4:H72	0.66	1.65	14	1
4:A:416:PX4:H48	4:A:422:PX4:H59	0.66	1.67	14	1
4:A:340:PX4:H43	4:A:407:PX4:H66	0.66	1.67	1	1
4:A:388:PX4:H16	4:A:395:PX4:H15	0.66	1.66	5	1
4:A:314:PX4:H58	4:A:364:PX4:H54	0.66	1.66	8	1
4:A:387:PX4:H15	4:A:411:PX4:H49	0.66	1.66	8	1
4:A:314:PX4:H64	4:A:422:PX4:H68	0.66	1.65	2	1
4:A:347:PX4:H16	4:A:348:PX4:H46	0.66	1.67	4	1
4:A:386:PX4:H17	4:A:387:PX4:H24	0.66	1.68	10	1
4:A:403:PX4:H56	4:A:404:PX4:H39	0.66	1.67	12	1
4:A:340:PX4:H58	4:A:341:PX4:H16	0.66	1.68	14	1
4:A:339:PX4:H30	4:A:355:PX4:H40	0.66	1.67	10	1
4:A:306:PX4:H16	4:A:322:PX4:H9	0.66	1.68	13	1
4:A:356:PX4:H32	4:A:362:PX4:H24	0.66	1.66	2	2
4:A:336:PX4:H27	4:A:344:PX4:H62	0.66	1.67	6	1
4:A:331:PX4:H21	4:A:340:PX4:H17	0.66	1.66	5	1
4:A:385:PX4:H71	4:A:399:PX4:H61	0.66	1.67	14	1
4:A:357:PX4:H58	4:A:357:PX4:H31	0.66	1.66	8	1
4:A:336:PX4:H65	4:A:344:PX4:H71	0.66	1.68	9	1
4:A:335:PX4:H42	4:A:337:PX4:H38	0.66	1.65	10	1
4:A:400:PX4:H17	4:A:401:PX4:H3	0.66	1.65	10	1
4:A:408:PX4:H50	4:A:409:PX4:H17	0.66	1.66	10	1
4:A:349:PX4:H36	4:A:350:PX4:H40	0.65	1.68	2	1
4:A:391:PX4:H19	4:A:414:PX4:H17	0.65	1.67	8	1
4:A:389:PX4:H42	4:A:389:PX4:H71	0.65	1.66	1	1
4:A:413:PX4:H41	4:A:421:PX4:H67	0.65	1.69	3	1
4:A:420:PX4:H51	4:A:427:PX4:H49	0.65	1.68	7	1
4:A:308:PX4:H66	4:A:410:PX4:H68	0.65	1.68	10	1
4:A:373:PX4:H21	4:A:381:PX4:H32	0.65	1.68	11	1
4:A:332:PX4:H37	4:A:340:PX4:H35	0.65	1.68	7	1
4:A:359:PX4:H37	4:A:412:PX4:H64	0.65	1.67	8	1
4:A:358:PX4:H71	4:A:358:PX4:H39	0.65	1.69	11	1
4:A:393:PX4:H18	4:A:394:PX4:H18	0.65	1.67	9	1
4:A:403:PX4:H16	4:A:404:PX4:H24	0.65	1.69	12	1
4:A:373:PX4:H46	4:A:382:PX4:H46	0.65	1.67	5	1
4:A:306:PX4:H54	4:A:321:PX4:H48	0.65	1.68	7	2
4:A:391:PX4:H53	4:A:408:PX4:H20	0.65	1.68	9	1
4:A:419:PX4:H46	4:A:427:PX4:H50	0.65	1.68	1	1
4:A:322:PX4:H62	4:A:361:PX4:H71	0.65	1.69	3	1
4:A:405:PX4:H21	4:A:415:PX4:H50	0.65	1.68	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:368:PX4:H25	4:A:429:PX4:H66	0.65	1.69	9	1
4:A:312:PX4:H38	4:A:366:PX4:H48	0.65	1.69	3	1
4:A:406:PX4:H37	4:A:423:PX4:H28	0.65	1.69	4	1
4:A:335:PX4:H16	4:A:344:PX4:H19	0.65	1.67	10	2
4:A:390:PX4:H44	4:A:407:PX4:H17	0.65	1.67	14	1
4:A:402:PX4:H52	4:A:403:PX4:H27	0.65	1.69	1	1
4:A:400:PX4:H20	4:A:401:PX4:H17	0.65	1.68	6	1
4:A:335:PX4:H34	4:A:343:PX4:H65	0.65	1.69	11	1
4:A:391:PX4:H47	4:A:394:PX4:H28	0.65	1.67	2	1
4:A:406:PX4:H46	4:A:421:PX4:H50	0.65	1.68	7	1
4:A:348:PX4:H26	4:A:355:PX4:H25	0.65	1.69	12	1
4:A:400:PX4:H28	4:A:401:PX4:H46	0.64	1.67	2	1
4:A:308:PX4:H19	4:A:364:PX4:H22	0.64	1.68	9	1
4:A:391:PX4:H50	4:A:393:PX4:H60	0.64	1.69	10	1
4:A:397:PX4:H53	4:A:402:PX4:H21	0.64	1.68	6	1
4:A:376:PX4:H20	4:A:377:PX4:H16	0.64	1.67	14	2
4:A:404:PX4:O1	4:A:419:PX4:H13	0.64	1.93	2	1
4:A:317:PX4:H40	4:A:342:PX4:H38	0.64	1.68	1	1
4:A:339:PX4:H23	4:A:347:PX4:H29	0.64	1.69	1	1
4:A:379:PX4:H19	4:A:384:PX4:H20	0.64	1.70	4	1
4:A:359:PX4:H36	4:A:366:PX4:H40	0.64	1.69	6	1
4:A:353:PX4:H46	4:A:354:PX4:H64	0.64	1.68	7	1
4:A:376:PX4:H35	4:A:383:PX4:H60	0.64	1.67	7	1
4:A:312:PX4:H55	4:A:359:PX4:H56	0.64	1.70	9	1
4:A:316:PX4:H56	4:A:316:PX4:H25	0.64	1.69	9	1
4:A:350:PX4:H51	4:A:363:PX4:H59	0.64	1.69	1	1
4:A:397:PX4:H28	4:A:398:PX4:H58	0.64	1.68	1	1
4:A:405:PX4:H4	4:A:414:PX4:H22	0.64	1.67	1	1
4:A:313:PX4:H53	4:A:359:PX4:H23	0.64	1.68	10	1
4:A:371:PX4:H31	4:A:376:PX4:H23	0.64	1.70	14	1
4:A:378:PX4:H63	4:A:418:PX4:H66	0.64	1.69	4	1
4:A:403:PX4:H24	4:A:404:PX4:H53	0.64	1.68	5	1
4:A:357:PX4:H45	4:A:365:PX4:H72	0.64	1.70	10	1
4:A:368:PX4:H4	4:A:418:PX4:H2	0.63	1.70	1	1
4:A:369:PX4:H25	4:A:429:PX4:H64	0.63	1.68	2	2
4:A:317:PX4:H55	4:A:342:PX4:H53	0.63	1.68	2	1
4:A:370:PX4:H46	4:A:411:PX4:H53	0.63	1.70	13	1
4:A:417:PX4:H50	4:A:426:PX4:H47	0.63	1.70	8	1
4:A:320:PX4:H36	4:A:418:PX4:H66	0.63	1.70	9	1
4:A:332:PX4:H41	4:A:407:PX4:H66	0.63	1.68	6	1
4:A:386:PX4:H17	4:A:387:PX4:H21	0.63	1.69	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PX4:H3	4:A:414:PX4:O6	0.63	1.94	13	1
4:A:416:PX4:H23	4:A:422:PX4:H52	0.63	1.70	2	1
4:A:428:PX4:H19	4:A:429:PX4:H37	0.63	1.69	7	2
4:A:355:PX4:H46	4:A:355:PX4:H10	0.63	1.70	8	1
4:A:375:PX4:H67	4:A:375:PX4:H36	0.63	1.71	14	1
4:A:312:PX4:H21	4:A:366:PX4:H17	0.63	1.70	2	2
4:A:370:PX4:H46	4:A:411:PX4:H49	0.63	1.69	14	1
4:A:386:PX4:H64	4:A:387:PX4:H34	0.63	1.69	2	1
4:A:367:PX4:H45	4:A:429:PX4:H31	0.63	1.70	3	1
4:A:376:PX4:H21	4:A:377:PX4:H20	0.63	1.71	5	1
4:A:406:PX4:H35	4:A:425:PX4:H68	0.63	1.70	10	1
4:A:314:PX4:H34	4:A:362:PX4:H14	0.63	1.70	9	1
4:A:314:PX4:H57	4:A:361:PX4:H27	0.63	1.70	9	1
4:A:355:PX4:H10	4:A:355:PX4:H49	0.63	1.68	12	1
4:A:355:PX4:H68	4:A:415:PX4:H64	0.63	1.71	13	1
4:A:398:PX4:H30	4:A:407:PX4:H53	0.63	1.71	14	1
4:A:407:PX4:H22	4:A:414:PX4:H50	0.63	1.69	12	1
4:A:332:PX4:H72	4:A:391:PX4:H25	0.63	1.70	14	1
4:A:378:PX4:H15	4:A:410:PX4:H47	0.62	1.69	3	1
4:A:406:PX4:H34	4:A:424:PX4:H35	0.62	1.71	5	1
4:A:378:PX4:H46	4:A:410:PX4:H17	0.62	1.70	10	1
4:A:329:PX4:H12	4:A:333:PX4:H41	0.62	1.71	12	1
4:A:307:PX4:H65	4:A:349:PX4:H22	0.62	1.71	14	1
4:A:393:PX4:H21	4:A:394:PX4:H29	0.62	1.69	11	1
4:A:309:PX4:H56	4:A:319:PX4:H48	0.62	1.70	13	1
4:A:313:PX4:H70	4:A:375:PX4:H69	0.62	1.71	6	1
4:A:338:PX4:H16	4:A:345:PX4:H49	0.62	1.71	7	1
4:A:308:PX4:H22	4:A:310:PX4:H65	0.62	1.70	3	1
4:A:313:PX4:H60	4:A:327:PX4:H32	0.62	1.70	9	1
4:A:419:PX4:H36	4:A:430:PX4:H27	0.62	1.71	1	1
4:A:375:PX4:H54	4:A:389:PX4:H60	0.61	1.70	3	1
4:A:334:PX4:H54	4:A:356:PX4:H8	0.61	1.69	9	1
4:A:339:PX4:H26	4:A:347:PX4:H54	0.61	1.71	12	1
4:A:310:PX4:H53	4:A:364:PX4:H31	0.61	1.70	13	1
4:A:345:PX4:H59	4:A:345:PX4:H22	0.61	1.72	3	1
4:A:353:PX4:H19	4:A:357:PX4:H46	0.61	1.72	5	1
4:A:315:PX4:H43	4:A:369:PX4:H28	0.61	1.70	7	1
4:A:347:PX4:H54	4:A:355:PX4:H22	0.61	1.71	10	1
4:A:326:PX4:H42	4:A:332:PX4:H51	0.61	1.70	4	1
4:A:355:PX4:H66	4:A:362:PX4:H64	0.61	1.73	4	1
4:A:375:PX4:H18	4:A:429:PX4:H24	0.61	1.71	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H26	4:A:342:PX4:H19	0.61	1.73	8	1
4:A:373:PX4:H39	4:A:402:PX4:H38	0.61	1.72	10	1
4:A:392:PX4:H7	4:A:392:PX4:H15	0.61	1.71	13	1
4:A:387:PX4:H47	4:A:411:PX4:H48	0.61	1.71	14	1
4:A:397:PX4:H31	4:A:398:PX4:H63	0.61	1.73	2	1
4:A:338:PX4:H25	4:A:347:PX4:H23	0.61	1.72	7	1
4:A:335:PX4:H31	4:A:337:PX4:H33	0.61	1.71	8	1
4:A:410:PX4:H59	4:A:417:PX4:H54	0.61	1.72	12	1
4:A:423:PX4:H16	4:A:424:PX4:H19	0.61	1.70	13	1
4:A:350:PX4:H37	4:A:408:PX4:H39	0.61	1.73	4	1
4:A:331:PX4:H14	4:A:347:PX4:H50	0.61	1.71	10	2
1:A:191:ILE:HD13	4:A:314:PX4:H21	0.61	1.72	14	3
4:A:315:PX4:H43	4:A:424:PX4:H71	0.61	1.72	10	1
4:A:380:PX4:H39	4:A:386:PX4:H38	0.61	1.73	12	1
4:A:325:PX4:H61	4:A:341:PX4:H60	0.61	1.72	10	1
4:A:396:PX4:H37	4:A:397:PX4:H42	0.61	1.72	12	1
4:A:395:PX4:H52	4:A:421:PX4:H50	0.61	1.73	2	1
4:A:306:PX4:H58	4:A:321:PX4:H21	0.61	1.72	10	1
4:A:337:PX4:H58	4:A:348:PX4:H32	0.61	1.73	12	1
4:A:330:PX4:H64	4:A:338:PX4:H39	0.61	1.72	1	1
4:A:407:PX4:H32	4:A:414:PX4:H55	0.61	1.72	4	1
4:A:319:PX4:H29	4:A:320:PX4:H28	0.61	1.72	6	1
4:A:360:PX4:H57	4:A:366:PX4:H56	0.61	1.73	12	1
4:A:368:PX4:H17	4:A:390:PX4:H50	0.61	1.73	1	1
4:A:407:PX4:H34	4:A:414:PX4:H65	0.61	1.73	1	1
4:A:349:PX4:H36	4:A:350:PX4:H37	0.61	1.71	11	1
4:A:421:PX4:H47	4:A:423:PX4:H66	0.61	1.73	11	1
4:A:331:PX4:H22	4:A:340:PX4:H17	0.61	1.73	13	1
4:A:355:PX4:H43	4:A:398:PX4:H70	0.60	1.71	3	1
4:A:316:PX4:H37	4:A:316:PX4:H72	0.60	1.72	6	1
4:A:407:PX4:H16	4:A:414:PX4:H49	0.60	1.73	10	3
4:A:334:PX4:H48	4:A:349:PX4:H20	0.60	1.71	11	1
4:A:335:PX4:H34	4:A:337:PX4:H34	0.60	1.74	2	1
4:A:345:PX4:H19	4:A:353:PX4:H47	0.60	1.71	12	1
4:A:387:PX4:H47	4:A:411:PX4:H52	0.60	1.73	13	1
4:A:331:PX4:H40	4:A:331:PX4:H69	0.60	1.73	1	1
4:A:357:PX4:H24	4:A:358:PX4:H22	0.60	1.73	6	1
4:A:387:PX4:H53	4:A:411:PX4:H50	0.60	1.72	9	1
4:A:338:PX4:H28	4:A:348:PX4:H57	0.60	1.72	11	1
4:A:428:PX4:H62	4:A:429:PX4:H50	0.60	1.73	1	1
4:A:314:PX4:H36	4:A:362:PX4:H16	0.60	1.72	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:360:PX4:H70	4:A:404:PX4:H42	0.60	1.74	14	1
4:A:307:PX4:H19	4:A:361:PX4:H15	0.60	1.73	14	4
4:A:376:PX4:H52	4:A:377:PX4:H19	0.60	1.72	8	1
4:A:331:PX4:H54	4:A:339:PX4:H35	0.60	1.72	13	1
4:A:392:PX4:H20	4:A:399:PX4:H48	0.60	1.74	1	1
4:A:368:PX4:H67	4:A:424:PX4:H17	0.60	1.72	8	1
4:A:327:PX4:H37	4:A:328:PX4:H53	0.60	1.72	12	1
4:A:335:PX4:H16	4:A:344:PX4:H22	0.60	1.72	7	1
4:A:410:PX4:H46	4:A:426:PX4:H15	0.60	1.72	13	2
4:A:332:PX4:H55	4:A:334:PX4:H36	0.60	1.74	11	1
4:A:350:PX4:H34	4:A:394:PX4:H43	0.59	1.73	2	1
1:A:191:ILE:HD12	4:A:314:PX4:H21	0.59	1.73	11	1
4:A:396:PX4:H20	4:A:396:PX4:H55	0.59	1.73	2	1
4:A:307:PX4:H43	4:A:410:PX4:H29	0.59	1.74	5	1
4:A:406:PX4:H21	4:A:423:PX4:H65	0.59	1.74	7	1
4:A:370:PX4:H70	4:A:402:PX4:H34	0.59	1.74	9	1
4:A:369:PX4:H61	4:A:425:PX4:H47	0.59	1.73	1	1
4:A:313:PX4:H63	4:A:328:PX4:H66	0.59	1.73	2	1
4:A:391:PX4:H25	4:A:392:PX4:H62	0.59	1.73	4	1
4:A:396:PX4:H53	4:A:398:PX4:H24	0.59	1.75	4	1
4:A:400:PX4:H11	4:A:401:PX4:O6	0.59	1.97	10	1
4:A:389:PX4:H53	4:A:398:PX4:H55	0.59	1.73	11	1
4:A:330:PX4:C9	4:A:344:PX4:H49	0.59	2.28	2	1
4:A:308:PX4:H23	4:A:364:PX4:H26	0.59	1.73	6	2
4:A:317:PX4:H53	4:A:342:PX4:H17	0.59	1.75	10	1
4:A:368:PX4:H62	4:A:424:PX4:H23	0.59	1.73	13	1
4:A:408:PX4:H40	4:A:422:PX4:H40	0.59	1.75	14	1
4:A:338:PX4:H53	4:A:346:PX4:H53	0.59	1.73	11	1
4:A:374:PX4:H30	4:A:427:PX4:H26	0.59	1.73	11	1
4:A:322:PX4:H64	4:A:361:PX4:H64	0.59	1.74	4	1
4:A:428:PX4:H56	4:A:429:PX4:H46	0.59	1.74	6	1
4:A:428:PX4:H23	4:A:429:PX4:H42	0.59	1.73	8	1
4:A:330:PX4:H52	4:A:338:PX4:H36	0.59	1.73	11	1
4:A:391:PX4:H20	4:A:392:PX4:H61	0.59	1.75	11	1
4:A:338:PX4:H60	4:A:355:PX4:H63	0.59	1.75	9	1
4:A:334:PX4:H69	4:A:349:PX4:H66	0.58	1.73	5	1
4:A:396:PX4:H69	4:A:398:PX4:H43	0.58	1.75	8	1
4:A:306:PX4:O8	4:A:322:PX4:H13	0.58	1.98	14	1
4:A:331:PX4:H10	4:A:347:PX4:H49	0.58	1.75	14	1
4:A:329:PX4:H42	4:A:336:PX4:H62	0.58	1.74	2	1
4:A:330:PX4:H50	4:A:337:PX4:H48	0.58	1.74	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:342:PX4:H16	4:A:351:PX4:H20	0.58	1.75	8	1
4:A:400:PX4:H47	4:A:409:PX4:H20	0.58	1.74	9	1
4:A:395:PX4:H33	4:A:405:PX4:H34	0.58	1.74	10	1
4:A:381:PX4:H50	4:A:397:PX4:H47	0.58	1.74	4	2
4:A:356:PX4:H12	4:A:356:PX4:H16	0.58	1.75	8	1
4:A:331:PX4:H65	4:A:339:PX4:H69	0.58	1.74	11	1
4:A:403:PX4:H29	4:A:404:PX4:H35	0.58	1.76	13	1
4:A:400:PX4:H22	4:A:408:PX4:H67	0.58	1.75	14	1
4:A:405:PX4:H4	4:A:414:PX4:H23	0.58	1.74	2	1
4:A:314:PX4:H45	4:A:346:PX4:H38	0.58	1.76	7	1
4:A:315:PX4:H35	4:A:322:PX4:H49	0.58	1.74	10	1
4:A:348:PX4:H27	4:A:348:PX4:H60	0.58	1.74	11	1
4:A:393:PX4:H23	4:A:394:PX4:H29	0.58	1.74	12	1
4:A:339:PX4:H21	4:A:347:PX4:H50	0.58	1.74	13	1
4:A:410:PX4:H48	4:A:426:PX4:H22	0.58	1.74	13	1
4:A:324:PX4:H61	4:A:341:PX4:H24	0.58	1.74	2	1
4:A:370:PX4:H35	4:A:427:PX4:H71	0.58	1.74	2	1
4:A:330:PX4:H41	4:A:336:PX4:H35	0.58	1.75	6	1
4:A:366:PX4:H27	4:A:427:PX4:H68	0.58	1.74	8	1
4:A:349:PX4:H15	4:A:356:PX4:H28	0.58	1.75	12	2
4:A:366:PX4:H38	4:A:412:PX4:H41	0.58	1.76	1	1
4:A:392:PX4:H48	4:A:393:PX4:H57	0.58	1.73	1	1
4:A:343:PX4:H9	4:A:344:PX4:H16	0.58	1.75	3	1
4:A:318:PX4:H47	4:A:327:PX4:H15	0.58	1.74	10	1
4:A:318:PX4:H18	4:A:327:PX4:H47	0.58	1.76	3	1
4:A:391:PX4:H16	4:A:393:PX4:H65	0.58	1.76	3	1
4:A:341:PX4:H40	4:A:385:PX4:H64	0.58	1.75	6	1
4:A:346:PX4:H43	4:A:356:PX4:H31	0.58	1.74	7	1
4:A:373:PX4:H29	4:A:384:PX4:H59	0.58	1.73	13	1
4:A:326:PX4:H50	4:A:351:PX4:H49	0.58	1.75	1	1
4:A:332:PX4:H10	4:A:356:PX4:O1	0.58	1.98	2	1
4:A:338:PX4:H46	4:A:355:PX4:H16	0.58	1.75	5	4
4:A:400:PX4:H22	4:A:408:PX4:H63	0.58	1.74	1	1
4:A:421:PX4:H4	4:A:423:PX4:H51	0.58	1.76	2	1
4:A:420:PX4:H47	4:A:427:PX4:H16	0.58	1.75	3	1
4:A:389:PX4:H25	4:A:398:PX4:H58	0.58	1.75	5	1
4:A:316:PX4:C24	4:A:319:PX4:H46	0.58	2.29	6	1
4:A:332:PX4:H70	4:A:425:PX4:H62	0.58	1.74	7	1
4:A:330:PX4:H63	4:A:337:PX4:H61	0.58	1.74	8	1
4:A:383:PX4:H35	4:A:407:PX4:H26	0.58	1.74	3	1
4:A:378:PX4:H69	4:A:410:PX4:H42	0.58	1.74	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PX4:H64	4:A:421:PX4:H62	0.58	1.76	4	1
4:A:326:PX4:H60	4:A:350:PX4:H71	0.58	1.74	8	1
4:A:310:PX4:H43	4:A:351:PX4:H66	0.58	1.74	12	1
4:A:310:PX4:H53	4:A:364:PX4:H25	0.58	1.76	12	1
4:A:404:PX4:H50	4:A:413:PX4:H26	0.58	1.75	12	1
4:A:383:PX4:H17	4:A:392:PX4:H26	0.58	1.75	14	1
4:A:390:PX4:H47	4:A:399:PX4:H24	0.58	1.76	14	1
4:A:310:PX4:H35	4:A:417:PX4:H31	0.57	1.75	2	1
4:A:372:PX4:H72	4:A:384:PX4:H38	0.57	1.75	11	1
4:A:378:PX4:H48	4:A:417:PX4:H72	0.57	1.74	7	1
4:A:380:PX4:H51	4:A:402:PX4:H24	0.57	1.74	7	1
4:A:383:PX4:H40	4:A:390:PX4:H41	0.57	1.76	8	1
4:A:332:PX4:H32	4:A:339:PX4:H44	0.57	1.76	13	1
4:A:310:PX4:H61	4:A:426:PX4:H44	0.57	1.76	1	1
4:A:338:PX4:H14	4:A:348:PX4:H4	0.57	1.75	2	1
4:A:345:PX4:H20	4:A:353:PX4:H52	0.57	1.75	3	1
4:A:368:PX4:H51	4:A:424:PX4:C30	0.57	2.29	3	1
4:A:330:PX4:H7	4:A:344:PX4:H49	0.57	1.75	5	1
4:A:326:PX4:H49	4:A:363:PX4:H55	0.57	1.75	7	1
4:A:389:PX4:H60	4:A:407:PX4:H55	0.57	1.75	12	1
4:A:355:PX4:H18	4:A:356:PX4:H15	0.57	1.75	13	1
4:A:331:PX4:H27	4:A:340:PX4:H53	0.57	1.76	14	1
4:A:393:PX4:H29	4:A:394:PX4:H56	0.57	1.75	5	1
4:A:368:PX4:H46	4:A:369:PX4:H22	0.57	1.74	8	1
4:A:331:PX4:H4	4:A:347:PX4:H50	0.57	1.74	9	1
4:A:316:PX4:H20	4:A:316:PX4:H49	0.57	1.74	10	1
4:A:395:PX4:H21	4:A:406:PX4:H51	0.57	1.77	10	1
4:A:423:PX4:H67	4:A:424:PX4:H37	0.57	1.75	14	1
4:A:370:PX4:H23	4:A:403:PX4:H17	0.57	1.75	10	1
4:A:378:PX4:H23	4:A:417:PX4:H64	0.57	1.75	10	1
4:A:404:PX4:H8	4:A:430:PX4:O6	0.57	2.00	6	2
4:A:337:PX4:H58	4:A:357:PX4:H56	0.57	1.75	8	1
4:A:396:PX4:H61	4:A:396:PX4:H29	0.57	1.77	11	1
4:A:412:PX4:H56	4:A:419:PX4:H35	0.57	1.76	13	1
4:A:376:PX4:H30	4:A:383:PX4:H64	0.57	1.76	2	1
4:A:403:PX4:H2	4:A:411:PX4:O3	0.57	1.99	2	1
4:A:423:PX4:H16	4:A:424:PX4:H26	0.57	1.74	2	1
4:A:307:PX4:H37	4:A:410:PX4:H44	0.57	1.75	12	1
4:A:378:PX4:H48	4:A:417:PX4:H67	0.57	1.77	13	1
4:A:317:PX4:H58	4:A:342:PX4:H24	0.57	1.76	3	1
4:A:335:PX4:H51	4:A:344:PX4:H24	0.57	1.77	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:332:PX4:H5	4:A:347:PX4:H61	0.57	1.75	10	1
1:A:165:ARG:NH1	4:A:362:PX4:H7	0.57	2.14	6	2
4:A:346:PX4:H35	4:A:354:PX4:H34	0.57	1.75	9	1
4:A:330:PX4:H22	4:A:344:PX4:H48	0.57	1.77	4	1
4:A:337:PX4:H61	4:A:345:PX4:H36	0.57	1.76	9	1
4:A:316:PX4:H45	4:A:418:PX4:H57	0.57	1.77	14	1
4:A:378:PX4:H51	4:A:418:PX4:H49	0.56	1.77	2	1
4:A:307:PX4:H67	4:A:314:PX4:H67	0.56	1.77	4	1
4:A:391:PX4:H22	4:A:414:PX4:H17	0.56	1.77	12	3
4:A:320:PX4:H34	4:A:378:PX4:H42	0.56	1.75	8	1
4:A:346:PX4:O6	4:A:346:PX4:H16	0.56	1.99	1	1
4:A:367:PX4:H17	4:A:430:PX4:H49	0.56	1.76	1	1
4:A:371:PX4:H8	4:A:377:PX4:O6	0.56	1.99	1	1
4:A:329:PX4:O6	4:A:336:PX4:H3	0.56	2.00	2	1
4:A:349:PX4:H70	4:A:422:PX4:H32	0.56	1.77	4	1
4:A:400:PX4:H1	4:A:409:PX4:H18	0.56	1.75	6	1
4:A:331:PX4:O1	4:A:332:PX4:H3	0.56	2.00	8	1
4:A:338:PX4:H57	4:A:346:PX4:H57	0.56	1.77	11	1
4:A:345:PX4:H65	4:A:348:PX4:H19	0.56	1.76	13	1
4:A:361:PX4:H64	4:A:425:PX4:H24	0.56	1.75	13	1
4:A:325:PX4:H47	4:A:341:PX4:H49	0.56	1.77	4	1
4:A:311:PX4:H22	4:A:311:PX4:H52	0.56	1.77	6	1
4:A:316:PX4:H68	4:A:368:PX4:H38	0.56	1.77	6	1
4:A:367:PX4:H23	4:A:368:PX4:H66	0.56	1.76	6	1
4:A:357:PX4:H29	4:A:357:PX4:H53	0.56	1.75	7	1
4:A:371:PX4:H52	4:A:377:PX4:H54	0.56	1.77	8	1
4:A:380:PX4:H21	4:A:381:PX4:H53	0.56	1.76	11	1
4:A:395:PX4:H50	4:A:402:PX4:H62	0.56	1.77	11	1
4:A:423:PX4:H49	4:A:424:PX4:H21	0.56	1.76	13	1
1:A:171:PHE:CZ	4:A:307:PX4:H17	0.56	2.36	1	2
4:A:400:PX4:H33	4:A:401:PX4:H60	0.56	1.77	4	1
4:A:376:PX4:H64	4:A:393:PX4:H50	0.56	1.77	2	1
4:A:403:PX4:H55	4:A:419:PX4:H59	0.56	1.77	4	1
4:A:368:PX4:H50	4:A:369:PX4:H25	0.56	1.76	9	1
4:A:393:PX4:H68	4:A:399:PX4:H68	0.56	1.78	14	1
4:A:312:PX4:H30	4:A:360:PX4:H53	0.56	1.76	1	1
4:A:321:PX4:H48	4:A:354:PX4:H23	0.56	1.77	3	1
4:A:329:PX4:H58	4:A:333:PX4:H43	0.56	1.78	3	1
4:A:306:PX4:H27	4:A:328:PX4:H41	0.56	1.78	8	1
4:A:306:PX4:H19	4:A:321:PX4:H23	0.56	1.76	12	2
4:A:370:PX4:H28	4:A:403:PX4:H17	0.56	1.77	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:396:PX4:H11	4:A:405:PX4:O8	0.56	2.00	13	1
4:A:345:PX4:H71	4:A:357:PX4:H57	0.56	1.78	1	1
4:A:314:PX4:C35	4:A:364:PX4:H29	0.56	2.30	6	1
4:A:339:PX4:H70	4:A:355:PX4:H43	0.56	1.78	8	1
4:A:370:PX4:H37	4:A:404:PX4:H29	0.56	1.76	11	1
4:A:354:PX4:H44	4:A:423:PX4:H36	0.56	1.78	14	1
4:A:332:PX4:H12	4:A:332:PX4:H16	0.56	1.77	1	1
4:A:371:PX4:H19	4:A:377:PX4:H17	0.56	1.77	1	1
4:A:380:PX4:H56	4:A:387:PX4:H64	0.56	1.78	2	1
4:A:316:PX4:H25	4:A:320:PX4:H30	0.56	1.78	3	1
4:A:314:PX4:H69	4:A:364:PX4:H29	0.56	1.77	6	1
4:A:342:PX4:H38	4:A:394:PX4:H70	0.56	1.78	9	1
4:A:325:PX4:H20	4:A:326:PX4:H22	0.56	1.75	10	1
4:A:355:PX4:H68	4:A:422:PX4:H37	0.56	1.77	1	1
4:A:330:PX4:H53	4:A:338:PX4:H21	0.56	1.76	4	1
4:A:406:PX4:H48	4:A:421:PX4:H53	0.56	1.78	11	1
4:A:412:PX4:H29	4:A:419:PX4:H49	0.56	1.78	12	1
4:A:322:PX4:H67	4:A:367:PX4:H30	0.56	1.77	13	1
4:A:359:PX4:H41	4:A:366:PX4:H44	0.56	1.78	1	1
4:A:343:PX4:H31	4:A:344:PX4:H32	0.56	1.78	3	1
4:A:374:PX4:H15	4:A:420:PX4:H19	0.56	1.76	12	2
4:A:306:PX4:H64	4:A:354:PX4:H19	0.56	1.76	10	1
4:A:311:PX4:H56	4:A:311:PX4:H25	0.56	1.75	14	1
4:A:348:PX4:H57	4:A:355:PX4:H32	0.55	1.77	3	1
4:A:329:PX4:H70	4:A:369:PX4:H41	0.55	1.78	6	1
4:A:421:PX4:H17	4:A:423:PX4:H52	0.55	1.77	7	2
4:A:374:PX4:H44	4:A:427:PX4:H17	0.55	1.76	7	1
4:A:412:PX4:H44	4:A:419:PX4:H39	0.55	1.79	12	1
4:A:388:PX4:H63	4:A:406:PX4:H62	0.55	1.78	13	1
4:A:313:PX4:H10	4:A:359:PX4:O2	0.55	2.01	14	1
4:A:391:PX4:H17	4:A:408:PX4:H20	0.55	1.78	6	1
4:A:331:PX4:H24	4:A:340:PX4:H17	0.55	1.78	7	1
4:A:309:PX4:H54	4:A:319:PX4:H53	0.55	1.78	12	1
4:A:308:PX4:H68	4:A:426:PX4:H51	0.55	1.78	7	1
4:A:349:PX4:H47	4:A:356:PX4:H38	0.55	1.79	11	1
4:A:422:PX4:H17	4:A:425:PX4:C29	0.55	2.30	13	1
4:A:308:PX4:H18	4:A:426:PX4:H43	0.55	1.79	2	1
4:A:406:PX4:H53	4:A:423:PX4:H61	0.55	1.77	2	1
4:A:349:PX4:O6	4:A:349:PX4:H6	0.55	2.02	5	2
4:A:423:PX4:H16	4:A:424:PX4:H23	0.55	1.79	4	1
4:A:421:PX4:H36	4:A:424:PX4:H37	0.55	1.77	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:336:PX4:H21	4:A:344:PX4:H56	0.55	1.77	9	1
4:A:420:PX4:H25	4:A:427:PX4:H31	0.55	1.77	12	1
4:A:341:PX4:H72	4:A:407:PX4:H40	0.55	1.78	1	1
4:A:371:PX4:H25	4:A:377:PX4:H21	0.55	1.79	8	1
4:A:342:PX4:H67	4:A:385:PX4:H43	0.55	1.77	10	1
4:A:405:PX4:H71	4:A:407:PX4:H54	0.55	1.78	12	1
4:A:309:PX4:H30	4:A:377:PX4:H70	0.55	1.78	1	1
4:A:400:PX4:H61	4:A:417:PX4:H25	0.55	1.78	4	1
4:A:388:PX4:H62	4:A:395:PX4:H55	0.55	1.79	6	1
4:A:417:PX4:H47	4:A:426:PX4:H51	0.55	1.77	6	1
4:A:363:PX4:H30	4:A:364:PX4:H32	0.55	1.79	10	1
4:A:404:PX4:H57	4:A:430:PX4:H27	0.55	1.78	12	1
4:A:310:PX4:H71	4:A:316:PX4:H22	0.55	1.78	13	1
4:A:348:PX4:H34	4:A:407:PX4:H70	0.55	1.79	1	1
4:A:404:PX4:H33	4:A:412:PX4:H35	0.55	1.77	7	1
4:A:342:PX4:H57	4:A:351:PX4:H36	0.55	1.78	8	1
4:A:338:PX4:H26	4:A:348:PX4:H22	0.55	1.78	12	1
4:A:312:PX4:H56	4:A:359:PX4:H50	0.55	1.79	1	1
4:A:349:PX4:H34	4:A:415:PX4:H45	0.55	1.79	2	1
4:A:412:PX4:H31	4:A:419:PX4:H47	0.55	1.77	4	1
4:A:327:PX4:H24	4:A:329:PX4:H31	0.55	1.79	5	1
4:A:371:PX4:H16	4:A:377:PX4:H47	0.55	1.79	5	2
4:A:391:PX4:H17	4:A:408:PX4:H19	0.55	1.78	8	1
4:A:339:PX4:H25	4:A:347:PX4:H53	0.55	1.79	1	1
4:A:308:PX4:O6	4:A:315:PX4:H11	0.55	2.02	3	1
4:A:372:PX4:H71	4:A:386:PX4:H37	0.55	1.78	4	1
4:A:374:PX4:H68	4:A:420:PX4:H41	0.55	1.77	4	1
4:A:391:PX4:H18	4:A:414:PX4:O2	0.55	2.02	7	1
4:A:400:PX4:H30	4:A:400:PX4:H59	0.55	1.77	7	1
4:A:325:PX4:H37	4:A:325:PX4:H67	0.55	1.79	10	1
4:A:306:PX4:H54	4:A:321:PX4:H49	0.55	1.78	5	1
4:A:313:PX4:H23	4:A:359:PX4:H21	0.55	1.78	6	1
4:A:423:PX4:H14	4:A:424:PX4:H19	0.55	1.78	7	1
4:A:386:PX4:H50	4:A:387:PX4:H58	0.55	1.77	9	1
4:A:321:PX4:H5	4:A:362:PX4:O1	0.54	2.02	4	2
4:A:317:PX4:H39	4:A:317:PX4:H68	0.54	1.79	3	1
4:A:380:PX4:H62	4:A:387:PX4:H30	0.54	1.79	7	1
4:A:335:PX4:H66	4:A:343:PX4:H45	0.54	1.80	8	1
4:A:359:PX4:H44	4:A:366:PX4:H30	0.54	1.78	8	1
4:A:366:PX4:H29	4:A:427:PX4:H67	0.54	1.77	9	1
4:A:343:PX4:H34	4:A:344:PX4:H37	0.54	1.76	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:392:PX4:H62	4:A:407:PX4:H33	0.54	1.79	2	1
4:A:338:PX4:H32	4:A:347:PX4:H28	0.54	1.79	8	1
4:A:374:PX4:H27	4:A:412:PX4:H46	0.54	1.78	9	1
4:A:357:PX4:H15	4:A:358:PX4:O1	0.54	2.02	11	1
4:A:392:PX4:H63	4:A:393:PX4:H57	0.54	1.78	11	1
4:A:309:PX4:H33	4:A:319:PX4:H37	0.54	1.78	13	1
4:A:357:PX4:H70	4:A:411:PX4:H42	0.54	1.78	4	1
4:A:405:PX4:H25	4:A:415:PX4:H54	0.54	1.80	4	1
4:A:421:PX4:H69	4:A:430:PX4:H44	0.54	1.78	4	1
4:A:327:PX4:H56	4:A:327:PX4:H19	0.54	1.80	5	1
4:A:404:PX4:H28	4:A:413:PX4:H32	0.54	1.79	5	1
4:A:342:PX4:H30	4:A:351:PX4:H33	0.54	1.78	7	1
4:A:369:PX4:H31	4:A:424:PX4:H71	0.54	1.77	11	1
4:A:306:PX4:H71	4:A:360:PX4:H30	0.54	1.79	13	1
4:A:338:PX4:H27	4:A:345:PX4:H63	0.54	1.80	13	1
4:A:348:PX4:H53	4:A:355:PX4:H28	0.54	1.79	3	1
4:A:332:PX4:H48	4:A:334:PX4:H38	0.54	1.80	5	1
4:A:370:PX4:H63	4:A:403:PX4:H33	0.54	1.80	7	1
4:A:395:PX4:H38	4:A:415:PX4:H62	0.54	1.77	9	1
4:A:381:PX4:H59	4:A:402:PX4:H27	0.54	1.79	10	1
4:A:367:PX4:H11	4:A:424:PX4:H18	0.54	1.78	2	1
4:A:383:PX4:H57	4:A:392:PX4:H31	0.54	1.80	2	1
1:A:119:ASN:OD1	4:A:355:PX4:H7	0.54	2.01	5	2
4:A:324:PX4:H67	4:A:341:PX4:H36	0.54	1.79	11	1
4:A:382:PX4:H57	4:A:427:PX4:H42	0.54	1.79	1	1
4:A:397:PX4:H39	4:A:398:PX4:H66	0.54	1.78	1	1
4:A:376:PX4:H17	4:A:383:PX4:H51	0.54	1.80	2	1
4:A:327:PX4:H21	4:A:329:PX4:H41	0.54	1.80	4	1
4:A:409:PX4:H50	4:A:422:PX4:H47	0.54	1.79	6	1
4:A:336:PX4:H28	4:A:339:PX4:H29	0.54	1.80	8	1
4:A:424:PX4:H60	4:A:429:PX4:H55	0.54	1.79	9	1
4:A:330:PX4:H30	4:A:336:PX4:H56	0.54	1.80	6	1
4:A:333:PX4:H53	4:A:341:PX4:H16	0.54	1.78	7	1
4:A:416:PX4:H47	4:A:422:PX4:H51	0.54	1.79	7	1
4:A:306:PX4:H14	4:A:321:PX4:C10	0.54	2.33	8	1
4:A:317:PX4:H52	4:A:324:PX4:H24	0.54	1.79	8	1
4:A:388:PX4:H18	4:A:396:PX4:H2	0.54	1.79	14	1
1:A:162:VAL:HG11	4:A:314:PX4:H34	0.54	1.80	2	1
4:A:400:PX4:H34	4:A:417:PX4:H32	0.54	1.79	8	1
4:A:380:PX4:H25	4:A:381:PX4:H56	0.54	1.80	11	1
4:A:337:PX4:H46	4:A:345:PX4:H56	0.54	1.79	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:420:PX4:H58	4:A:427:PX4:H52	0.54	1.78	3	1
4:A:391:PX4:H24	4:A:392:PX4:H61	0.54	1.79	7	1
4:A:400:PX4:H64	4:A:417:PX4:H27	0.54	1.78	8	1
4:A:326:PX4:H37	4:A:334:PX4:H24	0.54	1.79	12	1
4:A:332:PX4:H39	4:A:339:PX4:H39	0.54	1.78	1	1
4:A:320:PX4:H69	4:A:378:PX4:H33	0.54	1.79	3	1
4:A:328:PX4:H62	4:A:329:PX4:H25	0.54	1.80	4	1
4:A:326:PX4:H8	4:A:351:PX4:H22	0.54	1.80	5	1
4:A:393:PX4:H16	4:A:394:PX4:H24	0.54	1.79	6	1
4:A:313:PX4:H42	4:A:430:PX4:H41	0.54	1.79	7	1
4:A:358:PX4:H20	4:A:365:PX4:H17	0.54	1.78	11	1
4:A:389:PX4:H25	4:A:389:PX4:H59	0.53	1.81	3	1
4:A:388:PX4:H63	4:A:402:PX4:H72	0.53	1.79	5	1
4:A:349:PX4:H50	4:A:356:PX4:H5	0.53	1.79	2	1
4:A:367:PX4:H66	4:A:428:PX4:H27	0.53	1.80	5	1
4:A:415:PX4:H53	4:A:422:PX4:H25	0.53	1.79	9	1
4:A:391:PX4:H58	4:A:401:PX4:H26	0.53	1.80	4	1
4:A:339:PX4:H31	4:A:347:PX4:H56	0.53	1.81	9	1
4:A:388:PX4:H7	4:A:397:PX4:H49	0.53	1.80	9	1
4:A:374:PX4:H43	4:A:412:PX4:H32	0.53	1.79	11	1
4:A:363:PX4:H44	4:A:426:PX4:H70	0.53	1.78	12	1
4:A:373:PX4:H52	4:A:381:PX4:H33	0.53	1.79	12	1
4:A:377:PX4:H54	4:A:378:PX4:H25	0.53	1.80	13	1
1:A:165:ARG:CZ	4:A:362:PX4:H7	0.53	2.33	13	4
4:A:388:PX4:H59	4:A:402:PX4:H27	0.53	1.79	5	1
4:A:361:PX4:H26	4:A:362:PX4:H31	0.53	1.80	8	1
4:A:420:PX4:H30	4:A:427:PX4:H33	0.53	1.80	8	1
4:A:383:PX4:H27	4:A:399:PX4:H21	0.53	1.81	10	1
4:A:348:PX4:H16	4:A:355:PX4:H20	0.53	1.79	12	1
4:A:389:PX4:H53	4:A:398:PX4:H52	0.53	1.81	13	1
4:A:392:PX4:H24	4:A:399:PX4:H49	0.53	1.81	2	1
4:A:388:PX4:O1	4:A:396:PX4:H4	0.53	2.03	9	1
4:A:389:PX4:O2	4:A:398:PX4:H15	0.53	2.02	9	1
4:A:345:PX4:H16	4:A:346:PX4:O8	0.53	2.04	12	1
4:A:343:PX4:H69	4:A:344:PX4:H65	0.53	1.79	1	1
4:A:342:PX4:H49	4:A:351:PX4:H25	0.53	1.80	2	1
4:A:337:PX4:H54	4:A:345:PX4:H63	0.53	1.79	5	1
4:A:369:PX4:H44	4:A:430:PX4:H72	0.53	1.80	6	1
4:A:312:PX4:H17	4:A:359:PX4:H8	0.53	1.80	7	1
4:A:380:PX4:O2	4:A:381:PX4:H15	0.53	2.03	9	1
4:A:395:PX4:H42	4:A:415:PX4:H69	0.53	1.81	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H53	4:A:401:PX4:H25	0.53	1.79	13	1
4:A:326:PX4:O2	4:A:350:PX4:H6	0.53	2.03	3	1
4:A:316:PX4:H64	4:A:368:PX4:H42	0.53	1.81	6	1
4:A:367:PX4:H26	4:A:430:PX4:H69	0.53	1.78	6	1
4:A:368:PX4:O1	4:A:418:PX4:H7	0.53	2.04	10	1
4:A:328:PX4:H54	4:A:329:PX4:H22	0.53	1.80	13	1
4:A:395:PX4:H39	4:A:415:PX4:H59	0.53	1.80	5	1
4:A:393:PX4:H68	4:A:394:PX4:H41	0.53	1.80	6	1
4:A:313:PX4:H45	4:A:354:PX4:H58	0.53	1.79	9	1
4:A:412:PX4:H63	4:A:421:PX4:H45	0.53	1.79	9	1
4:A:389:PX4:H34	4:A:397:PX4:H34	0.53	1.79	10	1
4:A:366:PX4:H32	4:A:427:PX4:H64	0.53	1.81	11	1
4:A:350:PX4:H66	4:A:350:PX4:H33	0.53	1.81	13	1
4:A:339:PX4:H19	4:A:347:PX4:H22	0.53	1.80	14	1
4:A:326:PX4:H44	4:A:350:PX4:H28	0.53	1.79	1	1
4:A:340:PX4:H49	4:A:341:PX4:H46	0.53	1.81	7	1
4:A:317:PX4:H20	4:A:342:PX4:H22	0.53	1.80	5	1
4:A:397:PX4:H23	4:A:398:PX4:H53	0.53	1.81	5	1
4:A:421:PX4:H33	4:A:430:PX4:H63	0.53	1.81	12	1
4:A:306:PX4:H24	4:A:360:PX4:H43	0.52	1.80	4	1
4:A:325:PX4:H29	4:A:325:PX4:H58	0.52	1.80	9	1
4:A:351:PX4:H66	4:A:409:PX4:H42	0.52	1.80	4	1
4:A:385:PX4:H60	4:A:399:PX4:H62	0.52	1.82	5	1
4:A:346:PX4:H44	4:A:362:PX4:H67	0.52	1.81	8	1
4:A:308:PX4:H51	4:A:311:PX4:H14	0.52	1.82	9	1
4:A:332:PX4:H47	4:A:347:PX4:H66	0.52	1.80	14	1
4:A:337:PX4:H18	4:A:337:PX4:O3	0.52	2.03	6	1
4:A:406:PX4:H34	4:A:424:PX4:H38	0.52	1.81	6	1
4:A:388:PX4:H19	4:A:396:PX4:H48	0.52	1.80	8	1
4:A:355:PX4:H5	4:A:362:PX4:H46	0.52	1.81	9	1
4:A:311:PX4:H71	4:A:426:PX4:H59	0.52	1.82	12	1
4:A:358:PX4:H9	4:A:358:PX4:H16	0.52	1.81	2	1
4:A:380:PX4:H31	4:A:381:PX4:H65	0.52	1.81	2	1
4:A:367:PX4:H24	4:A:424:PX4:H50	0.52	1.82	3	1
4:A:319:PX4:H19	4:A:319:PX4:H58	0.52	1.82	7	1
4:A:310:PX4:H35	4:A:409:PX4:H38	0.52	1.80	9	1
4:A:307:PX4:H53	4:A:361:PX4:H24	0.52	1.80	8	1
4:A:315:PX4:H58	4:A:322:PX4:H24	0.52	1.80	9	1
4:A:390:PX4:H24	4:A:428:PX4:H53	0.52	1.82	9	1
4:A:337:PX4:H50	4:A:345:PX4:H34	0.52	1.81	12	1
4:A:404:PX4:H9	4:A:419:PX4:O1	0.52	2.05	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:330:PX4:H26	4:A:344:PX4:H52	0.52	1.81	4	1
4:A:309:PX4:H16	4:A:320:PX4:H23	0.52	1.82	5	1
4:A:322:PX4:H26	4:A:333:PX4:H38	0.52	1.80	5	1
4:A:400:PX4:O1	4:A:401:PX4:H2	0.52	2.05	5	1
4:A:310:PX4:H25	4:A:363:PX4:H42	0.52	1.82	7	1
4:A:424:PX4:H50	4:A:429:PX4:H51	0.52	1.80	8	1
4:A:307:PX4:H52	4:A:356:PX4:H42	0.52	1.81	10	1
4:A:396:PX4:O2	4:A:396:PX4:H16	0.52	2.05	12	1
4:A:368:PX4:H58	4:A:424:PX4:H48	0.52	1.82	7	1
4:A:408:PX4:H67	4:A:409:PX4:H32	0.52	1.81	7	1
4:A:404:PX4:H53	4:A:413:PX4:H26	0.52	1.81	13	1
4:A:350:PX4:H45	4:A:363:PX4:C29	0.52	2.33	1	1
4:A:400:PX4:C14	4:A:401:PX4:H46	0.52	2.34	2	1
4:A:418:PX4:H26	4:A:425:PX4:C12	0.52	2.33	4	1
4:A:361:PX4:H44	4:A:415:PX4:H42	0.52	1.81	6	1
4:A:331:PX4:H56	4:A:339:PX4:H59	0.52	1.82	9	1
4:A:369:PX4:H56	4:A:425:PX4:H29	0.52	1.81	13	1
4:A:383:PX4:O6	4:A:399:PX4:H16	0.52	2.05	1	1
4:A:405:PX4:H10	4:A:414:PX4:H27	0.52	1.80	2	1
4:A:337:PX4:O1	4:A:357:PX4:H15	0.52	2.04	3	1
4:A:350:PX4:H22	4:A:363:PX4:H57	0.52	1.82	9	1
4:A:325:PX4:H41	4:A:394:PX4:H41	0.51	1.80	1	1
4:A:428:PX4:H52	4:A:429:PX4:H46	0.51	1.81	12	1
4:A:348:PX4:H32	4:A:355:PX4:H35	0.51	1.83	14	1
4:A:400:PX4:H20	4:A:409:PX4:H23	0.51	1.81	3	1
4:A:388:PX4:H57	4:A:411:PX4:H41	0.51	1.80	8	1
4:A:380:PX4:H39	4:A:402:PX4:H35	0.51	1.82	9	1
4:A:380:PX4:H20	4:A:381:PX4:H48	0.51	1.82	3	1
4:A:306:PX4:H41	4:A:329:PX4:H70	0.51	1.81	5	1
4:A:362:PX4:H44	4:A:409:PX4:H70	0.51	1.81	5	1
4:A:364:PX4:H60	4:A:426:PX4:H37	0.51	1.82	5	1
4:A:330:PX4:H41	4:A:344:PX4:H64	0.51	1.82	8	1
4:A:340:PX4:H37	4:A:350:PX4:H42	0.51	1.80	10	1
4:A:367:PX4:H48	4:A:430:PX4:H49	0.51	1.81	10	1
4:A:338:PX4:C6	4:A:348:PX4:H15	0.51	2.35	13	1
4:A:388:PX4:H35	4:A:405:PX4:H61	0.51	1.81	14	1
4:A:408:PX4:H51	4:A:409:PX4:H48	0.51	1.81	4	1
4:A:331:PX4:O1	4:A:332:PX4:H7	0.51	2.05	5	2
4:A:375:PX4:H51	4:A:389:PX4:H49	0.51	1.83	5	1
4:A:313:PX4:H49	4:A:327:PX4:H25	0.51	1.81	6	1
4:A:314:PX4:H54	4:A:361:PX4:H30	0.51	1.82	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:316:PX4:H27	4:A:368:PX4:H42	0.51	1.82	10	1
4:A:315:PX4:H36	4:A:361:PX4:H61	0.51	1.82	11	1
4:A:367:PX4:H41	4:A:375:PX4:H64	0.51	1.81	11	1
4:A:356:PX4:H35	4:A:362:PX4:H28	0.51	1.81	14	1
4:A:419:PX4:H31	4:A:430:PX4:H29	0.51	1.82	14	1
4:A:326:PX4:H47	4:A:363:PX4:H67	0.51	1.82	1	1
4:A:369:PX4:H50	4:A:424:PX4:H20	0.51	1.83	4	2
4:A:355:PX4:H17	4:A:356:PX4:H15	0.51	1.82	5	1
4:A:387:PX4:H47	4:A:411:PX4:H47	0.51	1.82	8	1
4:A:349:PX4:H43	4:A:415:PX4:H32	0.51	1.82	11	1
4:A:330:PX4:H35	4:A:336:PX4:H52	0.51	1.83	11	1
4:A:317:PX4:H45	4:A:326:PX4:H52	0.51	1.81	12	1
4:A:406:PX4:H27	4:A:423:PX4:H62	0.51	1.83	1	1
4:A:326:PX4:H17	4:A:363:PX4:H61	0.51	1.82	4	1
4:A:321:PX4:H42	4:A:367:PX4:H68	0.51	1.81	6	1
4:A:326:PX4:H21	4:A:363:PX4:H63	0.51	1.83	8	1
4:A:348:PX4:H16	4:A:355:PX4:H19	0.51	1.82	8	1
4:A:385:PX4:H62	4:A:392:PX4:H34	0.51	1.82	9	1
4:A:313:PX4:H50	4:A:327:PX4:H34	0.51	1.81	12	1
4:A:403:PX4:H10	4:A:411:PX4:O2	0.51	2.05	4	1
4:A:317:PX4:H29	4:A:363:PX4:H71	0.51	1.82	5	1
4:A:308:PX4:H53	4:A:311:PX4:H19	0.51	1.83	6	1
4:A:392:PX4:H58	4:A:414:PX4:H51	0.51	1.83	12	1
4:A:388:PX4:H35	4:A:395:PX4:H34	0.51	1.82	1	1
4:A:405:PX4:H6	4:A:414:PX4:H26	0.51	1.82	1	1
4:A:324:PX4:H59	4:A:342:PX4:H26	0.51	1.82	3	1
4:A:402:PX4:H55	4:A:404:PX4:H49	0.51	1.82	10	1
4:A:348:PX4:H71	4:A:348:PX4:H44	0.51	1.83	12	1
4:A:306:PX4:H14	4:A:321:PX4:H19	0.51	1.82	8	1
4:A:307:PX4:H64	4:A:314:PX4:H67	0.51	1.83	8	1
4:A:330:PX4:H60	4:A:337:PX4:H29	0.51	1.82	9	1
4:A:344:PX4:H62	4:A:347:PX4:H36	0.51	1.82	12	1
4:A:413:PX4:H60	4:A:421:PX4:H57	0.50	1.83	4	1
4:A:334:PX4:H47	4:A:350:PX4:H16	0.50	1.83	6	1
4:A:390:PX4:H63	4:A:429:PX4:H68	0.50	1.81	7	1
4:A:346:PX4:H7	4:A:353:PX4:H48	0.50	1.84	8	1
4:A:309:PX4:H39	4:A:319:PX4:H35	0.50	1.83	9	1
4:A:342:PX4:H39	4:A:394:PX4:H39	0.50	1.81	10	1
4:A:391:PX4:H34	4:A:407:PX4:H46	0.50	1.82	10	1
4:A:314:PX4:H51	4:A:364:PX4:H46	0.50	1.82	14	1
4:A:313:PX4:H68	4:A:328:PX4:H44	0.50	1.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:428:PX4:H14	4:A:429:PX4:H22	0.50	1.83	4	1
4:A:317:PX4:H20	4:A:324:PX4:H56	0.50	1.83	10	1
4:A:337:PX4:H26	4:A:357:PX4:H35	0.50	1.83	12	1
4:A:310:PX4:H30	4:A:364:PX4:H39	0.50	1.83	2	1
4:A:332:PX4:H30	4:A:339:PX4:H39	0.50	1.82	5	1
4:A:317:PX4:O8	4:A:342:PX4:H17	0.50	2.06	6	1
4:A:367:PX4:H21	4:A:424:PX4:H55	0.50	1.82	7	1
4:A:331:PX4:H61	4:A:333:PX4:H21	0.50	1.81	8	1
4:A:408:PX4:H15	4:A:409:PX4:C1	0.50	2.28	10	1
4:A:307:PX4:H36	4:A:361:PX4:H54	0.50	1.83	11	1
4:A:368:PX4:H4	4:A:418:PX4:O1	0.50	2.06	12	1
4:A:331:PX4:H47	4:A:347:PX4:H54	0.50	1.83	13	1
4:A:331:PX4:H59	4:A:339:PX4:H38	0.50	1.84	14	1
4:A:374:PX4:H36	4:A:427:PX4:H21	0.50	1.84	1	1
4:A:380:PX4:H16	4:A:381:PX4:H47	0.50	1.83	1	2
4:A:412:PX4:H26	4:A:419:PX4:H26	0.50	1.81	1	1
4:A:330:PX4:H12	4:A:344:PX4:H46	0.50	1.84	3	1
4:A:400:PX4:C10	4:A:401:PX4:H17	0.50	2.35	6	1
4:A:306:PX4:H52	4:A:322:PX4:H61	0.50	1.84	8	1
4:A:411:PX4:H45	4:A:421:PX4:H53	0.50	1.84	9	1
4:A:387:PX4:H72	4:A:402:PX4:H38	0.50	1.82	12	1
4:A:400:PX4:O4	4:A:401:PX4:H3	0.50	2.07	12	1
4:A:410:PX4:H62	4:A:417:PX4:H58	0.50	1.82	12	1
4:A:373:PX4:H28	4:A:381:PX4:H46	0.50	1.82	13	1
4:A:420:PX4:H17	4:A:427:PX4:H19	0.50	1.83	1	1
4:A:309:PX4:H16	4:A:320:PX4:H22	0.50	1.83	2	1
4:A:386:PX4:O1	4:A:387:PX4:H13	0.50	2.07	2	1
4:A:379:PX4:H26	4:A:379:PX4:H56	0.50	1.82	3	1
4:A:389:PX4:H67	4:A:398:PX4:H37	0.50	1.84	5	1
4:A:338:PX4:H55	4:A:356:PX4:H55	0.50	1.82	6	1
4:A:359:PX4:H63	4:A:420:PX4:H64	0.50	1.83	7	1
4:A:365:PX4:C23	4:A:366:PX4:H51	0.50	2.36	8	1
4:A:318:PX4:H17	4:A:327:PX4:H49	0.50	1.82	13	2
4:A:350:PX4:H19	4:A:363:PX4:H64	0.50	1.84	1	1
4:A:355:PX4:O4	4:A:356:PX4:H15	0.50	2.06	14	2
4:A:367:PX4:H68	4:A:421:PX4:H29	0.50	1.83	1	1
4:A:408:PX4:O3	4:A:409:PX4:H1	0.50	2.05	1	1
4:A:370:PX4:H13	4:A:411:PX4:O8	0.50	2.07	2	1
4:A:383:PX4:H24	4:A:390:PX4:H56	0.50	1.84	8	1
4:A:380:PX4:H35	4:A:380:PX4:H64	0.50	1.84	12	1
4:A:368:PX4:H11	4:A:369:PX4:O6	0.50	2.07	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:378:PX4:H39	4:A:418:PX4:H67	0.50	1.83	4	1
4:A:317:PX4:H40	4:A:326:PX4:H61	0.50	1.83	5	1
4:A:321:PX4:H11	4:A:362:PX4:O1	0.50	2.07	8	1
4:A:337:PX4:H16	4:A:357:PX4:H47	0.50	1.84	9	2
4:A:379:PX4:H47	4:A:384:PX4:H16	0.50	1.83	9	1
4:A:378:PX4:H28	4:A:417:PX4:H63	0.50	1.83	12	1
4:A:348:PX4:H36	4:A:396:PX4:H43	0.50	1.82	13	1
4:A:336:PX4:H33	4:A:339:PX4:H67	0.50	1.84	1	1
4:A:339:PX4:H57	4:A:339:PX4:H41	0.50	1.84	2	1
4:A:383:PX4:H40	4:A:390:PX4:H39	0.50	1.82	13	2
4:A:384:PX4:H21	4:A:385:PX4:H20	0.50	1.82	5	1
4:A:393:PX4:H3	4:A:394:PX4:O4	0.50	2.07	5	1
4:A:395:PX4:H57	4:A:421:PX4:H67	0.50	1.82	5	1
4:A:348:PX4:H40	4:A:395:PX4:H64	0.50	1.83	7	1
4:A:309:PX4:H48	4:A:319:PX4:H26	0.50	1.83	9	1
4:A:398:PX4:H20	4:A:407:PX4:H15	0.50	1.84	13	1
4:A:404:PX4:H26	4:A:413:PX4:H24	0.50	1.82	13	1
4:A:410:PX4:H46	4:A:426:PX4:C6	0.50	2.37	13	1
4:A:346:PX4:O8	4:A:362:PX4:H13	0.50	2.07	11	2
4:A:307:PX4:H45	4:A:425:PX4:H23	0.50	1.84	10	1
4:A:342:PX4:H14	4:A:351:PX4:H20	0.50	1.83	12	1
4:A:387:PX4:H67	4:A:402:PX4:H34	0.50	1.83	12	1
4:A:388:PX4:H32	4:A:397:PX4:H64	0.49	1.83	1	1
4:A:395:PX4:H40	4:A:405:PX4:H36	0.49	1.83	2	1
4:A:374:PX4:H30	4:A:412:PX4:H52	0.49	1.83	5	1
4:A:380:PX4:H34	4:A:387:PX4:H70	0.49	1.84	7	1
4:A:370:PX4:H19	4:A:403:PX4:O7	0.49	2.07	13	1
4:A:306:PX4:H34	4:A:328:PX4:H36	0.49	1.84	1	1
4:A:335:PX4:H17	4:A:343:PX4:O1	0.49	2.07	1	1
4:A:338:PX4:H16	4:A:345:PX4:H53	0.49	1.82	2	1
4:A:402:PX4:H62	4:A:404:PX4:H58	0.49	1.83	3	1
4:A:405:PX4:H40	4:A:422:PX4:H38	0.49	1.82	8	1
4:A:317:PX4:H46	4:A:342:PX4:H12	0.49	1.84	10	1
4:A:313:PX4:O2	4:A:360:PX4:H12	0.49	2.07	12	1
4:A:340:PX4:H16	4:A:341:PX4:H50	0.49	1.82	12	1
4:A:371:PX4:H34	4:A:377:PX4:H30	0.49	1.83	12	1
4:A:404:PX4:H6	4:A:430:PX4:O6	0.49	2.07	12	1
4:A:326:PX4:H36	4:A:332:PX4:H46	0.49	1.83	13	1
4:A:349:PX4:H33	4:A:363:PX4:H17	0.49	1.84	14	1
4:A:399:PX4:H58	4:A:407:PX4:H32	0.49	1.84	1	1
4:A:378:PX4:H46	4:A:418:PX4:H47	0.49	1.83	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H54	4:A:416:PX4:H39	0.49	1.84	8	1
4:A:376:PX4:H35	4:A:418:PX4:H72	0.49	1.84	11	1
4:A:323:PX4:H26	4:A:333:PX4:H30	0.49	1.84	14	1
4:A:369:PX4:H56	4:A:423:PX4:H25	0.49	1.84	2	1
4:A:367:PX4:H54	4:A:412:PX4:H19	0.49	1.83	6	1
4:A:413:PX4:H21	4:A:430:PX4:H23	0.49	1.84	14	1
4:A:374:PX4:H45	4:A:419:PX4:H24	0.49	1.85	4	1
4:A:376:PX4:H44	4:A:377:PX4:H61	0.49	1.83	4	1
4:A:317:PX4:O7	4:A:324:PX4:H14	0.49	2.07	5	1
4:A:408:PX4:H32	4:A:425:PX4:H68	0.49	1.82	5	1
4:A:377:PX4:H55	4:A:378:PX4:H26	0.49	1.84	7	1
4:A:353:PX4:H20	4:A:366:PX4:H53	0.49	1.83	11	1
4:A:361:PX4:H59	4:A:425:PX4:H31	0.49	1.83	11	1
4:A:328:PX4:H24	4:A:360:PX4:H41	0.49	1.84	3	1
4:A:391:PX4:H42	4:A:414:PX4:H19	0.49	1.84	3	1
4:A:316:PX4:H58	4:A:316:PX4:H21	0.49	1.85	4	1
4:A:331:PX4:H15	4:A:332:PX4:H19	0.49	1.83	5	1
4:A:331:PX4:H29	4:A:340:PX4:H17	0.49	1.83	7	1
4:A:409:PX4:H13	4:A:409:PX4:H15	0.49	1.84	9	1
4:A:307:PX4:H48	4:A:361:PX4:H24	0.49	1.83	12	1
4:A:334:PX4:H48	4:A:349:PX4:O5	0.49	2.06	12	1
4:A:388:PX4:O2	4:A:395:PX4:H4	0.49	2.08	3	2
4:A:319:PX4:H39	4:A:377:PX4:H70	0.49	1.84	6	1
4:A:307:PX4:H46	4:A:314:PX4:H22	0.49	1.85	10	1
4:A:373:PX4:H15	4:A:373:PX4:H13	0.49	1.84	1	1
4:A:309:PX4:H15	4:A:319:PX4:O5	0.49	2.08	6	1
4:A:313:PX4:H54	4:A:327:PX4:H27	0.49	1.85	10	1
4:A:327:PX4:H32	4:A:329:PX4:H27	0.49	1.83	11	1
4:A:348:PX4:H26	4:A:355:PX4:C13	0.49	2.37	12	1
4:A:410:PX4:H54	4:A:417:PX4:H54	0.49	1.83	13	1
4:A:317:PX4:H55	4:A:342:PX4:H48	0.49	1.84	1	1
4:A:353:PX4:H28	4:A:366:PX4:H55	0.49	1.85	2	1
4:A:400:PX4:H1	4:A:401:PX4:O1	0.49	2.08	2	1
4:A:332:PX4:H62	4:A:415:PX4:H60	0.49	1.84	4	1
4:A:306:PX4:H72	4:A:354:PX4:H51	0.49	1.84	6	1
4:A:318:PX4:H63	4:A:329:PX4:H44	0.49	1.85	6	1
4:A:385:PX4:H55	4:A:393:PX4:H54	0.49	1.84	8	1
4:A:367:PX4:H28	4:A:424:PX4:H56	0.49	1.85	10	1
1:A:191:ILE:HG22	4:A:349:PX4:H3	0.49	1.85	12	1
4:A:370:PX4:H30	4:A:403:PX4:H26	0.49	1.85	14	1
4:A:325:PX4:H51	4:A:341:PX4:H49	0.49	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:348:PX4:H9	4:A:355:PX4:O2	0.49	2.08	3	2
4:A:371:PX4:H37	4:A:376:PX4:H42	0.49	1.84	5	1
4:A:354:PX4:H27	4:A:362:PX4:H60	0.49	1.85	11	1
4:A:355:PX4:H54	4:A:362:PX4:H53	0.49	1.84	11	1
4:A:376:PX4:H40	4:A:377:PX4:H57	0.49	1.83	11	1
4:A:405:PX4:H17	4:A:414:PX4:H22	0.49	1.85	14	1
4:A:315:PX4:H56	4:A:323:PX4:H16	0.48	1.85	4	1
4:A:346:PX4:H66	4:A:353:PX4:H66	0.48	1.83	6	1
4:A:403:PX4:O6	4:A:403:PX4:H1	0.48	2.08	10	1
4:A:418:PX4:H31	4:A:425:PX4:H22	0.48	1.85	13	1
4:A:391:PX4:H48	4:A:408:PX4:H20	0.48	1.83	14	1
4:A:306:PX4:H27	4:A:328:PX4:H53	0.48	1.84	3	1
4:A:388:PX4:H14	4:A:395:PX4:O3	0.48	2.08	13	3
4:A:310:PX4:H59	4:A:364:PX4:H30	0.48	1.83	7	1
4:A:306:PX4:H67	4:A:360:PX4:H30	0.48	1.86	8	1
4:A:315:PX4:H32	4:A:322:PX4:H48	0.48	1.83	9	1
4:A:306:PX4:H65	4:A:321:PX4:H17	0.48	1.84	10	1
4:A:321:PX4:H27	4:A:322:PX4:H59	0.48	1.84	13	1
4:A:331:PX4:H57	4:A:332:PX4:H29	0.48	1.85	5	1
4:A:353:PX4:H48	4:A:354:PX4:H62	0.48	1.84	12	1
4:A:346:PX4:H48	4:A:362:PX4:H50	0.48	1.85	4	1
4:A:380:PX4:H63	4:A:386:PX4:H20	0.48	1.85	7	1
4:A:313:PX4:H63	4:A:328:PX4:H38	0.48	1.84	10	1
4:A:328:PX4:H23	4:A:360:PX4:H33	0.48	1.85	14	1
1:A:163:PHE:CZ	1:A:212:LEU:HD11	0.48	2.43	9	1
4:A:370:PX4:H72	4:A:387:PX4:H71	0.48	1.84	9	1
4:A:318:PX4:H57	4:A:327:PX4:H54	0.48	1.84	10	1
4:A:322:PX4:H32	4:A:333:PX4:H55	0.48	1.86	14	1
4:A:306:PX4:H37	4:A:360:PX4:H38	0.48	1.83	2	1
4:A:322:PX4:H45	4:A:323:PX4:H65	0.48	1.84	4	1
4:A:358:PX4:H60	4:A:358:PX4:H36	0.48	1.86	4	1
4:A:417:PX4:H51	4:A:426:PX4:H46	0.48	1.85	4	1
4:A:316:PX4:H20	4:A:316:PX4:C25	0.48	2.38	10	1
4:A:328:PX4:H27	4:A:360:PX4:H36	0.48	1.85	13	1
4:A:343:PX4:H35	4:A:344:PX4:H28	0.48	1.84	13	1
4:A:332:PX4:O1	4:A:332:PX4:H7	0.48	2.09	2	1
4:A:393:PX4:H72	4:A:394:PX4:H32	0.48	1.84	2	1
4:A:405:PX4:H5	4:A:415:PX4:H17	0.48	1.85	7	1
4:A:368:PX4:H21	4:A:429:PX4:H62	0.48	1.84	9	1
4:A:323:PX4:H22	4:A:333:PX4:H49	0.48	1.86	12	1
4:A:351:PX4:H47	4:A:352:PX4:H19	0.48	1.86	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:309:PX4:H56	4:A:316:PX4:H50	0.48	1.84	8	1
4:A:333:PX4:H49	4:A:341:PX4:H14	0.48	1.85	8	1
4:A:336:PX4:H23	4:A:339:PX4:H57	0.48	1.86	9	1
4:A:350:PX4:H44	4:A:414:PX4:H42	0.48	1.84	9	1
4:A:343:PX4:H47	4:A:352:PX4:H53	0.48	1.84	11	1
4:A:345:PX4:H60	4:A:348:PX4:H22	0.48	1.85	11	1
4:A:358:PX4:H38	4:A:417:PX4:H45	0.48	1.84	12	1
4:A:400:PX4:H8	4:A:401:PX4:O6	0.48	2.09	13	1
4:A:349:PX4:H46	4:A:356:PX4:H11	0.48	1.86	4	1
4:A:392:PX4:H51	4:A:407:PX4:H23	0.48	1.86	4	1
4:A:336:PX4:H14	4:A:344:PX4:H51	0.48	1.86	5	1
4:A:377:PX4:H54	4:A:378:PX4:H30	0.48	1.85	6	1
4:A:400:PX4:H1	4:A:409:PX4:O1	0.48	2.09	9	1
4:A:396:PX4:H50	4:A:398:PX4:H28	0.48	1.85	1	1
4:A:388:PX4:H21	4:A:406:PX4:H70	0.48	1.85	5	1
4:A:388:PX4:H51	4:A:402:PX4:H19	0.48	1.85	5	1
4:A:393:PX4:H19	4:A:394:PX4:H48	0.48	1.85	8	1
4:A:382:PX4:H54	4:A:428:PX4:H27	0.48	1.84	12	1
4:A:381:PX4:H27	4:A:384:PX4:H54	0.48	1.84	13	1
4:A:318:PX4:H47	4:A:327:PX4:H46	0.48	1.85	14	1
4:A:393:PX4:H67	4:A:394:PX4:H33	0.47	1.84	1	1
4:A:392:PX4:H58	4:A:414:PX4:H50	0.47	1.86	4	1
4:A:387:PX4:H68	4:A:403:PX4:H36	0.47	1.86	10	1
4:A:330:PX4:H67	4:A:337:PX4:H36	0.47	1.86	12	1
4:A:308:PX4:H49	4:A:311:PX4:H4	0.47	1.85	13	1
4:A:319:PX4:H33	4:A:320:PX4:H29	0.47	1.85	14	1
4:A:317:PX4:H25	4:A:342:PX4:H28	0.47	1.83	1	1
4:A:314:PX4:H68	4:A:422:PX4:H64	0.47	1.85	2	1
1:A:138:PHE:CD1	1:A:149:PHE:CG	0.47	3.01	5	1
4:A:309:PX4:H17	4:A:319:PX4:H25	0.47	1.87	8	1
4:A:336:PX4:H52	4:A:344:PX4:H57	0.47	1.86	8	1
4:A:422:PX4:H47	4:A:425:PX4:H50	0.47	1.86	9	1
4:A:368:PX4:H8	4:A:369:PX4:O6	0.47	2.09	12	1
4:A:403:PX4:H8	4:A:411:PX4:O6	0.47	2.09	13	1
4:A:312:PX4:H48	4:A:359:PX4:H50	0.47	1.85	14	1
4:A:336:PX4:H38	4:A:344:PX4:H69	0.47	1.85	14	1
4:A:391:PX4:H44	4:A:395:PX4:H28	0.47	1.86	2	1
4:A:331:PX4:H5	4:A:348:PX4:O4	0.47	2.08	3	1
4:A:420:PX4:H27	4:A:427:PX4:H30	0.47	1.85	3	1
4:A:391:PX4:H62	4:A:415:PX4:H23	0.47	1.86	7	1
4:A:315:PX4:H65	4:A:323:PX4:H23	0.47	1.85	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:366:PX4:H44	4:A:374:PX4:H42	0.47	1.87	10	1
4:A:396:PX4:H65	4:A:396:PX4:H34	0.47	1.87	11	1
4:A:386:PX4:H46	4:A:387:PX4:H49	0.47	1.87	12	1
4:A:373:PX4:H28	4:A:381:PX4:C24	0.47	2.39	13	1
4:A:408:PX4:H17	4:A:415:PX4:O6	0.47	2.09	13	3
4:A:370:PX4:H23	4:A:403:PX4:H47	0.47	1.85	3	1
4:A:317:PX4:H32	4:A:363:PX4:H65	0.47	1.86	4	1
4:A:364:PX4:H68	4:A:422:PX4:H63	0.47	1.86	6	1
4:A:377:PX4:H46	4:A:378:PX4:H21	0.47	1.85	11	1
4:A:373:PX4:O2	4:A:381:PX4:H8	0.47	2.08	12	1
4:A:331:PX4:H63	4:A:331:PX4:H27	0.47	1.85	13	1
4:A:409:PX4:H55	4:A:416:PX4:H56	0.47	1.87	13	1
4:A:348:PX4:H44	4:A:405:PX4:H72	0.47	1.86	14	1
4:A:413:PX4:H56	4:A:430:PX4:H31	0.47	1.86	4	1
4:A:370:PX4:H20	4:A:403:PX4:H51	0.47	1.86	5	1
4:A:391:PX4:H39	4:A:414:PX4:H32	0.47	1.85	12	1
4:A:332:PX4:H60	4:A:393:PX4:H72	0.47	1.86	13	1
4:A:378:PX4:H47	4:A:410:PX4:H19	0.47	1.85	13	1
4:A:332:PX4:O1	4:A:356:PX4:H4	0.47	2.09	1	1
4:A:409:PX4:H52	4:A:415:PX4:H23	0.47	1.85	1	1
4:A:354:PX4:H65	4:A:366:PX4:H48	0.47	1.85	2	1
4:A:380:PX4:H51	4:A:381:PX4:H55	0.47	1.86	2	1
4:A:306:PX4:H23	4:A:360:PX4:H39	0.47	1.87	3	1
4:A:357:PX4:H40	4:A:357:PX4:H69	0.47	1.86	4	1
4:A:308:PX4:H57	4:A:310:PX4:H64	0.47	1.87	5	1
4:A:421:PX4:P1	4:A:423:PX4:H4	0.47	2.50	7	1
4:A:308:PX4:H13	4:A:310:PX4:H51	0.47	1.86	9	1
4:A:314:PX4:H68	4:A:361:PX4:H39	0.47	1.86	9	1
4:A:325:PX4:H57	4:A:341:PX4:H60	0.47	1.87	9	1
4:A:338:PX4:O7	4:A:348:PX4:H18	0.47	2.09	9	3
4:A:338:PX4:H30	4:A:348:PX4:H28	0.47	1.87	11	1
4:A:391:PX4:H71	4:A:408:PX4:H37	0.47	1.86	13	1
4:A:306:PX4:H58	4:A:321:PX4:H22	0.47	1.86	1	1
4:A:398:PX4:H19	4:A:407:PX4:H15	0.47	1.87	1	1
4:A:373:PX4:H54	4:A:375:PX4:H33	0.47	1.85	2	1
4:A:389:PX4:H63	4:A:389:PX4:H27	0.47	1.86	3	1
4:A:413:PX4:H54	4:A:423:PX4:H54	0.47	1.87	3	1
4:A:326:PX4:H40	4:A:350:PX4:H28	0.47	1.86	6	1
4:A:316:PX4:H36	4:A:378:PX4:H64	0.47	1.85	7	1
4:A:331:PX4:O1	4:A:332:PX4:H10	0.47	2.10	10	3
4:A:314:PX4:H70	4:A:349:PX4:H34	0.47	1.86	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:346:PX4:H60	4:A:362:PX4:H58	0.47	1.87	11	1
4:A:375:PX4:H48	4:A:382:PX4:H68	0.47	1.87	11	1
4:A:391:PX4:O2	4:A:414:PX4:H2	0.47	2.10	12	1
4:A:422:PX4:H67	4:A:426:PX4:H31	0.47	1.86	12	1
4:A:306:PX4:H38	4:A:329:PX4:H51	0.47	1.87	13	1
4:A:325:PX4:H22	4:A:326:PX4:H21	0.47	1.86	14	1
4:A:400:PX4:C11	4:A:408:PX4:H67	0.47	2.39	14	1
4:A:367:PX4:H65	4:A:421:PX4:H25	0.47	1.86	1	1
4:A:373:PX4:H36	4:A:397:PX4:H67	0.47	1.87	5	1
4:A:322:PX4:H17	4:A:333:PX4:H41	0.47	1.87	6	1
4:A:338:PX4:H62	4:A:356:PX4:H59	0.47	1.87	6	1
4:A:393:PX4:H13	4:A:394:PX4:O2	0.47	2.10	6	1
4:A:337:PX4:H31	4:A:343:PX4:H50	0.47	1.86	7	1
4:A:307:PX4:H50	4:A:314:PX4:H19	0.47	1.86	10	1
4:A:314:PX4:H71	4:A:409:PX4:H63	0.47	1.87	10	1
4:A:396:PX4:H30	4:A:397:PX4:H67	0.47	1.86	13	1
4:A:364:PX4:H45	4:A:426:PX4:H69	0.47	1.86	1	1
4:A:306:PX4:H3	4:A:329:PX4:O2	0.47	2.10	3	1
4:A:315:PX4:H2	4:A:316:PX4:H2	0.47	1.87	6	1
4:A:423:PX4:C7	4:A:424:PX4:H24	0.47	2.17	7	1
4:A:369:PX4:O1	4:A:425:PX4:H18	0.47	2.10	5	1
4:A:374:PX4:O2	4:A:420:PX4:H4	0.47	2.10	6	1
4:A:416:PX4:H5	4:A:426:PX4:O3	0.47	2.10	6	1
4:A:331:PX4:H57	4:A:332:PX4:H26	0.47	1.87	9	1
4:A:344:PX4:H50	4:A:347:PX4:H21	0.47	1.86	13	1
4:A:315:PX4:H7	4:A:316:PX4:O6	0.46	2.10	1	1
4:A:399:PX4:H54	4:A:407:PX4:H28	0.46	1.86	1	1
4:A:380:PX4:H68	4:A:386:PX4:H59	0.46	1.85	3	1
4:A:391:PX4:H33	4:A:407:PX4:H61	0.46	1.86	3	1
4:A:316:PX4:H44	4:A:316:PX4:H72	0.46	1.85	5	1
4:A:328:PX4:H11	4:A:360:PX4:H29	0.46	1.86	6	1
4:A:398:PX4:H21	4:A:407:PX4:H47	0.46	1.88	10	1
4:A:403:PX4:H29	4:A:413:PX4:H32	0.46	1.87	12	1
4:A:370:PX4:H22	4:A:403:PX4:H17	0.46	1.87	14	1
4:A:320:PX4:H40	4:A:418:PX4:H63	0.46	1.87	2	1
4:A:420:PX4:H40	4:A:427:PX4:H34	0.46	1.87	5	1
4:A:340:PX4:H44	4:A:399:PX4:H69	0.46	1.87	11	1
4:A:391:PX4:H17	4:A:408:PX4:H22	0.46	1.87	11	1
4:A:306:PX4:H70	4:A:328:PX4:H5	0.46	1.86	12	1
4:A:388:PX4:H51	4:A:406:PX4:H66	0.46	1.87	1	1
4:A:374:PX4:H39	4:A:427:PX4:H17	0.46	1.86	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H21	4:A:398:PX4:H54	0.46	1.87	5	1
4:A:406:PX4:O2	4:A:415:PX4:H2	0.46	2.10	6	1
4:A:325:PX4:H7	4:A:325:PX4:H15	0.46	1.86	13	2
4:A:345:PX4:O6	4:A:353:PX4:H15	0.46	2.10	13	2
4:A:348:PX4:H50	4:A:355:PX4:H27	0.46	1.87	8	1
4:A:416:PX4:H63	4:A:416:PX4:H44	0.46	1.87	9	1
4:A:388:PX4:H39	4:A:405:PX4:H65	0.46	1.86	14	1
4:A:335:PX4:H59	4:A:344:PX4:H37	0.46	1.86	2	1
4:A:399:PX4:O7	4:A:407:PX4:H19	0.46	2.11	3	1
4:A:401:PX4:H22	4:A:408:PX4:H66	0.46	1.87	3	1
4:A:315:PX4:H46	4:A:316:PX4:H59	0.46	1.88	4	1
4:A:335:PX4:O1	4:A:343:PX4:H4	0.46	2.10	7	1
4:A:353:PX4:H23	4:A:357:PX4:H27	0.46	1.86	7	1
4:A:353:PX4:H43	4:A:413:PX4:H37	0.46	1.86	7	1
4:A:329:PX4:H5	4:A:333:PX4:H30	0.46	1.86	10	1
4:A:372:PX4:H59	4:A:384:PX4:H25	0.46	1.86	12	1
4:A:317:PX4:H35	4:A:342:PX4:H33	0.46	1.86	1	1
4:A:307:PX4:H27	4:A:361:PX4:H23	0.46	1.87	2	1
4:A:378:PX4:C6	4:A:410:PX4:H47	0.46	2.39	3	1
4:A:400:PX4:H22	4:A:401:PX4:O7	0.46	2.11	3	1
4:A:330:PX4:H21	4:A:343:PX4:H61	0.46	1.86	4	1
4:A:397:PX4:H40	4:A:398:PX4:H71	0.46	1.86	4	1
4:A:311:PX4:O6	4:A:311:PX4:H48	0.46	2.11	2	1
4:A:388:PX4:H44	4:A:405:PX4:H72	0.46	1.87	7	1
4:A:331:PX4:H14	4:A:347:PX4:H51	0.46	1.87	8	1
4:A:355:PX4:H68	4:A:422:PX4:H42	0.46	1.88	9	1
4:A:393:PX4:H33	4:A:394:PX4:H34	0.46	1.88	10	1
4:A:367:PX4:H28	4:A:424:PX4:H52	0.46	1.88	12	1
4:A:380:PX4:H62	4:A:387:PX4:H66	0.46	1.88	14	1
1:A:167:ALA:O	4:A:307:PX4:H6	0.46	2.10	8	2
4:A:325:PX4:H66	4:A:340:PX4:H66	0.46	1.87	8	1
4:A:330:PX4:H17	4:A:348:PX4:C27	0.46	2.41	14	1
4:A:405:PX4:H22	4:A:406:PX4:H22	0.46	1.86	4	1
4:A:376:PX4:H53	4:A:377:PX4:H25	0.46	1.87	5	1
4:A:399:PX4:H10	4:A:399:PX4:O2	0.46	2.11	5	1
1:A:153:ASN:O	4:A:331:PX4:H11	0.46	2.11	8	1
4:A:367:PX4:H48	4:A:412:PX4:H18	0.46	1.87	8	1
4:A:409:PX4:H51	4:A:415:PX4:H29	0.46	1.87	8	1
4:A:362:PX4:H64	4:A:413:PX4:H69	0.46	1.85	10	1
4:A:407:PX4:C7	4:A:414:PX4:H49	0.46	2.40	10	1
4:A:422:PX4:H22	4:A:425:PX4:H69	0.46	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:412:PX4:H64	4:A:428:PX4:H45	0.46	1.87	12	1
4:A:374:PX4:H29	4:A:427:PX4:H45	0.46	1.88	3	1
4:A:312:PX4:H19	4:A:366:PX4:H17	0.46	1.88	4	1
4:A:322:PX4:H33	4:A:424:PX4:H69	0.46	1.88	4	1
4:A:378:PX4:H9	4:A:417:PX4:H53	0.46	1.88	5	1
4:A:400:PX4:H24	4:A:400:PX4:H59	0.46	1.87	5	1
4:A:332:PX4:H4	4:A:356:PX4:O3	0.46	2.11	7	1
4:A:387:PX4:H17	4:A:411:PX4:H55	0.46	1.88	12	2
4:A:377:PX4:H46	4:A:378:PX4:H24	0.46	1.87	13	1
4:A:388:PX4:H23	4:A:396:PX4:H9	0.46	1.86	13	1
4:A:316:PX4:H52	4:A:333:PX4:H63	0.46	1.87	1	1
4:A:366:PX4:H34	4:A:427:PX4:H60	0.46	1.89	5	1
4:A:354:PX4:H47	4:A:360:PX4:H21	0.46	1.87	7	1
4:A:367:PX4:H47	4:A:412:PX4:H53	0.46	1.87	7	1
4:A:400:PX4:H10	4:A:409:PX4:O6	0.46	2.10	7	1
4:A:400:PX4:H60	4:A:422:PX4:H71	0.46	1.87	12	1
4:A:373:PX4:H21	4:A:381:PX4:H21	0.46	1.86	13	1
4:A:307:PX4:H34	4:A:321:PX4:H68	0.45	1.88	2	1
4:A:321:PX4:H55	4:A:354:PX4:H34	0.45	1.87	4	1
4:A:353:PX4:H29	4:A:357:PX4:H57	0.45	1.85	4	1
4:A:378:PX4:O3	4:A:378:PX4:H18	0.45	2.11	4	1
4:A:392:PX4:H35	4:A:399:PX4:H61	0.45	1.87	5	1
4:A:334:PX4:H61	4:A:356:PX4:H39	0.45	1.88	7	1
4:A:348:PX4:H43	4:A:402:PX4:H41	0.45	1.88	7	1
4:A:416:PX4:H63	4:A:422:PX4:H65	0.45	1.88	8	1
4:A:388:PX4:H51	4:A:411:PX4:H31	0.45	1.88	9	1
4:A:315:PX4:H41	4:A:323:PX4:H65	0.45	1.88	10	1
4:A:361:PX4:H38	4:A:362:PX4:H40	0.45	1.88	10	1
4:A:422:PX4:H17	4:A:425:PX4:H64	0.45	1.88	10	1
4:A:378:PX4:H18	4:A:378:PX4:H1	0.45	1.88	11	1
4:A:413:PX4:H57	4:A:430:PX4:H32	0.45	1.88	11	1
4:A:371:PX4:H10	4:A:371:PX4:O6	0.45	2.11	13	1
4:A:329:PX4:H46	4:A:336:PX4:H20	0.45	1.88	3	1
4:A:339:PX4:C11	4:A:347:PX4:H53	0.45	2.42	3	1
4:A:361:PX4:H37	4:A:409:PX4:H68	0.45	1.89	3	1
4:A:325:PX4:H18	4:A:334:PX4:H11	0.45	1.88	6	1
4:A:332:PX4:O6	4:A:332:PX4:H1	0.45	2.11	7	1
4:A:322:PX4:H71	4:A:430:PX4:H65	0.45	1.89	8	1
4:A:408:PX4:O3	4:A:409:PX4:H2	0.45	2.11	8	1
4:A:328:PX4:H33	4:A:359:PX4:H40	0.45	1.87	10	1
4:A:385:PX4:H66	4:A:399:PX4:H63	0.45	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H52	4:A:345:PX4:H59	0.45	1.88	11	1
4:A:330:PX4:H34	4:A:343:PX4:H60	0.45	1.88	12	1
4:A:337:PX4:O1	4:A:338:PX4:H8	0.45	2.11	12	1
4:A:421:PX4:H45	4:A:430:PX4:H40	0.45	1.86	14	1
4:A:377:PX4:H51	4:A:378:PX4:H23	0.45	1.89	5	1
4:A:399:PX4:H39	4:A:407:PX4:H31	0.45	1.89	7	1
4:A:367:PX4:H34	4:A:428:PX4:H48	0.45	1.88	9	1
4:A:379:PX4:H24	4:A:384:PX4:H21	0.45	1.86	9	1
4:A:316:PX4:H41	4:A:368:PX4:H25	0.45	1.88	10	1
4:A:321:PX4:H8	4:A:362:PX4:O1	0.45	2.12	13	1
4:A:322:PX4:H69	4:A:413:PX4:H58	0.45	1.89	1	1
4:A:370:PX4:H40	4:A:404:PX4:H41	0.45	1.87	4	1
4:A:406:PX4:H31	4:A:424:PX4:H45	0.45	1.89	4	1
4:A:375:PX4:H27	4:A:382:PX4:H28	0.45	1.89	6	1
4:A:357:PX4:H49	4:A:357:PX4:H28	0.45	1.88	7	1
4:A:403:PX4:H54	4:A:419:PX4:H59	0.45	1.88	8	1
4:A:338:PX4:H23	4:A:348:PX4:H53	0.45	1.88	11	1
4:A:331:PX4:H61	4:A:339:PX4:H62	0.45	1.87	12	1
4:A:336:PX4:H34	4:A:339:PX4:H36	0.45	1.87	12	1
4:A:368:PX4:H50	4:A:369:PX4:H22	0.45	1.89	14	1
4:A:399:PX4:H10	4:A:399:PX4:H14	0.45	1.88	1	1
4:A:307:PX4:H12	4:A:361:PX4:O6	0.45	2.12	3	1
4:A:317:PX4:H54	4:A:342:PX4:H19	0.45	1.88	3	1
4:A:396:PX4:H52	4:A:398:PX4:H56	0.45	1.88	4	1
4:A:355:PX4:H61	4:A:405:PX4:H41	0.45	1.88	6	1
4:A:380:PX4:O8	4:A:381:PX4:H51	0.45	2.11	6	1
4:A:386:PX4:H58	4:A:411:PX4:H60	0.45	1.88	6	1
4:A:408:PX4:H29	4:A:415:PX4:H48	0.45	1.89	7	1
4:A:413:PX4:H70	4:A:430:PX4:H60	0.45	1.89	8	1
4:A:338:PX4:H69	4:A:346:PX4:H61	0.45	1.89	10	1
4:A:368:PX4:H51	4:A:369:PX4:H16	0.45	1.86	13	1
4:A:321:PX4:H47	4:A:354:PX4:H20	0.45	1.88	14	1
4:A:318:PX4:H53	4:A:336:PX4:H54	0.45	1.88	2	1
4:A:408:PX4:H51	4:A:415:PX4:H23	0.45	1.88	2	1
4:A:349:PX4:H71	4:A:356:PX4:H65	0.45	1.88	3	1
4:A:326:PX4:H40	4:A:350:PX4:H32	0.45	1.89	4	1
4:A:316:PX4:H46	4:A:319:PX4:H46	0.45	1.89	5	1
4:A:328:PX4:O6	4:A:328:PX4:H9	0.45	2.11	5	1
4:A:420:PX4:H48	4:A:427:PX4:H19	0.45	1.88	5	1
4:A:340:PX4:H54	4:A:341:PX4:H51	0.45	1.88	1	1
4:A:395:PX4:H59	4:A:406:PX4:H58	0.45	1.87	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.45	2.46	10	1
4:A:363:PX4:H23	4:A:364:PX4:H24	0.45	1.88	10	1
4:A:317:PX4:H54	4:A:324:PX4:H24	0.45	1.88	13	1
4:A:322:PX4:H68	4:A:430:PX4:H67	0.45	1.89	13	1
4:A:384:PX4:H7	4:A:386:PX4:O2	0.45	2.12	13	1
4:A:367:PX4:H23	4:A:368:PX4:H72	0.45	1.89	1	1
4:A:400:PX4:O2	4:A:409:PX4:H14	0.45	2.12	1	1
4:A:321:PX4:H25	4:A:322:PX4:H54	0.45	1.89	2	1
4:A:330:PX4:H28	4:A:344:PX4:H25	0.45	1.89	2	1
4:A:393:PX4:H32	4:A:394:PX4:H67	0.45	1.87	2	1
4:A:332:PX4:H35	4:A:355:PX4:H39	0.45	1.89	3	1
4:A:396:PX4:H45	4:A:398:PX4:H34	0.45	1.89	7	1
4:A:421:PX4:H42	4:A:423:PX4:H44	0.45	1.89	7	1
4:A:334:PX4:H70	4:A:406:PX4:H43	0.45	1.89	10	1
4:A:404:PX4:H10	4:A:430:PX4:O6	0.45	2.11	10	1
4:A:315:PX4:H29	4:A:425:PX4:H37	0.45	1.88	2	1
4:A:380:PX4:H19	4:A:381:PX4:H20	0.45	1.88	2	1
4:A:315:PX4:H64	4:A:316:PX4:H62	0.45	1.88	3	1
4:A:338:PX4:H59	4:A:345:PX4:H61	0.45	1.87	4	1
4:A:400:PX4:H59	4:A:400:PX4:H26	0.45	1.88	4	1
4:A:380:PX4:H52	4:A:386:PX4:H49	0.45	1.88	6	1
4:A:367:PX4:O5	4:A:428:PX4:H17	0.45	2.11	7	1
4:A:368:PX4:H24	4:A:390:PX4:H56	0.45	1.87	7	1
4:A:413:PX4:H22	4:A:430:PX4:H19	0.45	1.88	7	1
4:A:313:PX4:H52	4:A:328:PX4:H48	0.45	1.89	8	1
4:A:347:PX4:H41	4:A:348:PX4:H68	0.45	1.87	8	1
4:A:361:PX4:H29	4:A:362:PX4:H35	0.45	1.89	8	1
4:A:307:PX4:H13	4:A:361:PX4:O6	0.45	2.12	11	1
4:A:383:PX4:H22	4:A:399:PX4:H48	0.45	1.89	13	1
4:A:378:PX4:H3	4:A:410:PX4:O8	0.45	2.12	1	1
4:A:346:PX4:H14	4:A:362:PX4:H3	0.45	1.88	3	1
4:A:348:PX4:H1	4:A:355:PX4:H14	0.45	1.88	3	1
4:A:366:PX4:H34	4:A:427:PX4:H72	0.45	1.87	6	1
4:A:374:PX4:H17	4:A:382:PX4:H51	0.45	1.89	6	1
4:A:358:PX4:H22	4:A:365:PX4:H26	0.45	1.89	9	1
4:A:307:PX4:H42	4:A:364:PX4:H68	0.45	1.87	10	1
4:A:366:PX4:H43	4:A:412:PX4:H40	0.45	1.87	11	1
4:A:402:PX4:H67	4:A:421:PX4:H55	0.45	1.88	12	1
4:A:330:PX4:H53	4:A:338:PX4:C11	0.44	2.42	4	1
4:A:357:PX4:H20	4:A:358:PX4:H16	0.44	1.88	4	2
4:A:380:PX4:H16	4:A:381:PX4:H48	0.44	1.90	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:334:PX4:H52	4:A:349:PX4:H20	0.44	1.88	7	1
4:A:350:PX4:H22	4:A:363:PX4:H55	0.44	1.89	13	1
4:A:394:PX4:H19	4:A:401:PX4:H23	0.44	1.89	14	1
4:A:374:PX4:H17	4:A:382:PX4:H50	0.44	1.90	1	1
4:A:317:PX4:H19	4:A:325:PX4:H46	0.44	1.87	2	1
4:A:341:PX4:H70	4:A:407:PX4:H41	0.44	1.88	2	1
4:A:391:PX4:H35	4:A:415:PX4:H65	0.44	1.88	2	1
4:A:321:PX4:H59	4:A:354:PX4:H35	0.44	1.90	4	1
4:A:373:PX4:H36	4:A:396:PX4:H30	0.44	1.89	4	1
4:A:361:PX4:H30	4:A:362:PX4:H39	0.44	1.88	12	1
4:A:313:PX4:H31	4:A:360:PX4:H26	0.44	1.88	13	1
4:A:346:PX4:H21	4:A:362:PX4:H51	0.44	1.90	4	1
4:A:346:PX4:H20	4:A:362:PX4:H2	0.44	1.89	7	1
4:A:367:PX4:H68	4:A:428:PX4:H21	0.44	1.88	8	1
4:A:308:PX4:H41	4:A:310:PX4:H41	0.44	1.89	3	1
4:A:331:PX4:H24	4:A:331:PX4:H58	0.44	1.88	5	1
4:A:357:PX4:H35	4:A:358:PX4:H33	0.44	1.89	5	1
4:A:340:PX4:H2	4:A:340:PX4:O6	0.44	2.13	6	1
4:A:421:PX4:H19	4:A:430:PX4:H16	0.44	1.88	6	1
4:A:311:PX4:H10	4:A:320:PX4:H22	0.44	1.89	10	1
4:A:328:PX4:H17	4:A:360:PX4:H39	0.44	1.88	10	1
4:A:419:PX4:H56	4:A:427:PX4:H51	0.44	1.88	13	1
4:A:400:PX4:H22	4:A:408:PX4:H66	0.44	1.89	2	1
4:A:389:PX4:H57	4:A:390:PX4:H35	0.44	1.88	3	1
4:A:367:PX4:H62	4:A:430:PX4:H34	0.44	1.89	6	1
4:A:368:PX4:H52	4:A:369:PX4:H28	0.44	1.90	12	1
4:A:371:PX4:H14	4:A:377:PX4:H4	0.44	1.89	12	1
4:A:398:PX4:H32	4:A:398:PX4:H52	0.44	1.88	12	1
4:A:322:PX4:H70	4:A:421:PX4:H69	0.44	1.90	1	1
4:A:308:PX4:H24	4:A:364:PX4:H52	0.44	1.89	4	1
4:A:373:PX4:H38	4:A:402:PX4:H33	0.44	1.89	6	1
4:A:374:PX4:H27	4:A:427:PX4:H22	0.44	1.90	6	1
4:A:358:PX4:H40	4:A:366:PX4:H70	0.44	1.88	8	1
4:A:395:PX4:H62	4:A:406:PX4:H71	0.44	1.89	8	1
4:A:357:PX4:H23	4:A:358:PX4:H23	0.44	1.89	9	1
4:A:355:PX4:H17	4:A:356:PX4:H49	0.44	1.89	10	1
4:A:336:PX4:H39	4:A:389:PX4:H68	0.44	1.89	12	1
4:A:374:PX4:H27	4:A:428:PX4:H35	0.44	1.90	14	1
4:A:328:PX4:H28	4:A:360:PX4:H40	0.44	1.89	2	1
4:A:366:PX4:H43	4:A:419:PX4:H30	0.44	1.90	2	1
4:A:367:PX4:H19	4:A:368:PX4:H67	0.44	1.88	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:402:PX4:H17	4:A:411:PX4:H22	0.44	1.90	2	1
4:A:366:PX4:H37	4:A:412:PX4:H35	0.44	1.90	3	1
4:A:353:PX4:H57	4:A:354:PX4:H56	0.44	1.89	6	1
4:A:412:PX4:H27	4:A:419:PX4:H47	0.44	1.89	6	1
4:A:332:PX4:H1	4:A:356:PX4:O3	0.44	2.12	10	1
4:A:307:PX4:H52	4:A:314:PX4:H17	0.44	1.90	1	1
4:A:377:PX4:H60	4:A:418:PX4:H66	0.44	1.89	1	1
4:A:321:PX4:H7	4:A:354:PX4:O4	0.44	2.12	2	1
4:A:317:PX4:H26	4:A:325:PX4:H52	0.44	1.90	3	1
4:A:418:PX4:C13	4:A:425:PX4:H24	0.44	2.38	4	1
4:A:341:PX4:H70	4:A:393:PX4:H70	0.44	1.90	5	1
4:A:396:PX4:H62	4:A:398:PX4:H45	0.44	1.88	8	1
4:A:346:PX4:H39	4:A:355:PX4:H59	0.44	1.90	11	1
4:A:402:PX4:H59	4:A:404:PX4:H54	0.44	1.88	11	1
4:A:313:PX4:H6	4:A:359:PX4:O2	0.44	2.13	13	1
4:A:373:PX4:H27	4:A:396:PX4:H22	0.44	1.89	14	1
4:A:316:PX4:H25	4:A:320:PX4:H33	0.44	1.90	1	1
4:A:322:PX4:H19	4:A:323:PX4:H21	0.44	1.89	6	1
4:A:322:PX4:H36	4:A:333:PX4:H36	0.44	1.90	9	1
4:A:410:PX4:H31	4:A:416:PX4:H39	0.44	1.89	12	1
4:A:345:PX4:H46	4:A:348:PX4:H7	0.44	1.89	13	1
4:A:409:PX4:H66	4:A:409:PX4:H60	0.44	1.45	14	1
4:A:338:PX4:H62	4:A:345:PX4:H65	0.43	1.89	2	1
4:A:371:PX4:H10	4:A:377:PX4:O6	0.43	2.13	2	1
4:A:326:PX4:H37	4:A:414:PX4:H38	0.43	1.88	3	1
4:A:324:PX4:H68	4:A:325:PX4:H34	0.43	1.90	5	1
4:A:368:PX4:C27	4:A:424:PX4:H48	0.43	2.43	5	1
4:A:314:PX4:H50	4:A:361:PX4:H26	0.43	1.89	6	1
4:A:331:PX4:H24	4:A:340:PX4:C8	0.43	2.43	7	1
4:A:337:PX4:H27	4:A:357:PX4:H37	0.43	1.88	8	1
4:A:402:PX4:H67	4:A:411:PX4:H44	0.43	1.90	8	1
4:A:355:PX4:H68	4:A:422:PX4:C21	0.43	2.42	9	1
4:A:306:PX4:H69	4:A:354:PX4:H22	0.43	1.90	10	1
4:A:308:PX4:H53	4:A:311:PX4:H14	0.43	1.90	10	1
4:A:399:PX4:H51	4:A:407:PX4:H31	0.43	1.89	10	1
4:A:360:PX4:H62	4:A:366:PX4:H68	0.43	1.89	11	1
4:A:424:PX4:H58	4:A:428:PX4:C31	0.43	2.43	1	1
4:A:317:PX4:H65	4:A:342:PX4:H62	0.43	1.90	2	1
4:A:383:PX4:C18	4:A:407:PX4:H26	0.43	2.42	3	1
4:A:403:PX4:H12	4:A:403:PX4:O6	0.43	2.13	4	1
4:A:337:PX4:H27	4:A:337:PX4:H22	0.43	1.55	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:ARG:NH1	4:A:354:PX4:O1	0.43	2.52	6	2
4:A:360:PX4:H57	4:A:366:PX4:H20	0.43	1.90	9	1
4:A:322:PX4:H17	4:A:333:PX4:H44	0.43	1.89	10	1
4:A:420:PX4:H22	4:A:427:PX4:H27	0.43	1.90	12	1
4:A:334:PX4:H44	4:A:347:PX4:H65	0.43	1.89	14	1
4:A:308:PX4:H17	4:A:364:PX4:O1	0.43	2.12	1	1
4:A:334:PX4:H21	4:A:356:PX4:H10	0.43	1.89	12	2
4:A:421:PX4:H19	4:A:430:PX4:H21	0.43	1.90	5	1
4:A:316:PX4:H38	4:A:368:PX4:H30	0.43	1.89	8	1
4:A:335:PX4:H35	4:A:337:PX4:H37	0.43	1.91	8	1
4:A:343:PX4:H18	4:A:352:PX4:H57	0.43	1.91	10	1
4:A:370:PX4:H54	4:A:403:PX4:H26	0.43	1.90	10	1
4:A:314:PX4:O8	4:A:364:PX4:H4	0.43	2.13	11	1
4:A:325:PX4:H58	4:A:325:PX4:H26	0.43	1.90	12	1
4:A:385:PX4:H49	4:A:385:PX4:H54	0.43	1.54	12	1
4:A:353:PX4:O6	4:A:357:PX4:H46	0.43	2.13	14	1
4:A:311:PX4:H60	4:A:311:PX4:H27	0.43	1.89	2	1
4:A:308:PX4:H56	4:A:308:PX4:H63	0.43	1.47	4	1
4:A:370:PX4:H61	4:A:411:PX4:H54	0.43	1.90	4	1
4:A:392:PX4:H54	4:A:414:PX4:H47	0.43	1.89	4	1
4:A:315:PX4:H40	4:A:368:PX4:H45	0.43	1.91	6	1
4:A:316:PX4:H65	4:A:333:PX4:H72	0.43	1.90	6	1
4:A:370:PX4:H35	4:A:404:PX4:H27	0.43	1.89	8	1
4:A:405:PX4:H23	4:A:406:PX4:H17	0.43	1.89	8	1
4:A:424:PX4:H61	4:A:424:PX4:H66	0.43	1.54	9	1
4:A:326:PX4:H68	4:A:415:PX4:H42	0.43	1.90	10	1
4:A:331:PX4:H45	4:A:341:PX4:H68	0.43	1.90	10	1
4:A:380:PX4:H53	4:A:387:PX4:H57	0.43	1.91	10	1
4:A:336:PX4:H22	4:A:344:PX4:H55	0.43	1.90	11	1
4:A:400:PX4:H1	4:A:409:PX4:O4	0.43	2.13	11	1
4:A:422:PX4:C8	4:A:425:PX4:H56	0.43	2.33	13	1
4:A:315:PX4:H29	4:A:418:PX4:H42	0.43	1.91	14	1
4:A:314:PX4:H71	4:A:416:PX4:H38	0.43	1.90	1	1
4:A:409:PX4:H59	4:A:415:PX4:H34	0.43	1.91	1	1
4:A:318:PX4:H15	4:A:327:PX4:H15	0.43	1.91	3	1
4:A:348:PX4:H10	4:A:355:PX4:O2	0.43	2.13	4	1
4:A:330:PX4:H45	4:A:347:PX4:H38	0.43	1.90	5	1
4:A:367:PX4:H58	4:A:430:PX4:H26	0.43	1.90	6	1
4:A:428:PX4:H12	4:A:428:PX4:O2	0.43	2.14	6	1
4:A:400:PX4:H13	4:A:401:PX4:O1	0.43	2.13	10	1
4:A:360:PX4:H51	4:A:366:PX4:H18	0.43	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:361:PX4:H63	4:A:369:PX4:H34	0.43	1.90	11	1
4:A:310:PX4:C22	4:A:351:PX4:H66	0.43	2.43	12	1
4:A:330:PX4:H68	4:A:380:PX4:H44	0.43	1.90	12	1
4:A:356:PX4:H61	4:A:356:PX4:H66	0.43	1.59	12	1
4:A:349:PX4:H71	4:A:356:PX4:H55	0.43	1.88	13	1
4:A:354:PX4:H67	4:A:366:PX4:C27	0.43	2.43	13	1
4:A:338:PX4:O8	4:A:345:PX4:H49	0.43	2.13	2	1
4:A:380:PX4:C26	4:A:381:PX4:H55	0.43	2.44	2	1
4:A:372:PX4:C35	4:A:393:PX4:H41	0.43	2.44	3	1
4:A:378:PX4:H53	4:A:410:PX4:H58	0.43	1.90	3	1
4:A:369:PX4:H30	4:A:429:PX4:H57	0.43	1.91	6	1
4:A:375:PX4:H23	4:A:382:PX4:H24	0.43	1.89	6	1
4:A:410:PX4:H27	4:A:410:PX4:H34	0.43	1.58	14	2
4:A:331:PX4:H51	4:A:332:PX4:H21	0.43	1.89	10	1
4:A:334:PX4:H21	4:A:334:PX4:H53	0.43	1.91	11	1
4:A:351:PX4:H23	4:A:352:PX4:H17	0.43	1.91	12	1
4:A:406:PX4:H49	4:A:421:PX4:H49	0.43	1.91	13	1
4:A:417:PX4:H47	4:A:426:PX4:H52	0.43	1.89	13	1
4:A:326:PX4:H65	4:A:350:PX4:H37	0.43	1.91	1	1
4:A:388:PX4:H66	4:A:388:PX4:H38	0.43	1.91	4	1
4:A:404:PX4:H55	4:A:413:PX4:H25	0.43	1.90	4	1
4:A:330:PX4:H65	4:A:343:PX4:H65	0.43	1.90	6	1
4:A:373:PX4:H25	4:A:397:PX4:H23	0.43	1.90	8	1
4:A:388:PX4:H46	4:A:395:PX4:H47	0.43	1.90	8	1
4:A:392:PX4:H48	4:A:399:PX4:H56	0.43	1.89	8	1
4:A:337:PX4:H31	4:A:352:PX4:H54	0.43	1.89	9	1
4:A:391:PX4:C20	4:A:405:PX4:H69	0.43	2.40	9	1
4:A:321:PX4:H28	4:A:329:PX4:H72	0.43	1.89	10	1
4:A:385:PX4:H50	4:A:392:PX4:H16	0.43	1.90	13	1
4:A:317:PX4:H65	4:A:342:PX4:H60	0.43	1.89	14	1
4:A:375:PX4:H55	4:A:382:PX4:H71	0.43	1.89	14	1
4:A:318:PX4:H56	4:A:318:PX4:H63	0.43	1.60	1	1
4:A:403:PX4:H20	4:A:404:PX4:H22	0.43	1.89	2	1
4:A:370:PX4:H50	4:A:411:PX4:H59	0.43	1.90	7	1
4:A:422:PX4:H52	4:A:425:PX4:H48	0.43	1.90	8	1
4:A:317:PX4:H50	4:A:342:PX4:H47	0.43	1.90	9	1
4:A:327:PX4:H23	4:A:329:PX4:H36	0.43	1.91	9	1
4:A:367:PX4:H66	4:A:412:PX4:H63	0.43	1.91	11	1
4:A:306:PX4:H45	4:A:329:PX4:H55	0.43	1.91	13	1
4:A:369:PX4:O2	4:A:425:PX4:H10	0.43	2.14	1	1
4:A:411:PX4:H62	4:A:411:PX4:H69	0.43	1.47	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H31	4:A:329:PX4:H60	0.43	1.90	6	1
4:A:310:PX4:H54	4:A:364:PX4:H23	0.43	1.91	6	1
4:A:394:PX4:H15	4:A:401:PX4:H20	0.43	1.91	7	1
4:A:322:PX4:H41	4:A:323:PX4:H71	0.43	1.89	8	1
4:A:316:PX4:H23	4:A:418:PX4:H36	0.43	1.91	9	1
4:A:406:PX4:H28	4:A:423:PX4:H58	0.43	1.89	9	1
4:A:370:PX4:H19	4:A:370:PX4:H25	0.43	1.59	11	1
4:A:331:PX4:H49	4:A:336:PX4:H28	0.43	1.91	12	1
4:A:389:PX4:H26	4:A:397:PX4:H31	0.43	1.90	12	1
4:A:378:PX4:C25	4:A:417:PX4:H67	0.43	2.43	13	1
4:A:395:PX4:H41	4:A:406:PX4:H67	0.43	1.91	14	1
4:A:325:PX4:H38	4:A:326:PX4:H30	0.43	1.91	2	1
4:A:381:PX4:H61	4:A:396:PX4:H27	0.43	1.90	3	1
4:A:332:PX4:H62	4:A:414:PX4:H36	0.43	1.90	5	1
4:A:350:PX4:H41	4:A:414:PX4:H39	0.43	1.89	7	1
4:A:346:PX4:H16	4:A:362:PX4:H4	0.43	1.89	8	1
4:A:307:PX4:H56	4:A:349:PX4:H7	0.43	1.90	9	1
4:A:368:PX4:H53	4:A:424:PX4:H48	0.43	1.91	11	1
4:A:395:PX4:H61	4:A:406:PX4:H67	0.43	1.90	11	1
4:A:346:PX4:H52	4:A:362:PX4:H54	0.43	1.91	12	1
4:A:332:PX4:H15	4:A:334:PX4:H19	0.43	1.91	13	1
4:A:315:PX4:H60	4:A:323:PX4:H59	0.43	1.91	14	1
4:A:324:PX4:H42	4:A:372:PX4:H70	0.42	1.91	3	1
4:A:401:PX4:H66	4:A:401:PX4:H61	0.42	1.44	6	1
4:A:423:PX4:H19	4:A:425:PX4:H48	0.42	1.91	7	1
4:A:330:PX4:H39	4:A:344:PX4:H72	0.42	1.91	9	1
4:A:404:PX4:H28	4:A:419:PX4:H48	0.42	1.91	10	1
4:A:405:PX4:H48	4:A:414:PX4:H20	0.42	1.90	11	1
4:A:345:PX4:H31	4:A:357:PX4:H54	0.42	1.90	12	1
4:A:390:PX4:H45	4:A:407:PX4:H27	0.42	1.90	12	1
4:A:345:PX4:H33	4:A:354:PX4:H66	0.42	1.90	1	1
4:A:307:PX4:H22	4:A:361:PX4:H19	0.42	1.91	4	1
4:A:345:PX4:H53	4:A:346:PX4:H51	0.42	1.91	5	1
4:A:394:PX4:H2	4:A:401:PX4:O2	0.42	2.14	6	1
4:A:421:PX4:H23	4:A:430:PX4:H48	0.42	1.91	6	1
4:A:325:PX4:H35	4:A:341:PX4:H72	0.42	1.91	8	1
4:A:404:PX4:H13	4:A:430:PX4:O6	0.42	2.14	9	1
4:A:367:PX4:H50	4:A:419:PX4:H26	0.42	1.91	10	1
4:A:330:PX4:H56	4:A:357:PX4:H64	0.42	1.90	12	1
4:A:400:PX4:C31	4:A:422:PX4:H71	0.42	2.44	12	1
4:A:312:PX4:H31	4:A:366:PX4:H46	0.42	1.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:327:PX4:H30	4:A:359:PX4:H25	0.42	1.91	4	1
4:A:332:PX4:H44	4:A:340:PX4:H45	0.42	1.91	4	1
4:A:306:PX4:H44	4:A:367:PX4:C22	0.42	2.45	5	1
4:A:345:PX4:H9	4:A:353:PX4:O2	0.42	2.14	5	1
4:A:382:PX4:H45	4:A:397:PX4:H44	0.42	1.91	5	1
4:A:355:PX4:H30	4:A:356:PX4:H62	0.42	1.91	7	1
4:A:370:PX4:H67	4:A:403:PX4:H38	0.42	1.92	7	1
4:A:368:PX4:C34	4:A:424:PX4:H17	0.42	2.44	8	1
4:A:400:PX4:H44	4:A:400:PX4:H38	0.42	1.77	8	1
4:A:308:PX4:H29	4:A:416:PX4:H33	0.42	1.92	9	1
4:A:395:PX4:H36	4:A:406:PX4:H60	0.42	1.91	9	1
4:A:329:PX4:H64	4:A:329:PX4:H72	0.42	1.41	11	1
4:A:350:PX4:H54	4:A:363:PX4:H50	0.42	1.91	13	1
4:A:400:PX4:H62	4:A:400:PX4:H69	0.42	1.51	13	1
4:A:407:PX4:H27	4:A:407:PX4:H22	0.42	1.63	13	1
4:A:307:PX4:H18	4:A:314:PX4:H49	0.42	1.91	14	1
4:A:314:PX4:H36	4:A:356:PX4:H25	0.42	1.91	14	1
4:A:390:PX4:H59	4:A:390:PX4:H64	0.42	1.59	1	1
4:A:386:PX4:H59	4:A:387:PX4:H72	0.42	1.92	2	1
4:A:392:PX4:H59	4:A:407:PX4:H29	0.42	1.91	2	1
4:A:322:PX4:C18	4:A:424:PX4:H69	0.42	2.44	4	1
4:A:359:PX4:H10	4:A:359:PX4:O8	0.42	2.15	4	1
4:A:389:PX4:H47	4:A:398:PX4:H17	0.42	1.90	5	2
4:A:353:PX4:H70	4:A:424:PX4:H43	0.42	1.92	10	1
4:A:340:PX4:H56	4:A:341:PX4:H20	0.42	1.91	12	1
4:A:417:PX4:H46	4:A:426:PX4:H58	0.42	1.91	12	1
4:A:355:PX4:H5	4:A:362:PX4:O8	0.42	2.14	13	1
4:A:386:PX4:H48	4:A:387:PX4:H48	0.42	1.92	13	1
4:A:410:PX4:H23	4:A:410:PX4:H30	0.42	1.48	3	1
4:A:422:PX4:H22	4:A:425:PX4:H66	0.42	1.92	4	1
4:A:330:PX4:H46	4:A:337:PX4:H17	0.42	1.90	5	2
4:A:357:PX4:H39	4:A:358:PX4:H37	0.42	1.90	5	1
4:A:370:PX4:H32	4:A:404:PX4:H27	0.42	1.90	5	1
4:A:317:PX4:H29	4:A:317:PX4:H36	0.42	1.50	8	1
1:A:163:PHE:HZ	1:A:212:LEU:HD11	0.42	1.74	9	1
4:A:336:PX4:H25	4:A:344:PX4:H60	0.42	1.90	9	1
4:A:391:PX4:H26	4:A:414:PX4:H17	0.42	1.90	10	1
4:A:376:PX4:H14	4:A:377:PX4:O2	0.42	2.15	11	1
4:A:320:PX4:H43	4:A:376:PX4:H31	0.42	1.90	13	1
4:A:330:PX4:H16	4:A:343:PX4:H5	0.42	1.90	14	1
4:A:353:PX4:H36	4:A:413:PX4:H43	0.42	1.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:330:PX4:H51	4:A:337:PX4:H53	0.42	1.91	3	1
4:A:422:PX4:H20	4:A:422:PX4:H26	0.42	1.69	3	1
4:A:424:PX4:H64	4:A:429:PX4:H59	0.42	1.92	3	1
4:A:335:PX4:H42	4:A:344:PX4:H37	0.42	1.92	5	1
4:A:328:PX4:H19	4:A:360:PX4:H21	0.42	1.92	10	1
4:A:306:PX4:H58	4:A:306:PX4:H65	0.42	1.65	11	1
4:A:332:PX4:H49	4:A:334:PX4:H32	0.42	1.92	11	1
4:A:334:PX4:H70	4:A:349:PX4:H61	0.42	1.92	1	1
4:A:388:PX4:H50	4:A:397:PX4:H58	0.42	1.91	1	1
4:A:384:PX4:H23	4:A:385:PX4:H24	0.42	1.91	3	1
1:A:116:TYR:CD2	1:A:138:PHE:CE2	0.42	3.07	4	1
4:A:322:PX4:H36	4:A:323:PX4:H57	0.42	1.91	4	1
4:A:315:PX4:H44	4:A:315:PX4:H64	0.42	1.91	8	1
4:A:346:PX4:H22	4:A:354:PX4:H20	0.42	1.91	8	1
4:A:322:PX4:H17	4:A:333:PX4:C22	0.42	2.44	10	1
1:A:165:ARG:NH1	4:A:354:PX4:H10	0.42	2.30	12	1
4:A:314:PX4:H63	4:A:314:PX4:H56	0.42	1.62	1	1
4:A:388:PX4:H56	4:A:402:PX4:H57	0.42	1.91	1	1
4:A:424:PX4:H54	4:A:428:PX4:H61	0.42	1.92	1	1
4:A:319:PX4:H37	4:A:319:PX4:H31	0.42	1.73	2	1
4:A:391:PX4:H63	4:A:391:PX4:H56	0.42	1.60	2	1
4:A:315:PX4:H29	4:A:425:PX4:H44	0.42	1.92	3	1
4:A:309:PX4:H54	4:A:316:PX4:H57	0.42	1.92	4	1
4:A:370:PX4:H36	4:A:404:PX4:H37	0.42	1.91	4	1
4:A:340:PX4:H49	4:A:340:PX4:H54	0.42	1.70	5	1
4:A:346:PX4:H6	4:A:360:PX4:O8	0.42	2.15	7	1
4:A:349:PX4:H32	4:A:349:PX4:H37	0.42	1.60	8	1
4:A:395:PX4:H58	4:A:406:PX4:H66	0.42	1.90	8	1
4:A:320:PX4:H37	4:A:378:PX4:H39	0.42	1.91	9	1
4:A:332:PX4:H63	4:A:415:PX4:H63	0.42	1.91	9	1
4:A:395:PX4:H19	4:A:405:PX4:H16	0.42	1.92	9	1
4:A:331:PX4:C21	4:A:332:PX4:H42	0.42	2.45	11	1
4:A:368:PX4:H10	4:A:418:PX4:O1	0.42	2.15	12	1
4:A:312:PX4:H65	4:A:312:PX4:H58	0.42	1.68	13	1
4:A:396:PX4:H47	4:A:405:PX4:H47	0.42	1.91	2	1
4:A:417:PX4:H34	4:A:426:PX4:H65	0.42	1.92	2	1
4:A:404:PX4:H12	4:A:419:PX4:O1	0.42	2.15	3	1
4:A:355:PX4:O8	4:A:355:PX4:H3	0.42	2.14	5	1
4:A:400:PX4:H28	4:A:400:PX4:H63	0.42	1.92	5	1
4:A:328:PX4:H7	4:A:354:PX4:O8	0.42	2.15	6	1
4:A:429:PX4:H51	4:A:429:PX4:H56	0.42	1.63	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:363:PX4:H19	4:A:364:PX4:H36	0.42	1.90	7	1
4:A:408:PX4:H65	4:A:409:PX4:H28	0.42	1.91	8	1
4:A:415:PX4:H24	4:A:425:PX4:H66	0.42	1.91	11	1
4:A:329:PX4:H53	4:A:329:PX4:H59	0.42	1.62	12	1
4:A:333:PX4:H27	4:A:333:PX4:H21	0.42	1.45	14	1
4:A:380:PX4:H8	4:A:402:PX4:O6	0.42	2.15	14	1
4:A:315:PX4:H40	4:A:361:PX4:C3	0.42	2.44	1	1
4:A:306:PX4:H38	4:A:328:PX4:H37	0.42	1.92	3	1
4:A:346:PX4:O8	4:A:362:PX4:H9	0.42	2.14	3	1
4:A:321:PX4:H68	4:A:425:PX4:H37	0.42	1.90	4	1
4:A:394:PX4:H55	4:A:394:PX4:H49	0.42	1.73	4	1
4:A:420:PX4:H17	4:A:427:PX4:H22	0.42	1.90	4	1
4:A:306:PX4:H18	4:A:322:PX4:H50	0.42	1.92	5	1
4:A:321:PX4:H48	4:A:354:PX4:H30	0.42	1.91	5	1
4:A:355:PX4:H11	4:A:362:PX4:O8	0.42	2.15	7	1
4:A:374:PX4:H25	4:A:412:PX4:H56	0.42	1.91	7	1
4:A:417:PX4:H25	4:A:417:PX4:H20	0.42	1.48	9	1
4:A:333:PX4:H59	4:A:333:PX4:H52	0.42	1.57	11	1
4:A:421:PX4:H24	4:A:430:PX4:H21	0.42	1.91	11	1
4:A:307:PX4:H38	4:A:364:PX4:H58	0.42	1.91	12	1
4:A:416:PX4:H12	4:A:426:PX4:O2	0.42	2.15	12	1
4:A:307:PX4:H60	4:A:349:PX4:H5	0.41	1.92	1	1
4:A:337:PX4:H59	4:A:338:PX4:H58	0.41	1.92	1	1
4:A:370:PX4:H64	4:A:370:PX4:H59	0.41	1.59	3	1
4:A:345:PX4:H35	4:A:353:PX4:H32	0.41	1.92	4	1
4:A:425:PX4:H32	4:A:425:PX4:H38	0.41	1.56	4	1
4:A:307:PX4:H70	4:A:350:PX4:H58	0.41	1.91	6	1
4:A:354:PX4:H36	4:A:355:PX4:H72	0.41	1.92	6	1
4:A:380:PX4:H23	4:A:381:PX4:H21	0.41	1.92	6	1
4:A:347:PX4:H24	4:A:348:PX4:H51	0.41	1.92	7	1
4:A:339:PX4:H20	4:A:347:PX4:H48	0.41	1.90	9	1
4:A:421:PX4:O6	4:A:423:PX4:H46	0.41	2.15	9	1
4:A:313:PX4:H53	4:A:359:PX4:C12	0.41	2.42	10	1
4:A:313:PX4:H57	4:A:359:PX4:H26	0.41	1.92	10	1
4:A:335:PX4:H26	4:A:335:PX4:H19	0.41	1.54	10	1
4:A:319:PX4:H23	4:A:320:PX4:H43	0.41	1.91	12	1
4:A:320:PX4:H70	4:A:371:PX4:H67	0.41	1.92	12	1
4:A:331:PX4:H37	4:A:331:PX4:H31	0.41	1.55	12	1
4:A:391:PX4:H57	4:A:391:PX4:H62	0.41	1.65	12	1
4:A:326:PX4:H35	4:A:340:PX4:H38	0.41	1.91	13	1
1:A:191:ILE:O	4:A:314:PX4:H7	0.41	2.16	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H52	4:A:308:PX4:H59	0.41	1.72	4	1
4:A:388:PX4:H33	4:A:406:PX4:H64	0.41	1.93	4	1
4:A:312:PX4:H48	4:A:312:PX4:H55	0.41	1.65	6	1
4:A:314:PX4:H42	4:A:355:PX4:H11	0.41	1.91	7	1
4:A:322:PX4:H11	4:A:361:PX4:O8	0.41	2.15	7	1
4:A:330:PX4:H55	4:A:337:PX4:H52	0.41	1.91	7	1
4:A:325:PX4:H32	4:A:341:PX4:H67	0.41	1.91	8	1
4:A:426:PX4:H39	4:A:426:PX4:H34	0.41	1.75	10	1
4:A:347:PX4:C29	4:A:355:PX4:H25	0.41	2.24	11	1
4:A:379:PX4:H33	4:A:379:PX4:H28	0.41	1.60	11	1
4:A:307:PX4:H51	4:A:356:PX4:H37	0.41	1.92	12	1
4:A:319:PX4:H55	4:A:319:PX4:H22	0.41	1.92	13	1
4:A:366:PX4:H53	4:A:366:PX4:H47	0.41	1.69	14	1
4:A:402:PX4:H48	4:A:411:PX4:H25	0.41	1.92	14	1
1:A:191:ILE:O	4:A:314:PX4:H3	0.41	2.15	1	1
4:A:367:PX4:H52	4:A:430:PX4:H50	0.41	1.90	2	1
4:A:369:PX4:H27	4:A:369:PX4:H21	0.41	1.70	2	1
4:A:330:PX4:H22	4:A:343:PX4:H8	0.41	1.91	3	1
4:A:336:PX4:H39	4:A:428:PX4:H42	0.41	1.92	3	1
4:A:388:PX4:H36	4:A:406:PX4:H60	0.41	1.91	3	1
4:A:400:PX4:H64	4:A:417:PX4:H29	0.41	1.90	4	1
4:A:405:PX4:H33	4:A:415:PX4:H64	0.41	1.91	4	1
4:A:401:PX4:H63	4:A:401:PX4:H56	0.41	1.53	5	1
4:A:360:PX4:H47	4:A:366:PX4:H18	0.41	1.93	6	1
4:A:387:PX4:H55	4:A:411:PX4:H50	0.41	1.92	7	1
4:A:409:PX4:H59	4:A:409:PX4:H52	0.41	1.60	7	1
4:A:314:PX4:H43	4:A:349:PX4:H47	0.41	1.92	8	1
4:A:367:PX4:H46	4:A:367:PX4:H53	0.41	1.55	8	1
4:A:389:PX4:H52	4:A:398:PX4:H65	0.41	1.91	9	1
4:A:405:PX4:H30	4:A:422:PX4:H33	0.41	1.93	10	1
4:A:405:PX4:H52	4:A:405:PX4:H59	0.41	1.69	11	1
4:A:388:PX4:H55	4:A:402:PX4:H28	0.41	1.91	12	1
4:A:392:PX4:H54	4:A:407:PX4:H21	0.41	1.91	12	1
4:A:404:PX4:H23	4:A:419:PX4:H46	0.41	1.90	12	1
4:A:307:PX4:H20	4:A:307:PX4:H25	0.41	1.66	13	1
4:A:329:PX4:H45	4:A:359:PX4:H23	0.41	1.92	1	1
4:A:349:PX4:H71	4:A:355:PX4:H71	0.41	1.91	1	1
4:A:346:PX4:H33	4:A:362:PX4:H25	0.41	1.92	2	1
4:A:368:PX4:H17	4:A:390:PX4:H48	0.41	1.92	2	1
4:A:311:PX4:H26	4:A:311:PX4:H56	0.41	1.91	6	1
4:A:309:PX4:O1	4:A:319:PX4:H18	0.41	2.15	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:395:PX4:H21	4:A:406:PX4:C26	0.41	2.43	10	1
4:A:417:PX4:H47	4:A:417:PX4:H52	0.41	1.67	10	1
4:A:368:PX4:H3	4:A:369:PX4:O3	0.41	2.14	11	1
4:A:398:PX4:H27	4:A:398:PX4:H52	0.41	1.92	11	1
4:A:408:PX4:H24	4:A:415:PX4:H17	0.41	1.92	12	1
4:A:410:PX4:H54	4:A:426:PX4:H51	0.41	1.91	12	1
4:A:318:PX4:H71	4:A:318:PX4:H65	0.41	1.56	14	1
4:A:428:PX4:H49	4:A:429:PX4:H21	0.41	1.92	1	1
4:A:306:PX4:O8	4:A:322:PX4:H9	0.41	2.15	2	1
4:A:322:PX4:H19	4:A:333:PX4:H37	0.41	1.91	2	1
4:A:368:PX4:H50	4:A:369:PX4:H30	0.41	1.92	2	1
4:A:391:PX4:H47	4:A:391:PX4:H53	0.41	1.60	2	1
4:A:339:PX4:H65	4:A:339:PX4:H58	0.41	1.68	3	1
4:A:346:PX4:H26	4:A:354:PX4:H25	0.41	1.90	4	1
4:A:384:PX4:H22	4:A:385:PX4:H24	0.41	1.92	8	1
4:A:307:PX4:H41	4:A:425:PX4:H30	0.41	1.91	9	1
4:A:336:PX4:H35	4:A:336:PX4:H30	0.41	1.62	11	1
4:A:390:PX4:H25	4:A:390:PX4:H19	0.41	1.64	12	1
4:A:319:PX4:H46	4:A:333:PX4:H54	0.41	1.92	13	1
4:A:334:PX4:H26	4:A:334:PX4:H59	0.41	1.91	13	1
4:A:356:PX4:H31	4:A:356:PX4:H25	0.41	1.78	13	1
4:A:312:PX4:O1	4:A:366:PX4:H18	0.41	2.16	1	1
4:A:353:PX4:H50	4:A:353:PX4:H57	0.41	1.62	1	1
4:A:325:PX4:H55	4:A:325:PX4:H49	0.41	1.66	2	1
4:A:351:PX4:H19	4:A:351:PX4:H26	0.41	1.66	4	1
4:A:353:PX4:H27	4:A:365:PX4:H51	0.41	1.92	4	1
4:A:385:PX4:H8	4:A:393:PX4:O1	0.41	2.16	5	1
4:A:365:PX4:H16	4:A:366:PX4:H5	0.41	1.93	8	2
4:A:371:PX4:H25	4:A:377:PX4:C11	0.41	2.45	8	1
4:A:325:PX4:H62	4:A:325:PX4:H33	0.41	1.91	10	1
4:A:307:PX4:H18	4:A:314:PX4:O8	0.41	2.15	12	1
4:A:406:PX4:H61	4:A:421:PX4:H71	0.41	1.93	12	1
4:A:315:PX4:H59	4:A:368:PX4:H44	0.41	1.93	13	1
4:A:373:PX4:O6	4:A:397:PX4:H1	0.41	2.16	14	1
4:A:322:PX4:H16	4:A:323:PX4:H49	0.41	1.91	1	1
4:A:408:PX4:H37	4:A:425:PX4:H62	0.41	1.93	1	1
4:A:321:PX4:O1	4:A:328:PX4:H10	0.41	2.15	2	1
4:A:321:PX4:H61	4:A:361:PX4:H30	0.41	1.91	2	1
4:A:336:PX4:C36	4:A:344:PX4:H35	0.41	2.46	5	1
4:A:321:PX4:H62	4:A:425:PX4:H43	0.41	1.92	6	1
4:A:360:PX4:H17	4:A:366:PX4:O6	0.41	2.16	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:388:PX4:H14	4:A:395:PX4:O1	0.41	2.15	6	1
4:A:360:PX4:H68	4:A:413:PX4:H35	0.41	1.91	8	1
4:A:421:PX4:H30	4:A:421:PX4:H35	0.41	1.67	11	1
4:A:310:PX4:H70	4:A:364:PX4:H52	0.41	1.92	12	1
4:A:405:PX4:H17	4:A:414:PX4:H24	0.41	1.93	12	1
4:A:406:PX4:H33	4:A:425:PX4:H63	0.41	1.92	12	1
4:A:314:PX4:H55	4:A:364:PX4:H46	0.41	1.92	13	1
4:A:330:PX4:H36	4:A:347:PX4:H37	0.41	1.92	13	1
4:A:331:PX4:H15	4:A:332:PX4:O6	0.41	2.15	14	1
4:A:379:PX4:H53	4:A:379:PX4:H46	0.41	1.60	14	1
4:A:343:PX4:H44	4:A:343:PX4:H38	0.41	1.73	1	1
4:A:317:PX4:H56	4:A:324:PX4:H40	0.41	1.93	2	1
4:A:383:PX4:H49	4:A:392:PX4:H26	0.41	1.93	2	1
4:A:339:PX4:H21	4:A:348:PX4:H50	0.41	1.91	3	1
4:A:379:PX4:H68	4:A:379:PX4:H41	0.41	1.91	3	1
4:A:430:PX4:H52	4:A:430:PX4:H47	0.41	1.63	3	1
4:A:316:PX4:H69	4:A:368:PX4:H30	0.41	1.91	4	1
4:A:334:PX4:H52	4:A:349:PX4:H21	0.41	1.93	4	1
4:A:376:PX4:H39	4:A:377:PX4:H61	0.41	1.93	4	1
4:A:400:PX4:H50	4:A:416:PX4:H34	0.41	1.91	4	1
4:A:325:PX4:O6	4:A:334:PX4:H7	0.41	2.16	5	1
4:A:347:PX4:H58	4:A:355:PX4:H23	0.41	1.91	6	1
4:A:353:PX4:H50	4:A:353:PX4:H56	0.41	1.67	8	1
4:A:348:PX4:H42	4:A:388:PX4:H69	0.41	1.93	9	1
4:A:390:PX4:H38	4:A:390:PX4:H44	0.41	1.48	10	1
4:A:325:PX4:H43	4:A:393:PX4:H63	0.41	1.92	11	1
4:A:332:PX4:H4	4:A:356:PX4:O1	0.41	2.16	11	1
4:A:343:PX4:C24	4:A:352:PX4:H56	0.41	2.45	11	1
4:A:354:PX4:H39	4:A:423:PX4:H41	0.41	1.92	11	1
4:A:374:PX4:H33	4:A:428:PX4:H44	0.41	1.93	12	1
4:A:384:PX4:H19	4:A:386:PX4:O6	0.41	2.16	12	1
4:A:359:PX4:H54	4:A:359:PX4:H48	0.41	1.49	13	1
4:A:330:PX4:H58	4:A:357:PX4:H61	0.41	1.93	1	1
4:A:416:PX4:H18	4:A:425:PX4:H15	0.41	1.93	1	1
4:A:317:PX4:H16	4:A:342:PX4:O6	0.41	2.16	2	1
4:A:392:PX4:H47	4:A:392:PX4:H52	0.41	1.69	3	1
4:A:392:PX4:H15	4:A:392:PX4:H12	0.41	1.92	3	1
4:A:313:PX4:H47	4:A:327:PX4:H25	0.41	1.93	5	1
4:A:335:PX4:H46	4:A:343:PX4:H23	0.41	1.91	5	1
4:A:310:PX4:H37	4:A:364:PX4:H36	0.41	1.92	6	1
4:A:397:PX4:H60	4:A:406:PX4:H71	0.41	1.92	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:PX4:H31	4:A:411:PX4:H26	0.41	1.67	6	1
4:A:306:PX4:H19	4:A:360:PX4:H42	0.41	1.93	7	1
4:A:312:PX4:O2	4:A:312:PX4:H9	0.41	2.16	7	1
4:A:316:PX4:H69	4:A:377:PX4:H38	0.41	1.92	8	1
4:A:369:PX4:O1	4:A:425:PX4:H2	0.41	2.16	8	1
4:A:413:PX4:H71	4:A:424:PX4:H33	0.41	1.92	8	1
4:A:421:PX4:H20	4:A:430:PX4:H16	0.41	1.92	8	1
4:A:329:PX4:H62	4:A:428:PX4:H62	0.41	1.93	9	1
4:A:388:PX4:H64	4:A:402:PX4:H36	0.41	1.93	9	1
4:A:317:PX4:O8	4:A:342:PX4:H4	0.41	2.16	10	1
4:A:378:PX4:H63	4:A:378:PX4:H56	0.41	1.50	10	1
4:A:315:PX4:O7	4:A:316:PX4:H16	0.41	2.15	11	1
4:A:337:PX4:H69	4:A:395:PX4:H67	0.41	1.90	11	1
4:A:372:PX4:H36	4:A:372:PX4:H41	0.41	1.73	11	1
4:A:383:PX4:H17	4:A:392:PX4:H22	0.41	1.92	12	1
4:A:416:PX4:H21	4:A:425:PX4:O7	0.41	2.16	12	1
4:A:361:PX4:H30	4:A:364:PX4:H72	0.41	1.92	13	1
4:A:373:PX4:H38	4:A:373:PX4:H44	0.41	1.55	13	1
4:A:390:PX4:H5	4:A:407:PX4:O1	0.41	2.16	13	1
4:A:374:PX4:H28	4:A:427:PX4:H25	0.41	1.92	14	1
4:A:393:PX4:H55	4:A:399:PX4:H63	0.41	1.93	3	1
4:A:428:PX4:H51	4:A:429:PX4:H22	0.41	1.92	3	1
4:A:360:PX4:H49	4:A:360:PX4:H22	0.41	1.93	5	1
4:A:316:PX4:H72	4:A:316:PX4:C19	0.41	2.43	6	1
4:A:350:PX4:H63	4:A:363:PX4:H58	0.41	1.92	6	1
4:A:416:PX4:H27	4:A:426:PX4:H21	0.41	1.91	6	1
4:A:392:PX4:H60	4:A:393:PX4:H63	0.41	1.92	7	1
4:A:314:PX4:H67	4:A:314:PX4:H60	0.41	1.70	8	1
4:A:395:PX4:C19	4:A:415:PX4:H62	0.41	2.45	9	1
4:A:326:PX4:H55	4:A:363:PX4:H48	0.41	1.91	10	1
4:A:410:PX4:H58	4:A:426:PX4:H51	0.41	1.91	11	1
1:A:153:ASN:O	4:A:331:PX4:H12	0.41	2.16	14	1
4:A:306:PX4:H22	4:A:322:PX4:H57	0.41	1.90	14	1
4:A:384:PX4:H34	4:A:384:PX4:H40	0.41	1.72	14	1
4:A:416:PX4:H17	4:A:426:PX4:H25	0.41	1.91	14	1
4:A:396:PX4:H67	4:A:398:PX4:H65	0.40	1.93	1	1
4:A:348:PX4:H42	4:A:398:PX4:H45	0.40	1.91	3	1
4:A:393:PX4:H3	4:A:394:PX4:P1	0.40	2.56	4	1
4:A:428:PX4:H54	4:A:429:PX4:H48	0.40	1.93	4	1
4:A:330:PX4:O8	4:A:337:PX4:H10	0.40	2.16	5	1
4:A:322:PX4:H60	4:A:361:PX4:H52	0.40	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:334:PX4:H58	4:A:349:PX4:H48	0.40	1.92	7	1
4:A:337:PX4:H4	4:A:337:PX4:O6	0.40	2.16	7	1
4:A:330:PX4:H26	4:A:330:PX4:H31	0.40	1.59	8	1
4:A:333:PX4:H60	4:A:340:PX4:H60	0.40	1.92	8	1
4:A:306:PX4:H22	4:A:329:PX4:H63	0.40	1.92	10	1
4:A:349:PX4:H24	4:A:350:PX4:H52	0.40	1.93	10	1
4:A:385:PX4:H54	4:A:385:PX4:H48	0.40	1.59	11	1
4:A:423:PX4:H52	4:A:423:PX4:H47	0.40	1.69	11	1
4:A:355:PX4:H9	4:A:356:PX4:O6	0.40	2.16	12	1
4:A:378:PX4:H52	4:A:378:PX4:H47	0.40	1.76	12	1
4:A:325:PX4:H61	4:A:341:PX4:H29	0.40	1.93	13	1
4:A:389:PX4:O6	4:A:397:PX4:H8	0.40	2.16	13	1
4:A:367:PX4:H17	4:A:430:PX4:H50	0.40	1.91	14	1
4:A:389:PX4:H56	4:A:389:PX4:H51	0.40	1.63	14	1
4:A:325:PX4:H23	4:A:325:PX4:H30	0.40	1.29	2	1
4:A:315:PX4:H27	4:A:315:PX4:H21	0.40	1.73	3	1
4:A:399:PX4:H14	4:A:399:PX4:H6	0.40	1.94	3	1
4:A:321:PX4:H60	4:A:321:PX4:H67	0.40	1.45	6	1
4:A:392:PX4:H30	4:A:392:PX4:H35	0.40	1.73	6	1
4:A:327:PX4:H55	4:A:327:PX4:H48	0.40	1.54	9	1
4:A:328:PX4:H68	4:A:328:PX4:H62	0.40	1.73	9	1
4:A:345:PX4:H23	4:A:345:PX4:H30	0.40	1.74	11	1
4:A:313:PX4:H27	4:A:360:PX4:H21	0.40	1.93	12	1
4:A:307:PX4:H37	4:A:361:PX4:H55	0.40	1.92	13	1
4:A:317:PX4:H17	4:A:324:PX4:H52	0.40	1.93	14	1
4:A:379:PX4:H12	4:A:385:PX4:O1	0.40	2.16	14	1
4:A:395:PX4:H22	4:A:395:PX4:H27	0.40	1.68	14	1
4:A:307:PX4:H41	4:A:315:PX4:H28	0.40	1.93	1	1
4:A:322:PX4:H72	4:A:413:PX4:H63	0.40	1.92	2	1
4:A:331:PX4:H3	4:A:347:PX4:H46	0.40	1.93	2	1
4:A:370:PX4:H66	4:A:411:PX4:H31	0.40	1.93	4	1
4:A:375:PX4:H47	4:A:389:PX4:H21	0.40	1.93	4	1
4:A:422:PX4:H40	4:A:423:PX4:H69	0.40	1.93	5	1
4:A:346:PX4:H67	4:A:362:PX4:H68	0.40	1.92	6	1
1:A:160:LEU:CD2	4:A:356:PX4:H23	0.40	2.47	8	1
4:A:340:PX4:H20	4:A:341:PX4:H55	0.40	1.92	10	1
1:A:123:PRO:HB3	4:A:345:PX4:H4	0.40	1.93	13	1
4:A:346:PX4:H46	4:A:355:PX4:C4	0.40	2.46	13	1
4:A:369:PX4:O2	4:A:425:PX4:H2	0.40	2.16	13	1
4:A:359:PX4:H29	4:A:359:PX4:H24	0.40	1.64	14	1
4:A:345:PX4:H46	4:A:348:PX4:H6	0.40	1.94	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:349:PX4:H32	4:A:350:PX4:H35	0.40	1.92	2	1
4:A:422:PX4:H30	4:A:425:PX4:H67	0.40	1.93	2	1
4:A:371:PX4:H33	4:A:377:PX4:H26	0.40	1.93	3	1
4:A:356:PX4:H59	4:A:356:PX4:H53	0.40	1.60	4	1
4:A:370:PX4:H36	4:A:413:PX4:H36	0.40	1.92	7	1
4:A:406:PX4:H19	4:A:422:PX4:H19	0.40	1.92	7	1
4:A:386:PX4:H55	4:A:387:PX4:H22	0.40	1.92	9	1
4:A:387:PX4:H46	4:A:387:PX4:H53	0.40	1.81	10	1
4:A:391:PX4:H18	4:A:405:PX4:H3	0.40	1.94	10	1
4:A:313:PX4:H47	4:A:328:PX4:C7	0.40	2.35	12	1
4:A:374:PX4:H30	4:A:428:PX4:H39	0.40	1.92	12	1
4:A:334:PX4:H31	4:A:349:PX4:H57	0.40	1.91	13	1
4:A:347:PX4:H55	4:A:355:PX4:H27	0.40	1.92	13	1
4:A:373:PX4:H19	4:A:397:PX4:H15	0.40	1.93	13	1
4:A:378:PX4:O1	4:A:410:PX4:H7	0.40	2.15	13	1
4:A:315:PX4:H65	4:A:323:PX4:H35	0.40	1.92	3	1
4:A:403:PX4:H27	4:A:411:PX4:H28	0.40	1.94	3	1
4:A:403:PX4:H49	4:A:419:PX4:H51	0.40	1.94	3	1
4:A:319:PX4:H48	4:A:319:PX4:H55	0.40	1.79	4	1
4:A:374:PX4:H21	4:A:374:PX4:H13	0.40	1.93	4	1
4:A:419:PX4:H17	4:A:427:PX4:H15	0.40	1.92	4	1
4:A:330:PX4:H11	4:A:336:PX4:O1	0.40	2.17	5	1
4:A:316:PX4:C14	4:A:320:PX4:H40	0.40	2.47	8	1
4:A:328:PX4:H60	4:A:328:PX4:H55	0.40	1.62	8	1
4:A:375:PX4:H55	4:A:375:PX4:H48	0.40	1.63	8	1
4:A:380:PX4:H35	4:A:380:PX4:H42	0.40	1.60	8	1
4:A:403:PX4:H18	4:A:403:PX4:H1	0.40	1.94	9	1
4:A:391:PX4:H26	4:A:391:PX4:H19	0.40	1.43	10	1
4:A:411:PX4:H19	4:A:411:PX4:H26	0.40	1.65	10	1
4:A:316:PX4:H68	4:A:368:PX4:H32	0.40	1.93	11	1
4:A:383:PX4:H29	4:A:399:PX4:H25	0.40	1.93	12	1
4:A:390:PX4:H50	4:A:399:PX4:H34	0.40	1.93	13	1
4:A:401:PX4:H53	4:A:401:PX4:H58	0.40	1.81	13	1
4:A:421:PX4:H17	4:A:423:PX4:H55	0.40	1.93	14	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	162/164 (99%)	151±2 (93±1%)	10±2 (6±1%)	2±1 (1±1%)	20	68
All	All	2268/2296 (99%)	2109 (93%)	136 (6%)	23 (1%)	20	68

All 8 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	173	ALA	11
1	A	179	GLY	4
1	A	172	HIS	2
1	A	170	ASP	2
1	A	109	TRP	1
1	A	107	PRO	1
1	A	171	PHE	1
1	A	110	ARG	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	130/131 (99%)	123±1 (95±1%)	7±1 (5±1%)	27	77
All	All	1820/1834 (99%)	1728 (95%)	92 (5%)	27	77

All 26 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	165	ARG	14
1	A	199	GLU	14
1	A	170	ASP	12
1	A	172	HIS	11
1	A	244	ASP	6
1	A	253	ASP	5
1	A	109	TRP	4
1	A	101	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	129	ASP	2
1	A	201	GLU	2
1	A	136	LYS	2
1	A	251	SER	2
1	A	260	SER	2
1	A	191	ILE	1
1	A	108	VAL	1
1	A	261	LEU	1
1	A	102	GLU	1
1	A	131	ASP	1
1	A	223	SER	1
1	A	140	VAL	1
1	A	162	VAL	1
1	A	171	PHE	1
1	A	110	ARG	1
1	A	236	MET	1
1	A	200	ASP	1
1	A	202	PHE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 5 are monoatomic - leaving 125 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	348	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.63±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	374	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.64±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	351	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.64±0.03	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	355	-	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	348	-	51,53,53	1.42±0.17	8±2 (15±4%)
4	PX4	A	380	-	51,53,53	1.50±0.16	10±2 (19±4%)
4	PX4	A	352	-	51,53,53	1.48±0.16	9±2 (16±3%)
4	PX4	A	307	-	51,53,53	1.44±0.19	8±3 (16±5%)
4	PX4	A	376	-	51,53,53	1.48±0.15	10±2 (18±4%)
4	PX4	A	410	-	51,53,53	1.44±0.16	9±2 (17±3%)
4	PX4	A	414	-	51,53,53	1.51±0.15	9±2 (17±4%)
4	PX4	A	338	-	51,53,53	1.46±0.11	9±2 (16±4%)
4	PX4	A	413	-	51,53,53	1.55±0.15	10±2 (19±4%)
4	PX4	A	420	-	51,53,53	1.53±0.16	10±2 (19±4%)
4	PX4	A	426	-	51,53,53	1.48±0.14	9±2 (18±4%)
4	PX4	A	306	-	51,53,53	1.42±0.13	8±3 (14±4%)
4	PX4	A	366	-	51,53,53	1.55±0.16	9±2 (18±4%)
4	PX4	A	311	-	51,53,53	1.51±0.14	9±2 (18±3%)
4	PX4	A	330	-	51,53,53	1.41±0.16	8±3 (14±5%)
4	PX4	A	356	-	51,53,53	1.46±0.13	8±2 (16±4%)
4	PX4	A	409	-	51,53,53	1.45±0.17	8±2 (16±4%)
4	PX4	A	418	-	51,53,53	1.48±0.12	8±2 (16±3%)
4	PX4	A	342	-	51,53,53	1.46±0.14	9±2 (17±3%)
4	PX4	A	389	-	51,53,53	1.49±0.09	8±2 (16±4%)
4	PX4	A	419	-	51,53,53	1.44±0.10	9±2 (16±3%)
4	PX4	A	429	-	51,53,53	1.45±0.15	8±3 (16±5%)
4	PX4	A	337	-	51,53,53	1.43±0.12	8±2 (14±4%)
4	PX4	A	365	-	51,53,53	1.41±0.09	8±3 (14±4%)
4	PX4	A	367	-	51,53,53	1.46±0.10	8±2 (16±3%)
4	PX4	A	388	-	51,53,53	1.52±0.11	10±2 (19±4%)
4	PX4	A	359	-	51,53,53	1.47±0.12	9±2 (17±3%)
4	PX4	A	361	-	51,53,53	1.58±0.14	10±2 (20±4%)
4	PX4	A	396	-	51,53,53	1.44±0.15	7±2 (14±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	362	-	51,53,53	1.45±0.12	8±2 (16±4%)
4	PX4	A	335	-	51,53,53	1.52±0.15	9±2 (18±3%)
4	PX4	A	378	-	51,53,53	1.55±0.14	9±2 (18±4%)
4	PX4	A	377	-	51,53,53	1.43±0.13	8±2 (16±4%)
4	PX4	A	383	-	51,53,53	1.42±0.12	8±2 (16±4%)
4	PX4	A	391	-	51,53,53	1.48±0.14	8±3 (16±5%)
4	PX4	A	364	-	51,53,53	1.47±0.13	8±3 (15±5%)
4	PX4	A	308	-	51,53,53	1.53±0.12	9±2 (18±3%)
4	PX4	A	340	-	51,53,53	1.44±0.13	8±2 (16±4%)
4	PX4	A	310	-	51,53,53	1.48±0.12	9±2 (17±3%)
4	PX4	A	386	-	51,53,53	1.51±0.14	9±2 (17±4%)
4	PX4	A	374	-	51,53,53	1.45±0.14	8±3 (15±5%)
4	PX4	A	407	-	51,53,53	1.52±0.11	9±2 (17±4%)
4	PX4	A	322	-	51,53,53	1.47±0.10	9±2 (18±4%)
4	PX4	A	379	-	51,53,53	1.62±0.17	10±3 (19±5%)
4	PX4	A	346	-	51,53,53	1.46±0.12	9±2 (16±4%)
4	PX4	A	425	-	51,53,53	1.48±0.14	8±2 (16±4%)
4	PX4	A	315	-	51,53,53	1.41±0.09	8±2 (15±3%)
4	PX4	A	371	-	51,53,53	1.49±0.15	9±3 (16±5%)
4	PX4	A	408	-	51,53,53	1.54±0.16	10±3 (19±6%)
4	PX4	A	427	-	51,53,53	1.57±0.12	9±2 (17±3%)
4	PX4	A	347	-	51,53,53	1.49±0.18	9±3 (17±5%)
4	PX4	A	402	-	51,53,53	1.57±0.15	9±2 (18±4%)
4	PX4	A	392	-	51,53,53	1.46±0.10	9±2 (17±3%)
4	PX4	A	390	-	51,53,53	1.47±0.11	8±2 (16±4%)
4	PX4	A	363	-	51,53,53	1.56±0.08	10±1 (20±2%)
4	PX4	A	411	-	51,53,53	1.54±0.23	10±4 (19±7%)
4	PX4	A	372	-	51,53,53	1.43±0.20	8±4 (15±7%)
4	PX4	A	314	-	51,53,53	1.56±0.12	9±1 (17±2%)
4	PX4	A	398	-	51,53,53	1.53±0.16	9±3 (18±5%)
4	PX4	A	400	-	51,53,53	1.46±0.16	9±2 (17±4%)
4	PX4	A	370	-	51,53,53	1.51±0.17	9±2 (16±4%)
4	PX4	A	394	-	51,53,53	1.42±0.14	8±2 (14±3%)
4	PX4	A	405	-	51,53,53	1.39±0.14	7±2 (14±3%)
4	PX4	A	368	-	51,53,53	1.46±0.14	8±2 (16±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	353	-	51,53,53	1.49±0.11	9±2 (18±3%)
4	PX4	A	415	-	51,53,53	1.53±0.14	9±3 (18±5%)
4	PX4	A	349	-	51,53,53	1.49±0.11	9±2 (17±3%)
4	PX4	A	397	-	51,53,53	1.46±0.15	8±2 (15±4%)
4	PX4	A	326	-	51,53,53	1.46±0.14	8±2 (16±3%)
4	PX4	A	399	-	51,53,53	1.47±0.09	8±2 (16±3%)
4	PX4	A	334	-	51,53,53	1.45±0.12	8±2 (16±3%)
4	PX4	A	417	-	51,53,53	1.51±0.16	10±3 (19±5%)
4	PX4	A	328	-	51,53,53	1.47±0.13	9±3 (17±5%)
4	PX4	A	336	-	51,53,53	1.40±0.09	8±3 (15±5%)
4	PX4	A	381	-	51,53,53	1.49±0.15	9±2 (18±4%)
4	PX4	A	343	-	51,53,53	1.49±0.15	9±2 (17±4%)
4	PX4	A	319	-	51,53,53	1.41±0.10	8±2 (15±3%)
4	PX4	A	354	-	51,53,53	1.60±0.11	10±3 (20±6%)
4	PX4	A	385	-	51,53,53	1.48±0.13	9±2 (17±4%)
4	PX4	A	428	-	51,53,53	1.49±0.13	9±2 (17±4%)
4	PX4	A	341	-	51,53,53	1.44±0.12	7±2 (13±4%)
4	PX4	A	344	-	51,53,53	1.54±0.10	8±2 (16±4%)
4	PX4	A	393	-	51,53,53	1.43±0.13	8±2 (15±4%)
4	PX4	A	351	-	51,53,53	1.44±0.12	8±2 (16±3%)
4	PX4	A	401	-	51,53,53	1.43±0.16	8±2 (16±4%)
4	PX4	A	333	-	51,53,53	1.47±0.16	9±3 (18±5%)
4	PX4	A	416	-	51,53,53	1.54±0.15	10±2 (19±4%)
4	PX4	A	404	-	51,53,53	1.49±0.14	8±2 (14±3%)
4	PX4	A	350	-	51,53,53	1.45±0.11	8±2 (15±3%)
4	PX4	A	329	-	51,53,53	1.47±0.15	9±3 (16±5%)
4	PX4	A	324	-	51,53,53	1.40±0.12	7±2 (14±4%)
4	PX4	A	339	-	51,53,53	1.53±0.15	10±3 (18±5%)
4	PX4	A	412	-	51,53,53	1.52±0.17	10±3 (18±5%)
4	PX4	A	323	-	51,53,53	1.47±0.14	9±2 (17±4%)
4	PX4	A	325	-	51,53,53	1.48±0.14	8±2 (15±3%)
4	PX4	A	375	-	51,53,53	1.53±0.22	10±4 (18±7%)
4	PX4	A	327	-	51,53,53	1.47±0.14	9±3 (17±5%)
4	PX4	A	345	-	51,53,53	1.34±0.09	7±1 (13±2%)
4	PX4	A	309	-	51,53,53	1.52±0.14	10±3 (18±5%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	369	-	51,53,53	1.51±0.09	9±1 (17±2%)
4	PX4	A	312	-	51,53,53	1.49±0.12	8±2 (16±3%)
4	PX4	A	313	-	51,53,53	1.48±0.13	9±3 (16±5%)
4	PX4	A	423	-	51,53,53	1.50±0.11	8±2 (16±3%)
4	PX4	A	406	-	51,53,53	1.45±0.13	8±2 (15±3%)
4	PX4	A	421	-	51,53,53	1.50±0.16	9±3 (18±5%)
4	PX4	A	403	-	51,53,53	1.51±0.16	9±2 (18±4%)
4	PX4	A	395	-	51,53,53	1.43±0.11	8±2 (16±3%)
4	PX4	A	358	-	51,53,53	1.36±0.10	7±2 (14±4%)
4	PX4	A	332	-	51,53,53	1.49±0.14	9±2 (18±4%)
4	PX4	A	357	-	51,53,53	1.52±0.08	9±2 (17±3%)
4	PX4	A	316	-	51,53,53	1.38±0.12	8±2 (14±3%)
4	PX4	A	321	-	51,53,53	1.55±0.14	9±2 (18±4%)
4	PX4	A	387	-	51,53,53	1.45±0.19	8±3 (16±5%)
4	PX4	A	382	-	51,53,53	1.51±0.12	10±2 (19±4%)
4	PX4	A	384	-	51,53,53	1.44±0.13	8±2 (15±4%)
4	PX4	A	331	-	51,53,53	1.45±0.12	8±2 (16±3%)
4	PX4	A	373	-	51,53,53	1.48±0.11	8±2 (16±3%)
4	PX4	A	320	-	51,53,53	1.50±0.12	9±2 (18±4%)
4	PX4	A	422	-	51,53,53	1.48±0.16	9±3 (17±5%)
4	PX4	A	424	-	51,53,53	1.45±0.15	8±2 (14±3%)
4	PX4	A	360	-	51,53,53	1.50±0.12	9±2 (16±3%)
4	PX4	A	318	-	51,53,53	1.44±0.14	8±2 (16±3%)
4	PX4	A	430	-	51,53,53	1.49±0.11	9±2 (17±3%)
4	PX4	A	317	-	51,53,53	1.45±0.11	8±1 (15±2%)
4	PX4	A	355	-	51,53,53	1.47±0.17	8±3 (16±5%)

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	418	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	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	328	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	371	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	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	307	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	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	307	PX4	C8-C7-C6	7.73	93.49	111.79	5	5
4	A	314	PX4	C8-C7-C6	7.54	93.95	111.79	11	10
4	A	378	PX4	C8-C7-C6	7.49	94.07	111.79	2	10
4	A	341	PX4	C7-O7-C23	7.48	136.20	117.79	2	9
4	A	371	PX4	C8-C7-C6	7.35	94.42	111.79	3	12
4	A	416	PX4	C8-C7-C6	7.34	94.43	111.79	6	11
4	A	323	PX4	C8-C7-C6	7.22	94.70	111.79	12	10
4	A	380	PX4	O7-C23-C24	7.17	126.95	111.50	10	5
4	A	400	PX4	C8-C7-C6	6.98	95.28	111.79	6	9
4	A	379	PX4	O3-P1-O2	6.97	81.85	109.07	3	7
4	A	350	PX4	O5-C8-C7	6.63	127.73	108.43	4	5
4	A	427	PX4	C8-C7-C6	6.59	96.20	111.79	3	7
4	A	372	PX4	O7-C23-C24	6.54	125.60	111.50	3	8
4	A	405	PX4	O7-C23-C24	6.48	125.46	111.50	9	4
4	A	313	PX4	C8-C7-C6	6.47	96.47	111.79	8	10
4	A	420	PX4	C8-C7-C6	6.41	96.63	111.79	1	6
4	A	318	PX4	C8-C7-C6	6.41	96.64	111.79	5	10
4	A	376	PX4	C8-C7-C6	6.37	96.72	111.79	3	10
4	A	333	PX4	C8-C7-C6	6.34	96.80	111.79	1	9
4	A	338	PX4	O5-C8-C7	6.32	126.83	108.43	4	5
4	A	408	PX4	O3-P1-O2	6.31	84.43	109.07	2	11
4	A	413	PX4	C8-C7-C6	6.25	97.01	111.79	3	9
4	A	353	PX4	O7-C23-C24	6.21	124.88	111.50	13	9
4	A	326	PX4	O7-C23-C24	6.14	124.73	111.50	11	8
4	A	321	PX4	O5-C8-C7	6.12	126.24	108.43	13	7
4	A	402	PX4	C8-C7-C6	6.11	97.34	111.79	6	13
4	A	335	PX4	O7-C23-C24	6.09	124.63	111.50	3	9
4	A	337	PX4	C8-C7-C6	6.07	97.43	111.79	7	6
4	A	342	PX4	O7-C23-C24	6.05	124.54	111.50	8	3
4	A	355	PX4	C8-C7-C6	6.02	97.56	111.79	14	11
4	A	426	PX4	C7-O7-C23	6.01	132.58	117.79	8	3
4	A	414	PX4	C8-C7-C6	5.98	97.64	111.79	4	7
4	A	353	PX4	O7-C23-O8	5.97	109.28	123.70	13	3
4	A	331	PX4	O5-C8-C7	5.92	125.67	108.43	14	10
4	A	414	PX4	O7-C23-C24	5.91	124.23	111.50	5	9
4	A	347	PX4	C8-C7-C6	5.89	97.86	111.79	9	10
4	A	415	PX4	O3-P1-O2	5.88	86.07	109.07	13	8
4	A	423	PX4	O7-C23-O8	5.88	109.49	123.70	3	2
4	A	311	PX4	O7-C23-O8	5.87	109.52	123.70	3	7
4	A	416	PX4	O5-C8-C7	5.85	125.48	108.43	8	7
4	A	396	PX4	C8-C7-C6	5.85	97.95	111.79	13	10
4	A	386	PX4	O3-P1-O2	5.84	86.26	109.07	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	O5-C8-C7	5.83	125.40	108.43	14	8
4	A	332	PX4	O7-C23-C24	5.81	124.02	111.50	9	10
4	A	399	PX4	C8-C7-C6	5.78	98.13	111.79	11	11
4	A	381	PX4	O7-C23-C24	5.74	123.87	111.50	5	9
4	A	376	PX4	O3-P1-O2	5.73	86.67	109.07	13	6
4	A	359	PX4	O5-C9-O6	5.68	109.26	123.59	13	5
4	A	355	PX4	C4-N1-C3	5.67	94.39	108.97	2	5
4	A	401	PX4	O7-C23-C24	5.66	123.70	111.50	6	5
4	A	389	PX4	O7-C23-C24	5.65	123.69	111.50	10	9
4	A	354	PX4	C7-O7-C23	5.65	131.70	117.79	13	9
4	A	320	PX4	O7-C23-C24	5.63	123.64	111.50	3	8
4	A	317	PX4	C8-C7-C6	5.63	98.48	111.79	9	9
4	A	361	PX4	O5-C8-C7	5.62	124.79	108.43	3	8
4	A	325	PX4	C8-C7-C6	5.61	98.52	111.79	14	7
4	A	386	PX4	C5-N1-C3	5.60	94.57	108.97	5	3
4	A	390	PX4	C7-O7-C23	5.58	131.53	117.79	10	6
4	A	422	PX4	O3-P1-O2	5.58	87.27	109.07	1	3
4	A	398	PX4	O7-C23-C24	5.57	123.51	111.50	2	9
4	A	418	PX4	O7-C23-C24	5.57	123.51	111.50	13	7
4	A	375	PX4	O3-P1-O2	5.55	87.39	109.07	8	5
4	A	393	PX4	C8-C7-C6	5.55	98.67	111.79	13	7
4	A	344	PX4	C8-C7-C6	5.54	98.68	111.79	1	10
4	A	424	PX4	O7-C23-C24	5.52	123.41	111.50	9	5
4	A	312	PX4	O5-C8-C7	5.52	124.49	108.43	3	13
4	A	410	PX4	C8-C7-C6	5.51	98.74	111.79	9	7
4	A	309	PX4	O7-C23-C24	5.51	123.38	111.50	4	7
4	A	379	PX4	C8-C7-C6	5.51	98.75	111.79	9	10
4	A	368	PX4	O5-C8-C7	5.51	124.46	108.43	3	10
4	A	412	PX4	C8-C7-C6	5.51	98.77	111.79	4	11
4	A	313	PX4	O5-C8-C7	5.49	124.40	108.43	7	9
4	A	369	PX4	O1-P1-O3	5.48	82.28	107.75	13	1
4	A	310	PX4	O5-C9-O6	5.48	109.77	123.59	5	3
4	A	309	PX4	C8-C7-C6	5.46	98.88	111.79	9	8
4	A	316	PX4	O7-C7-C8	5.44	128.12	108.40	4	9
4	A	404	PX4	C8-C7-C6	5.44	98.91	111.79	3	8
4	A	413	PX4	C7-O7-C23	5.44	104.39	117.79	5	3
4	A	348	PX4	O7-C23-C24	5.44	123.22	111.50	3	6
4	A	371	PX4	C4-N1-C3	5.44	94.99	108.97	6	3
4	A	363	PX4	O7-C23-C24	5.43	123.21	111.50	5	9
4	A	334	PX4	C8-C7-C6	5.40	99.00	111.79	3	9
4	A	308	PX4	C8-C7-C6	5.40	99.02	111.79	10	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	367	PX4	O5-C8-C7	5.39	124.12	108.43	1	11
4	A	366	PX4	C8-C7-C6	5.39	99.05	111.79	8	9
4	A	341	PX4	O7-C7-C8	5.38	127.88	108.40	3	7
4	A	327	PX4	C8-C7-C6	5.38	99.07	111.79	8	9
4	A	306	PX4	C7-O7-C23	5.37	131.02	117.79	11	3
4	A	430	PX4	O7-C23-C24	5.37	123.08	111.50	7	6
4	A	415	PX4	C8-C7-C6	5.35	99.13	111.79	7	7
4	A	421	PX4	O7-C23-C24	5.34	123.00	111.50	14	5
4	A	357	PX4	C8-C7-C6	5.33	99.19	111.79	4	8
4	A	387	PX4	O1-P1-O3	5.30	83.11	107.75	12	2
4	A	321	PX4	C8-C7-C6	5.29	99.29	111.79	3	8
4	A	330	PX4	O5-C8-C7	5.28	123.81	108.43	9	8
4	A	356	PX4	O7-C23-C24	5.28	122.88	111.50	10	7
4	A	327	PX4	O7-C23-C24	5.26	122.84	111.50	11	8
4	A	344	PX4	O5-C8-C7	5.26	123.73	108.43	6	8
4	A	360	PX4	O5-C8-C7	5.26	123.73	108.43	5	12
4	A	312	PX4	C8-C7-C6	5.25	99.36	111.79	4	7
4	A	317	PX4	P1-O3-C1	5.25	95.77	121.59	6	10
4	A	356	PX4	P1-O3-C1	5.24	95.78	121.59	7	9
4	A	360	PX4	O7-C23-C24	5.24	122.79	111.50	11	9
4	A	332	PX4	C8-C7-C6	5.23	99.41	111.79	4	3
4	A	367	PX4	C8-C7-C6	5.23	99.42	111.79	6	8
4	A	373	PX4	O5-C8-C7	5.22	123.63	108.43	7	11
4	A	403	PX4	C8-C7-C6	5.22	99.44	111.79	11	9
4	A	411	PX4	C5-N1-C3	5.22	95.56	108.97	1	3
4	A	329	PX4	O7-C23-C24	5.21	122.73	111.50	2	6
4	A	375	PX4	C8-C7-C6	5.21	99.47	111.79	4	8
4	A	306	PX4	C8-C7-C6	5.21	99.48	111.79	14	6
4	A	411	PX4	C8-C7-C6	5.20	99.49	111.79	1	10
4	A	384	PX4	P1-O3-C1	5.20	96.00	121.59	4	9
4	A	366	PX4	O7-C23-C24	5.19	122.68	111.50	12	7
4	A	409	PX4	C8-C7-C6	5.18	99.54	111.79	1	12
4	A	417	PX4	O1-P1-O3	5.18	83.69	107.75	14	3
4	A	395	PX4	C8-C7-C6	5.18	99.55	111.79	4	10
4	A	366	PX4	O5-C8-C7	5.17	123.48	108.43	2	11
4	A	370	PX4	O5-C9-O6	5.17	110.55	123.59	3	7
4	A	398	PX4	C5-N1-C4	5.16	95.71	108.97	9	7
4	A	311	PX4	C8-C7-C6	5.16	99.59	111.79	8	11
4	A	380	PX4	C8-C7-C6	5.15	99.60	111.79	9	9
4	A	400	PX4	O5-C8-C7	5.15	123.43	108.43	5	9
4	A	320	PX4	C8-C7-C6	5.15	99.61	111.79	11	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	378	PX4	O7-C23-C24	5.15	122.59	111.50	13	8
4	A	418	PX4	O5-C8-C7	5.13	123.37	108.43	1	6
4	A	335	PX4	O7-C23-O8	5.13	111.31	123.70	3	5
4	A	324	PX4	C8-C7-C6	5.12	99.67	111.79	14	11
4	A	331	PX4	O7-C7-C8	5.12	126.95	108.40	3	8
4	A	417	PX4	C8-C7-C6	5.12	99.67	111.79	4	9
4	A	387	PX4	C8-C7-C6	5.12	99.69	111.79	6	8
4	A	332	PX4	O5-C8-C7	5.11	123.30	108.43	6	8
4	A	390	PX4	C8-C7-C6	5.10	99.72	111.79	8	8
4	A	337	PX4	O7-C23-O8	5.10	111.38	123.70	2	6
4	A	410	PX4	O7-C23-C24	5.10	122.48	111.50	4	9
4	A	349	PX4	O7-C23-C24	5.09	122.47	111.50	2	9
4	A	369	PX4	C7-O7-C23	5.09	130.32	117.79	7	4
4	A	394	PX4	O7-C23-C24	5.09	122.46	111.50	6	5
4	A	319	PX4	O3-P1-O2	5.08	89.20	109.07	2	4
4	A	392	PX4	C5-N1-C4	5.08	95.90	108.97	8	4
4	A	409	PX4	O5-C8-C7	5.08	123.23	108.43	9	6
4	A	397	PX4	O5-C8-C7	5.08	123.21	108.43	10	5
4	A	352	PX4	C8-C7-C6	5.07	99.80	111.79	2	12
4	A	331	PX4	O7-C23-C24	5.07	122.42	111.50	8	5
4	A	361	PX4	C7-O7-C23	5.07	130.27	117.79	11	4
4	A	368	PX4	C8-C7-C6	5.07	99.80	111.79	6	11
4	A	367	PX4	C26-C25-C24	5.06	94.99	113.19	9	3
4	A	415	PX4	O7-C23-O8	5.06	111.47	123.70	4	7
4	A	362	PX4	C7-O7-C23	5.05	130.23	117.79	11	6
4	A	389	PX4	C8-C7-C6	5.05	99.84	111.79	5	7
4	A	420	PX4	C5-N1-C3	5.05	95.99	108.97	7	4
4	A	328	PX4	C8-C7-C6	5.04	99.86	111.79	2	12
4	A	333	PX4	O5-C8-C7	5.04	123.11	108.43	11	9
4	A	309	PX4	C7-O7-C23	5.03	130.17	117.79	8	6
4	A	343	PX4	O5-C8-C7	5.03	123.07	108.43	11	7
4	A	335	PX4	O3-P1-O2	5.03	89.43	109.07	7	4
4	A	353	PX4	O5-C9-O6	5.03	110.91	123.59	6	5
4	A	330	PX4	O7-C23-C24	5.02	122.33	111.50	11	7
4	A	429	PX4	C7-O7-C23	5.02	130.15	117.79	1	2
4	A	406	PX4	C8-C7-C6	5.02	99.92	111.79	1	8
4	A	412	PX4	O7-C23-C24	5.00	122.28	111.50	7	7
4	A	394	PX4	O5-C8-C7	5.00	122.98	108.43	3	8
4	A	370	PX4	C8-C7-C6	4.99	99.98	111.79	4	11
4	A	421	PX4	O5-C8-C7	4.99	122.96	108.43	13	8
4	A	424	PX4	O5-C8-C7	4.98	122.93	108.43	13	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	400	PX4	C4-N1-C3	4.98	96.18	108.97	2	4
4	A	319	PX4	C7-O7-C23	4.97	130.02	117.79	12	3
4	A	319	PX4	O5-C8-C7	4.96	122.88	108.43	6	9
4	A	322	PX4	C8-C7-C6	4.96	100.05	111.79	9	11
4	A	334	PX4	O5-C8-C7	4.96	122.88	108.43	13	6
4	A	344	PX4	O7-C23-C24	4.96	122.20	111.50	8	9
4	A	397	PX4	O7-C23-C24	4.96	122.19	111.50	14	6
4	A	382	PX4	O7-C23-C24	4.96	122.18	111.50	3	4
4	A	420	PX4	P1-O3-C1	4.95	97.20	121.59	14	9
4	A	422	PX4	O7-C23-C24	4.95	122.17	111.50	5	3
4	A	309	PX4	O5-C8-C7	4.95	122.84	108.43	7	8
4	A	337	PX4	O5-C8-C7	4.95	122.83	108.43	12	9
4	A	339	PX4	C4-N1-C3	4.95	121.69	108.97	5	3
4	A	342	PX4	C8-C7-C6	4.94	100.09	111.79	2	11
4	A	425	PX4	P1-O4-C6	4.94	92.71	121.68	10	10
4	A	365	PX4	P1-O3-C1	4.93	97.31	121.59	4	12
4	A	354	PX4	C8-C7-C6	4.93	100.13	111.79	11	9
4	A	328	PX4	P1-O3-C1	4.93	97.33	121.59	5	12
4	A	324	PX4	O5-C8-C7	4.93	122.77	108.43	14	7
4	A	346	PX4	O5-C8-C7	4.93	122.77	108.43	3	6
4	A	351	PX4	C8-C7-C6	4.92	100.14	111.79	6	8
4	A	386	PX4	C8-C7-C6	4.92	100.16	111.79	12	11
4	A	397	PX4	O7-C23-O8	4.92	111.82	123.70	14	4
4	A	340	PX4	C8-C7-C6	4.92	100.16	111.79	2	9
4	A	359	PX4	C8-C7-C6	4.90	100.19	111.79	14	11
4	A	402	PX4	C1-C2-N1	4.89	132.12	115.78	2	4
4	A	413	PX4	P1-O3-C1	4.89	97.52	121.59	11	12
4	A	355	PX4	C5-N1-C4	4.88	96.42	108.97	5	3
4	A	361	PX4	O5-C9-O6	4.88	111.27	123.59	10	3
4	A	312	PX4	O3-P1-O2	4.88	90.00	109.07	13	5
4	A	419	PX4	P1-O3-C1	4.88	97.57	121.59	7	9
4	A	402	PX4	O3-P1-O2	4.88	90.01	109.07	4	6
4	A	426	PX4	O1-P1-O3	4.88	85.09	107.75	8	3
4	A	411	PX4	P1-O3-C1	4.88	97.59	121.59	5	11
4	A	374	PX4	C5-N1-C3	4.87	96.45	108.97	11	3
4	A	415	PX4	P1-O3-C1	4.87	97.61	121.59	12	12
4	A	363	PX4	O5-C8-C7	4.87	122.60	108.43	11	10
4	A	421	PX4	C8-C7-C6	4.86	100.28	111.79	14	10
4	A	414	PX4	O5-C8-C7	4.86	122.59	108.43	6	10
4	A	389	PX4	O5-C8-C7	4.86	122.58	108.43	13	10
4	A	426	PX4	O7-C23-C24	4.86	121.97	111.50	9	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	329	PX4	C7-O7-C23	4.85	129.73	117.79	4	3
4	A	362	PX4	C8-C7-C6	4.85	100.32	111.79	2	9
4	A	423	PX4	C8-C7-C6	4.85	100.32	111.79	13	11
4	A	381	PX4	O7-C7-C8	4.85	125.95	108.40	2	6
4	A	391	PX4	O5-C8-C7	4.84	122.53	108.43	4	9
4	A	402	PX4	O7-C23-C24	4.84	121.93	111.50	12	7
4	A	407	PX4	O7-C23-C24	4.84	121.92	111.50	12	10
4	A	422	PX4	C8-C7-C6	4.84	100.35	111.79	13	12
4	A	346	PX4	C7-O7-C23	4.83	129.69	117.79	9	4
4	A	362	PX4	C5-N1-C4	4.83	96.55	108.97	1	8
4	A	340	PX4	O7-C23-C24	4.83	121.91	111.50	7	8
4	A	354	PX4	C5-N1-C3	4.83	96.56	108.97	5	3
4	A	407	PX4	C8-C7-C6	4.82	100.38	111.79	4	7
4	A	328	PX4	O5-C8-C7	4.81	122.43	108.43	9	7
4	A	385	PX4	O5-C8-C7	4.81	122.43	108.43	12	7
4	A	370	PX4	O5-C8-C7	4.81	122.42	108.43	2	7
4	A	419	PX4	C8-C7-C6	4.81	100.42	111.79	8	11
4	A	402	PX4	O5-C8-C7	4.80	122.42	108.43	7	10
4	A	308	PX4	O7-C23-C24	4.80	121.85	111.50	11	7
4	A	423	PX4	C5-N1-C4	4.79	96.65	108.97	5	1
4	A	383	PX4	O7-C7-C6	4.79	125.74	108.40	9	7
4	A	414	PX4	O1-P1-O2	4.79	135.91	112.24	11	8
4	A	329	PX4	P1-O3-C1	4.78	98.03	121.59	7	11
4	A	430	PX4	C8-C7-C6	4.78	100.49	111.79	9	10
4	A	407	PX4	C7-O7-C23	4.77	129.54	117.79	2	3
4	A	309	PX4	C5-N1-C4	4.77	96.71	108.97	7	3
4	A	335	PX4	O5-C8-C7	4.77	122.31	108.43	3	8
4	A	361	PX4	O1-P1-O3	4.77	85.61	107.75	14	6
4	A	383	PX4	O7-C23-C24	4.76	121.77	111.50	4	5
4	A	388	PX4	O7-C23-C24	4.76	121.77	111.50	7	8
4	A	398	PX4	C8-C7-C6	4.76	100.53	111.79	2	8
4	A	427	PX4	P1-O3-C1	4.76	98.16	121.59	12	10
4	A	374	PX4	C8-C7-C6	4.75	100.55	111.79	7	9
4	A	308	PX4	O3-P1-O2	4.75	90.51	109.07	4	7
4	A	339	PX4	O7-C23-C24	4.75	121.74	111.50	3	7
4	A	424	PX4	C12-C11-C10	4.75	96.11	113.19	6	2
4	A	308	PX4	C4-N1-C3	4.75	96.77	108.97	4	3
4	A	411	PX4	O7-C7-C8	4.75	125.58	108.40	1	8
4	A	413	PX4	O5-C8-C7	4.74	122.23	108.43	8	6
4	A	423	PX4	O7-C23-C24	4.74	121.72	111.50	11	8
4	A	428	PX4	C8-C7-C6	4.74	100.57	111.79	2	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	O5-C8-C7	4.74	122.23	108.43	12	10
4	A	416	PX4	C5-N1-C4	4.74	96.79	108.97	6	2
4	A	343	PX4	C7-O7-C23	4.73	129.44	117.79	5	3
4	A	394	PX4	O3-P1-O2	4.73	90.59	109.07	11	3
4	A	340	PX4	P1-O3-C1	4.72	98.35	121.59	6	11
4	A	352	PX4	O5-C8-C7	4.72	122.17	108.43	2	5
4	A	361	PX4	O7-C7-C6	4.72	125.48	108.40	8	8
4	A	389	PX4	O3-P1-O2	4.72	90.63	109.07	7	3
4	A	428	PX4	O5-C8-C7	4.72	122.17	108.43	5	8
4	A	318	PX4	O7-C23-C24	4.72	121.67	111.50	11	8
4	A	327	PX4	C7-O7-C23	4.72	129.40	117.79	14	5
4	A	406	PX4	O5-C8-C7	4.70	122.12	108.43	2	4
4	A	425	PX4	C8-C7-C6	4.70	100.66	111.79	1	7
4	A	371	PX4	O7-C23-C24	4.70	121.63	111.50	13	11
4	A	422	PX4	P1-O3-C1	4.70	98.45	121.59	3	10
4	A	412	PX4	O7-C7-C8	4.69	125.40	108.40	6	6
4	A	335	PX4	C8-C7-C6	4.69	100.69	111.79	5	9
4	A	418	PX4	P1-O3-C1	4.69	98.51	121.59	6	14
4	A	351	PX4	O5-C8-C7	4.68	122.07	108.43	14	5
4	A	404	PX4	P1-O3-C1	4.68	98.53	121.59	12	8
4	A	374	PX4	O5-C8-C7	4.68	122.06	108.43	4	10
4	A	325	PX4	O3-P1-O2	4.68	90.78	109.07	8	2
4	A	359	PX4	P1-O3-C1	4.68	98.55	121.59	12	11
4	A	366	PX4	P1-O3-C1	4.68	98.55	121.59	10	11
4	A	426	PX4	O5-C9-O6	4.68	111.78	123.59	14	5
4	A	353	PX4	C7-O7-C23	4.68	106.28	117.79	2	4
4	A	388	PX4	C8-C7-C6	4.67	100.73	111.79	8	11
4	A	369	PX4	O5-C8-C7	4.67	122.03	108.43	8	11
4	A	327	PX4	C5-N1-C4	4.67	96.97	108.97	3	2
4	A	372	PX4	O5-C8-C7	4.67	122.03	108.43	1	4
4	A	379	PX4	O7-C23-O8	4.67	112.42	123.70	2	4
4	A	384	PX4	C8-C7-C6	4.67	100.74	111.79	11	7
4	A	425	PX4	O7-C23-C24	4.67	121.56	111.50	2	6
4	A	355	PX4	C1-C2-N1	4.67	131.36	115.78	10	4
4	A	330	PX4	C4-N1-C3	4.66	120.95	108.97	6	3
4	A	331	PX4	C4-N1-C3	4.65	97.01	108.97	13	4
4	A	323	PX4	O7-C7-C6	4.65	125.24	108.40	12	7
4	A	421	PX4	C26-C25-C24	4.65	96.47	113.19	12	2
4	A	399	PX4	O7-C23-C24	4.65	121.52	111.50	12	5
4	A	356	PX4	C8-C7-C6	4.64	100.81	111.79	1	9
4	A	418	PX4	C8-C7-C6	4.64	100.82	111.79	11	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	411	PX4	C7-O7-C23	4.63	106.38	117.79	11	6
4	A	413	PX4	C1-C2-N1	4.63	131.25	115.78	4	3
4	A	423	PX4	P1-O3-C1	4.63	98.80	121.59	6	11
4	A	398	PX4	C5-N1-C3	4.63	120.88	108.97	7	4
4	A	381	PX4	O5-C8-C7	4.62	121.89	108.43	4	8
4	A	373	PX4	O7-C23-C24	4.62	121.46	111.50	13	9
4	A	362	PX4	O7-C23-C24	4.62	121.46	111.50	9	8
4	A	408	PX4	P1-O3-C1	4.62	98.86	121.59	6	11
4	A	325	PX4	O5-C8-C7	4.61	121.86	108.43	5	5
4	A	341	PX4	O7-C23-C24	4.61	121.44	111.50	5	6
4	A	411	PX4	O5-C8-C7	4.61	121.85	108.43	1	8
4	A	326	PX4	O3-P1-O2	4.61	91.07	109.07	11	4
4	A	353	PX4	C8-C7-C6	4.61	100.89	111.79	7	9
4	A	314	PX4	O7-C23-C24	4.60	121.42	111.50	13	9
4	A	418	PX4	C5-N1-C3	4.60	97.14	108.97	2	6
4	A	401	PX4	C4-N1-C3	4.60	97.15	108.97	2	4
4	A	346	PX4	O7-C23-C24	4.60	121.41	111.50	14	6
4	A	316	PX4	C8-C7-C6	4.59	100.92	111.79	6	9
4	A	407	PX4	O7-C7-C8	4.59	125.03	108.40	14	2
4	A	372	PX4	C8-C7-C6	4.59	100.93	111.79	4	8
4	A	412	PX4	O5-C8-C7	4.59	121.79	108.43	10	8
4	A	393	PX4	O5-C8-C7	4.59	121.79	108.43	9	6
4	A	420	PX4	O5-C8-C7	4.59	121.79	108.43	4	7
4	A	404	PX4	O7-C23-C24	4.59	121.39	111.50	7	7
4	A	354	PX4	O5-C9-O6	4.58	112.03	123.59	11	2
4	A	425	PX4	O5-C9-O6	4.58	112.04	123.59	2	5
4	A	312	PX4	C5-N1-C4	4.57	97.21	108.97	3	4
4	A	408	PX4	C8-C7-C6	4.57	100.98	111.79	5	9
4	A	357	PX4	O7-C23-C24	4.57	121.34	111.50	1	10
4	A	376	PX4	C8-O5-C9	4.57	100.21	117.12	11	1
4	A	415	PX4	O1-P1-O2	4.57	134.82	112.24	10	8
4	A	388	PX4	O5-C8-C7	4.57	121.72	108.43	5	8
4	A	419	PX4	O5-C8-C7	4.56	121.72	108.43	8	7
4	A	321	PX4	C25-C24-C23	4.56	97.03	113.62	4	1
4	A	350	PX4	O7-C23-C24	4.56	121.34	111.50	6	10
4	A	380	PX4	O5-C8-C7	4.56	121.72	108.43	3	8
4	A	395	PX4	O5-C9-O6	4.56	112.08	123.59	9	3
4	A	321	PX4	O7-C23-C24	4.56	121.32	111.50	11	4
4	A	348	PX4	C8-C7-C6	4.56	101.01	111.79	2	9
4	A	411	PX4	O3-P1-O2	4.55	91.28	109.07	12	6
4	A	413	PX4	C11-C10-C9	4.55	97.06	113.62	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	422	PX4	O5-C9-O6	4.55	112.10	123.59	10	4
4	A	428	PX4	O7-C23-C24	4.55	121.31	111.50	11	8
4	A	313	PX4	O7-C7-C8	4.55	124.87	108.40	9	6
4	A	416	PX4	C11-C10-C9	4.54	130.14	113.62	9	1
4	A	314	PX4	O5-C8-C7	4.54	121.64	108.43	8	5
4	A	357	PX4	O5-C8-C7	4.54	121.64	108.43	7	8
4	A	385	PX4	C8-C7-C6	4.54	101.06	111.79	1	11
4	A	410	PX4	C7-O7-C23	4.53	106.63	117.79	13	5
4	A	324	PX4	C7-O7-C23	4.53	128.94	117.79	1	3
4	A	374	PX4	P1-O3-C1	4.53	99.30	121.59	9	9
4	A	386	PX4	O7-C23-C24	4.52	121.25	111.50	12	8
4	A	343	PX4	P1-O3-C1	4.52	99.33	121.59	8	9
4	A	325	PX4	P1-O4-C6	4.52	95.19	121.68	10	11
4	A	347	PX4	O7-C7-C8	4.51	124.75	108.40	9	8
4	A	391	PX4	P1-O3-C1	4.51	99.37	121.59	10	9
4	A	310	PX4	O7-C23-C24	4.51	121.22	111.50	9	7
4	A	349	PX4	O5-C9-O6	4.51	112.21	123.59	11	5
4	A	332	PX4	O3-P1-O2	4.51	91.46	109.07	9	3
4	A	350	PX4	O3-P1-O2	4.51	91.46	109.07	11	5
4	A	378	PX4	C7-O7-C23	4.50	128.87	117.79	5	6
4	A	377	PX4	P1-O3-C1	4.50	99.44	121.59	6	11
4	A	392	PX4	O5-C8-C7	4.50	121.52	108.43	7	5
4	A	424	PX4	O7-C7-C6	4.49	124.67	108.40	13	4
4	A	345	PX4	O7-C23-O8	4.49	112.85	123.70	6	3
4	A	346	PX4	P1-O3-C1	4.49	99.48	121.59	8	13
4	A	343	PX4	C8-C7-C6	4.49	101.17	111.79	6	10
4	A	348	PX4	O5-C8-C7	4.48	121.49	108.43	12	7
4	A	307	PX4	O5-C8-C7	4.48	121.48	108.43	1	10
4	A	364	PX4	C8-C7-C6	4.48	101.20	111.79	8	8
4	A	404	PX4	O7-C23-O8	4.48	112.88	123.70	7	4
4	A	319	PX4	C8-C7-C6	4.48	101.20	111.79	7	7
4	A	406	PX4	O3-P1-O2	4.48	91.57	109.07	14	5
4	A	391	PX4	O7-C23-C24	4.47	121.14	111.50	3	7
4	A	313	PX4	C4-N1-C3	4.47	97.48	108.97	1	3
4	A	352	PX4	O7-C23-C24	4.47	121.13	111.50	7	7
4	A	427	PX4	O5-C8-C7	4.46	121.42	108.43	12	10
4	A	427	PX4	O1-P1-O3	4.46	87.04	107.75	5	3
4	A	344	PX4	C5-N1-C4	4.46	97.52	108.97	9	3
4	A	378	PX4	P1-O3-C1	4.45	99.69	121.59	5	9
4	A	416	PX4	O3-P1-O2	4.44	91.71	109.07	14	7
4	A	352	PX4	C26-C25-C24	4.44	97.24	113.19	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	361	PX4	O3-P1-O2	4.44	91.73	109.07	9	9
4	A	369	PX4	O7-C23-C24	4.44	121.06	111.50	9	5
4	A	422	PX4	O4-P1-O2	4.43	126.39	109.07	1	1
4	A	396	PX4	P1-O4-C6	4.43	95.71	121.68	9	9
4	A	369	PX4	C8-C7-C6	4.43	101.32	111.79	14	7
4	A	408	PX4	C5-N1-C3	4.43	120.35	108.97	3	3
4	A	413	PX4	O7-C7-C8	4.43	124.43	108.40	12	7
4	A	352	PX4	P1-O3-C1	4.43	99.80	121.59	6	10
4	A	314	PX4	P1-O3-C1	4.42	99.81	121.59	7	13
4	A	332	PX4	C5-N1-C3	4.42	120.35	108.97	2	4
4	A	324	PX4	O7-C7-C8	4.42	124.41	108.40	12	7
4	A	383	PX4	O4-P1-O2	4.42	126.35	109.07	9	3
4	A	314	PX4	C7-O7-C23	4.42	128.67	117.79	11	3
4	A	407	PX4	C5-N1-C4	4.42	97.62	108.97	5	3
4	A	387	PX4	O5-C8-C7	4.42	121.28	108.43	3	8
4	A	398	PX4	O3-P1-O2	4.41	91.82	109.07	7	5
4	A	328	PX4	O5-C9-O6	4.41	112.46	123.59	3	6
4	A	336	PX4	C12-C11-C10	4.41	97.33	113.19	6	3
4	A	370	PX4	O7-C23-C24	4.41	121.01	111.50	5	10
4	A	376	PX4	P1-O4-C6	4.41	95.80	121.68	5	14
4	A	424	PX4	C8-C7-C6	4.41	101.36	111.79	7	11
4	A	311	PX4	P1-O3-C1	4.41	99.89	121.59	3	13
4	A	395	PX4	P1-O3-C1	4.41	99.90	121.59	9	9
4	A	418	PX4	O7-C23-O8	4.41	113.06	123.70	8	8
4	A	320	PX4	O7-C7-C8	4.40	124.34	108.40	6	5
4	A	429	PX4	C5-N1-C4	4.40	97.66	108.97	12	5
4	A	364	PX4	C5-N1-C4	4.40	97.67	108.97	9	2
4	A	326	PX4	P1-O3-C1	4.40	99.95	121.59	1	6
4	A	361	PX4	C26-C25-C24	4.39	97.40	113.19	10	2
4	A	404	PX4	C7-O7-C23	4.39	128.61	117.79	5	6
4	A	415	PX4	O7-C7-C8	4.39	124.29	108.40	3	7
4	A	325	PX4	C5-N1-C3	4.39	97.70	108.97	9	7
4	A	330	PX4	P1-O3-C1	4.38	100.00	121.59	3	11
4	A	338	PX4	C8-C7-C6	4.38	101.42	111.79	14	10
4	A	317	PX4	O5-C9-O6	4.37	112.56	123.59	13	4
4	A	362	PX4	C4-N1-C3	4.37	120.22	108.97	6	4
4	A	384	PX4	O5-C8-C7	4.37	121.16	108.43	4	9
4	A	375	PX4	O7-C23-C24	4.36	120.90	111.50	14	8
4	A	397	PX4	C8-C7-C6	4.36	101.47	111.79	5	7
4	A	403	PX4	P1-O3-C1	4.36	100.13	121.59	3	9
4	A	377	PX4	O7-C23-C24	4.36	120.89	111.50	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	422	PX4	O5-C8-C7	4.36	121.12	108.43	13	7
4	A	405	PX4	C1-C2-N1	4.35	130.32	115.78	4	5
4	A	317	PX4	O7-C23-C24	4.35	120.88	111.50	10	6
4	A	323	PX4	O7-C23-C24	4.35	120.88	111.50	4	5
4	A	375	PX4	O5-C8-C7	4.34	121.08	108.43	7	8
4	A	411	PX4	C5-N1-C4	4.34	97.81	108.97	12	1
4	A	308	PX4	O5-C8-C7	4.33	121.04	108.43	9	9
4	A	391	PX4	O3-P1-O2	4.33	92.15	109.07	12	6
4	A	350	PX4	C5-N1-C3	4.33	97.85	108.97	7	4
4	A	416	PX4	O7-C23-C24	4.33	120.83	111.50	14	9
4	A	404	PX4	O3-P1-O2	4.33	92.16	109.07	3	4
4	A	383	PX4	C5-N1-C4	4.32	97.86	108.97	14	2
4	A	402	PX4	O1-P1-O4	4.32	127.82	107.75	8	3
4	A	411	PX4	C4-N1-C3	4.32	97.86	108.97	5	4
4	A	425	PX4	C7-O7-C23	4.32	107.17	117.79	9	3
4	A	404	PX4	O5-C9-O6	4.31	112.71	123.59	12	2
4	A	403	PX4	O7-C7-C6	4.31	124.00	108.40	6	6
4	A	307	PX4	O7-C7-C6	4.31	124.00	108.40	5	9
4	A	377	PX4	C8-C7-C6	4.31	101.60	111.79	13	9
4	A	405	PX4	C7-O7-C23	4.31	128.40	117.79	11	4
4	A	306	PX4	P1-O3-C1	4.31	100.39	121.59	6	10
4	A	320	PX4	C5-N1-C3	4.31	120.05	108.97	12	5
4	A	407	PX4	O5-C9-O6	4.30	112.73	123.59	6	2
4	A	382	PX4	O5-C8-C7	4.30	120.95	108.43	3	8
4	A	419	PX4	C7-O7-C23	4.30	128.38	117.79	1	4
4	A	360	PX4	C7-O7-C23	4.29	107.22	117.79	6	3
4	A	399	PX4	P1-O3-C1	4.29	100.45	121.59	7	9
4	A	311	PX4	O5-C8-C7	4.29	120.93	108.43	2	10
4	A	339	PX4	C5-N1-C3	4.29	97.94	108.97	4	3
4	A	358	PX4	O5-C8-C7	4.29	120.92	108.43	9	6
4	A	423	PX4	O5-C8-C7	4.29	120.92	108.43	1	7
4	A	384	PX4	O7-C7-C8	4.29	123.93	108.40	6	5
4	A	331	PX4	P1-O3-C1	4.29	100.48	121.59	5	10
4	A	409	PX4	O7-C7-C8	4.29	123.93	108.40	8	6
4	A	421	PX4	P1-O3-C1	4.29	100.49	121.59	9	10
4	A	397	PX4	P1-O3-C1	4.28	100.50	121.59	1	10
4	A	339	PX4	C5-N1-C4	4.28	97.97	108.97	5	3
4	A	329	PX4	C8-C7-C6	4.28	101.67	111.79	5	8
4	A	370	PX4	C7-O7-C23	4.28	128.32	117.79	4	3
4	A	379	PX4	O7-C7-C8	4.27	123.88	108.40	2	9
4	A	381	PX4	C8-C7-C6	4.27	101.68	111.79	6	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	O7-C23-C24	4.27	120.71	111.50	11	8
4	A	371	PX4	P1-O3-C1	4.27	100.56	121.59	11	8
4	A	369	PX4	P1-O3-C1	4.27	100.57	121.59	8	9
4	A	348	PX4	O7-C23-O8	4.27	113.39	123.70	5	4
4	A	360	PX4	P1-O3-C1	4.27	100.58	121.59	9	11
4	A	394	PX4	C5-N1-C4	4.26	98.01	108.97	7	3
4	A	383	PX4	O5-C8-C7	4.26	120.84	108.43	11	6
4	A	400	PX4	P1-O3-C1	4.26	100.61	121.59	12	9
4	A	310	PX4	P1-O4-C6	4.26	96.70	121.68	2	10
4	A	345	PX4	P1-O3-C1	4.26	100.63	121.59	8	9
4	A	333	PX4	P1-O4-C6	4.26	96.73	121.68	4	9
4	A	336	PX4	O3-P1-O2	4.25	92.45	109.07	12	5
4	A	397	PX4	C5-N1-C4	4.25	98.04	108.97	3	3
4	A	429	PX4	O5-C9-O6	4.25	112.86	123.59	7	4
4	A	416	PX4	P1-O3-C1	4.25	100.66	121.59	3	10
4	A	379	PX4	P1-O3-C1	4.25	100.69	121.59	7	11
4	A	362	PX4	O4-P1-O2	4.24	125.65	109.07	11	5
4	A	394	PX4	P1-O3-C1	4.25	100.69	121.59	5	12
4	A	379	PX4	O4-P1-O2	4.24	125.65	109.07	2	2
4	A	370	PX4	P1-O3-C1	4.24	100.71	121.59	11	9
4	A	361	PX4	C4-N1-C3	4.24	98.07	108.97	7	2
4	A	329	PX4	O5-C8-C7	4.24	120.77	108.43	4	7
4	A	376	PX4	O5-C8-C7	4.24	120.77	108.43	4	7
4	A	406	PX4	C26-C25-C24	4.24	97.96	113.19	11	3
4	A	338	PX4	P1-O3-C1	4.23	100.76	121.59	2	11
4	A	426	PX4	C5-N1-C3	4.23	98.09	108.97	13	3
4	A	390	PX4	P1-O3-C1	4.23	100.78	121.59	6	11
4	A	408	PX4	O7-C23-C24	4.23	120.61	111.50	3	7
4	A	361	PX4	C5-N1-C3	4.23	119.84	108.97	8	6
4	A	415	PX4	C4-N1-C3	4.22	98.12	108.97	1	3
4	A	349	PX4	P1-O3-C1	4.21	100.87	121.59	11	13
4	A	393	PX4	P1-O3-C1	4.21	100.87	121.59	10	8
4	A	316	PX4	O5-C8-C7	4.21	120.68	108.43	3	10
4	A	343	PX4	O7-C23-C24	4.21	120.57	111.50	13	9
4	A	347	PX4	O7-C23-C24	4.21	120.57	111.50	7	6
4	A	322	PX4	O7-C23-C24	4.20	120.56	111.50	13	8
4	A	334	PX4	O7-C23-C24	4.21	120.56	111.50	14	8
4	A	363	PX4	C8-C7-C6	4.21	101.84	111.79	5	8
4	A	369	PX4	O1-P1-O2	4.20	133.01	112.24	13	9
4	A	387	PX4	O5-C9-C10	4.20	125.09	111.91	9	4
4	A	314	PX4	P1-O4-C6	4.20	97.05	121.68	9	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	351	PX4	O7-C7-C8	4.20	123.61	108.40	13	7
4	A	403	PX4	C7-O7-C23	4.20	128.13	117.79	14	5
4	A	312	PX4	P1-O3-C1	4.20	100.93	121.59	3	8
4	A	389	PX4	P1-O3-C1	4.20	100.93	121.59	13	10
4	A	357	PX4	C7-O7-C23	4.19	107.47	117.79	5	4
4	A	307	PX4	O7-C23-C24	4.19	120.54	111.50	11	9
4	A	315	PX4	O7-C23-C24	4.19	120.54	111.50	8	9
4	A	430	PX4	O5-C9-C10	4.19	125.07	111.91	12	1
4	A	335	PX4	C5-N1-C4	4.19	98.20	108.97	12	3
4	A	347	PX4	O7-C7-C6	4.18	123.55	108.40	14	3
4	A	350	PX4	P1-O4-C6	4.18	97.15	121.68	9	6
4	A	379	PX4	O1-P1-O2	4.18	132.92	112.24	13	8
4	A	412	PX4	P1-O3-C1	4.18	101.00	121.59	14	11
4	A	417	PX4	C5-N1-C4	4.18	119.73	108.97	8	3
4	A	426	PX4	O5-C8-C7	4.18	120.61	108.43	6	7
4	A	347	PX4	C5-N1-C4	4.18	119.72	108.97	10	3
4	A	358	PX4	C8-C7-C6	4.18	101.91	111.79	14	9
4	A	405	PX4	C5-N1-C3	4.18	98.23	108.97	13	3
4	A	418	PX4	C7-O7-C23	4.18	128.08	117.79	4	3
4	A	361	PX4	O7-C23-C24	4.18	120.50	111.50	1	10
4	A	342	PX4	P1-O3-C1	4.17	101.04	121.59	8	10
4	A	323	PX4	P1-O3-C1	4.17	101.05	121.59	13	10
4	A	376	PX4	P1-O3-C1	4.17	101.04	121.59	9	11
4	A	379	PX4	C25-C24-C23	4.17	98.44	113.62	12	4
4	A	402	PX4	O7-C7-C6	4.17	123.50	108.40	12	7
4	A	354	PX4	O5-C8-C7	4.17	120.57	108.43	7	6
4	A	336	PX4	O7-C23-C24	4.17	120.48	111.50	1	11
4	A	390	PX4	O7-C23-C24	4.17	120.48	111.50	6	8
4	A	358	PX4	P1-O3-C1	4.17	101.08	121.59	13	12
4	A	402	PX4	C8-O5-C9	4.17	132.54	117.12	1	2
4	A	389	PX4	O7-C23-O8	4.16	113.64	123.70	10	7
4	A	426	PX4	C8-C7-C6	4.16	101.94	111.79	6	9
4	A	359	PX4	C7-O7-C23	4.16	128.04	117.79	2	7
4	A	314	PX4	C4-N1-C3	4.16	98.28	108.97	4	4
4	A	351	PX4	C5-N1-C3	4.16	98.28	108.97	2	3
4	A	362	PX4	O5-C8-C7	4.16	120.54	108.43	13	4
4	A	430	PX4	O5-C9-O6	4.16	113.10	123.59	11	6
4	A	405	PX4	C8-C7-C6	4.15	101.96	111.79	11	8
4	A	412	PX4	O7-C23-O8	4.15	113.67	123.70	13	4
4	A	399	PX4	O5-C9-O6	4.15	113.12	123.59	5	2
4	A	401	PX4	O5-C9-C10	4.15	124.93	111.91	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	320	PX4	P1-O4-C6	4.15	97.36	121.68	9	9
4	A	339	PX4	O3-P1-O2	4.15	92.86	109.07	14	6
4	A	376	PX4	O1-P1-O2	4.15	132.74	112.24	13	8
4	A	428	PX4	P1-O4-C6	4.15	97.37	121.68	11	10
4	A	310	PX4	C4-N1-C3	4.14	98.32	108.97	8	4
4	A	348	PX4	C4-N1-C3	4.14	98.32	108.97	5	3
4	A	427	PX4	P1-O4-C6	4.14	97.40	121.68	6	13
4	A	428	PX4	C5-N1-C3	4.14	98.34	108.97	4	2
4	A	428	PX4	O1-P1-O3	4.13	88.55	107.75	5	3
4	A	338	PX4	O7-C23-C24	4.13	120.40	111.50	6	8
4	A	326	PX4	O5-C9-C10	4.13	124.86	111.91	7	6
4	A	349	PX4	C31-C30-C29	4.13	93.46	114.42	9	2
4	A	377	PX4	O5-C8-C7	4.13	120.44	108.43	7	8
4	A	310	PX4	P1-O3-C1	4.12	101.29	121.59	11	11
4	A	369	PX4	O3-P1-O2	4.12	92.96	109.07	6	5
4	A	403	PX4	C5-N1-C3	4.12	98.37	108.97	3	7
4	A	383	PX4	C8-C7-C6	4.12	102.04	111.79	13	10
4	A	392	PX4	P1-O4-C6	4.12	97.52	121.68	9	10
4	A	424	PX4	O7-C23-O8	4.12	113.74	123.70	1	3
4	A	413	PX4	O1-P1-O4	4.12	126.87	107.75	8	4
4	A	419	PX4	C5-N1-C4	4.12	98.39	108.97	8	3
4	A	339	PX4	O4-P1-O2	4.12	125.15	109.07	14	3
4	A	351	PX4	P1-O3-C1	4.11	101.33	121.59	9	11
4	A	392	PX4	C4-N1-C3	4.11	98.39	108.97	7	2
4	A	339	PX4	C8-C7-C6	4.11	102.06	111.79	6	8
4	A	365	PX4	C5-N1-C3	4.11	98.41	108.97	14	3
4	A	373	PX4	C8-C7-C6	4.11	102.07	111.79	5	9
4	A	331	PX4	C8-C7-C6	4.10	102.08	111.79	9	8
4	A	417	PX4	C4-N1-C3	4.10	98.42	108.97	14	7
4	A	333	PX4	C25-C24-C23	4.10	98.70	113.62	2	3
4	A	362	PX4	O7-C7-C8	4.10	123.25	108.40	2	8
4	A	326	PX4	O5-C8-C7	4.10	120.36	108.43	9	4
4	A	315	PX4	P1-O3-C1	4.09	101.44	121.59	5	8
4	A	405	PX4	C8-O5-C9	4.09	101.96	117.12	13	3
4	A	332	PX4	P1-O3-C1	4.09	101.45	121.59	8	9
4	A	354	PX4	O7-C23-C24	4.09	120.32	111.50	7	6
4	A	363	PX4	O7-C7-C8	4.09	123.21	108.40	1	4
4	A	429	PX4	O7-C23-C24	4.09	120.32	111.50	1	7
4	A	352	PX4	C7-O7-C23	4.09	127.85	117.79	1	4
4	A	410	PX4	O7-C23-O8	4.09	113.83	123.70	5	8
4	A	312	PX4	O7-C7-C8	4.08	123.19	108.40	1	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	O1-P1-O2	4.08	132.43	112.24	14	4
4	A	398	PX4	P1-O3-C1	4.08	101.49	121.59	1	10
4	A	333	PX4	O7-C23-C24	4.08	120.30	111.50	1	6
4	A	404	PX4	O5-C8-C7	4.08	120.31	108.43	12	10
4	A	375	PX4	C4-N1-C3	4.08	98.48	108.97	12	2
4	A	384	PX4	O7-C23-C24	4.08	120.29	111.50	5	8
4	A	344	PX4	P1-O3-C1	4.08	101.52	121.59	12	10
4	A	421	PX4	O7-C23-O8	4.08	113.85	123.70	14	7
4	A	326	PX4	O7-C23-O8	4.07	113.86	123.70	2	5
4	A	388	PX4	O1-P1-O3	4.07	88.82	107.75	1	2
4	A	334	PX4	O1-P1-O2	4.07	132.36	112.24	5	8
4	A	357	PX4	P1-O3-C1	4.07	101.55	121.59	3	11
4	A	379	PX4	O1-P1-O3	4.07	88.84	107.75	13	5
4	A	407	PX4	O5-C8-C7	4.07	120.28	108.43	2	5
4	A	392	PX4	O7-C7-C6	4.07	123.13	108.40	9	7
4	A	341	PX4	P1-O3-C1	4.06	101.58	121.59	8	10
4	A	396	PX4	O7-C23-O8	4.07	113.88	123.70	9	3
4	A	321	PX4	O5-C9-O6	4.06	113.34	123.59	8	4
4	A	361	PX4	O7-C7-C8	4.06	123.11	108.40	13	5
4	A	396	PX4	O5-C8-C7	4.06	120.26	108.43	7	8
4	A	390	PX4	P1-O4-C6	4.06	97.87	121.68	5	10
4	A	400	PX4	C5-N1-C3	4.06	98.53	108.97	14	3
4	A	404	PX4	C5-N1-C4	4.06	98.53	108.97	6	4
4	A	308	PX4	O5-C9-O6	4.06	113.35	123.59	3	3
4	A	327	PX4	O7-C7-C8	4.06	123.10	108.40	13	5
4	A	392	PX4	O7-C23-C24	4.06	120.25	111.50	9	6
4	A	397	PX4	O5-C9-O6	4.06	113.35	123.59	8	6
4	A	415	PX4	O7-C23-C24	4.06	120.25	111.50	1	8
4	A	307	PX4	O7-C23-O8	4.06	113.90	123.70	12	8
4	A	424	PX4	P1-O3-C1	4.06	101.61	121.59	13	7
4	A	340	PX4	C12-C11-C10	4.06	98.61	113.19	11	2
4	A	391	PX4	C8-C7-C6	4.06	102.19	111.79	14	9
4	A	335	PX4	P1-O3-C1	4.05	101.63	121.59	2	10
4	A	353	PX4	O3-P1-O2	4.05	93.23	109.07	14	4
4	A	317	PX4	O5-C8-C7	4.05	96.64	108.43	4	8
4	A	340	PX4	O7-C7-C8	4.05	123.07	108.40	12	8
4	A	412	PX4	O7-C7-C6	4.05	123.07	108.40	5	7
4	A	358	PX4	C31-C30-C29	4.05	93.86	114.42	12	1
4	A	413	PX4	C5-N1-C3	4.05	119.39	108.97	6	2
4	A	336	PX4	O5-C8-C7	4.05	120.21	108.43	4	5
4	A	345	PX4	C8-C7-C6	4.05	102.22	111.79	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	403	PX4	O7-C23-C24	4.05	120.22	111.50	6	6
4	A	385	PX4	C5-N1-C4	4.05	98.57	108.97	6	5
4	A	390	PX4	O7-C7-C8	4.05	123.05	108.40	4	7
4	A	315	PX4	C8-C7-C6	4.04	102.23	111.79	14	7
4	A	386	PX4	P1-O3-C1	4.04	101.70	121.59	7	10
4	A	396	PX4	C5-N1-C3	4.04	98.59	108.97	13	3
4	A	417	PX4	O4-P1-O2	4.04	124.84	109.07	1	2
4	A	327	PX4	P1-O3-C1	4.03	101.72	121.59	14	13
4	A	320	PX4	P1-O3-C1	4.03	101.74	121.59	1	7
4	A	323	PX4	C26-C25-C24	4.03	98.70	113.19	14	1
4	A	365	PX4	O7-C23-O8	4.03	113.96	123.70	1	6
4	A	396	PX4	O7-C7-C8	4.03	123.00	108.40	10	5
4	A	411	PX4	O5-C9-O6	4.03	113.42	123.59	10	5
4	A	365	PX4	O7-C23-C24	4.03	120.19	111.50	2	7
4	A	307	PX4	O7-C7-C8	4.03	122.98	108.40	9	4
4	A	406	PX4	O4-P1-O2	4.03	124.80	109.07	11	3
4	A	413	PX4	C20-C19-C18	4.03	93.98	114.42	13	1
4	A	323	PX4	O5-C8-C7	4.02	120.14	108.43	2	8
4	A	321	PX4	P1-O4-C6	4.02	98.10	121.68	4	10
4	A	427	PX4	C1-C2-N1	4.02	129.20	115.78	4	5
4	A	346	PX4	C8-C7-C6	4.02	102.29	111.79	3	4
4	A	358	PX4	O7-C23-C24	4.02	120.16	111.50	1	4
4	A	407	PX4	O3-P1-O2	4.02	93.38	109.07	3	6
4	A	364	PX4	O5-C8-C7	4.01	120.11	108.43	5	9
4	A	387	PX4	P1-O4-C6	4.01	98.16	121.68	14	10
4	A	419	PX4	O7-C23-C24	4.01	120.15	111.50	3	7
4	A	394	PX4	C8-C7-C6	4.01	102.31	111.79	4	8
4	A	353	PX4	O5-C8-C7	4.01	120.09	108.43	1	5
4	A	429	PX4	O1-P1-O3	4.01	89.13	107.75	9	3
4	A	428	PX4	P1-O3-C1	4.01	101.87	121.59	13	11
4	A	404	PX4	O4-P1-O2	4.00	124.72	109.07	13	3
4	A	321	PX4	O7-C7-C6	4.00	122.89	108.40	2	4
4	A	400	PX4	C5-N1-C4	4.00	98.68	108.97	5	2
4	A	339	PX4	P1-O3-C1	4.00	101.90	121.59	5	13
4	A	378	PX4	O7-C23-O8	4.00	114.04	123.70	13	6
4	A	382	PX4	O7-C7-C6	4.00	122.88	108.40	12	6
4	A	342	PX4	O7-C23-O8	4.00	114.04	123.70	7	5
4	A	421	PX4	P1-O4-C6	3.99	98.26	121.68	8	8
4	A	321	PX4	P1-O3-C1	3.99	101.94	121.59	12	11
4	A	339	PX4	O5-C8-C7	3.99	120.05	108.43	3	6
4	A	360	PX4	C8-C7-C6	3.99	102.36	111.79	4	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	327	PX4	C1-C2-N1	3.98	129.09	115.78	4	3
4	A	346	PX4	P1-O4-C6	3.98	98.32	121.68	5	9
4	A	376	PX4	O7-C23-O8	3.98	114.08	123.70	5	3
4	A	385	PX4	C7-O7-C23	3.98	127.60	117.79	1	5
4	A	410	PX4	P1-O3-C1	3.98	101.97	121.59	6	10
4	A	344	PX4	C1-C2-N1	3.98	129.08	115.78	10	4
4	A	380	PX4	P1-O3-C1	3.98	101.98	121.59	11	13
4	A	385	PX4	O7-C23-C24	3.98	120.09	111.50	4	6
4	A	352	PX4	P1-O4-C6	3.98	98.33	121.68	9	6
4	A	352	PX4	C5-N1-C4	3.98	119.21	108.97	6	2
4	A	393	PX4	O7-C23-C24	3.98	120.08	111.50	2	9
4	A	413	PX4	O7-C23-C24	3.98	120.08	111.50	8	9
4	A	337	PX4	O4-P1-O2	3.98	124.61	109.07	10	2
4	A	360	PX4	O7-C23-O8	3.98	114.08	123.70	2	7
4	A	411	PX4	O7-C23-C24	3.98	120.08	111.50	8	3
4	A	368	PX4	O1-P1-O2	3.98	131.90	112.24	4	7
4	A	386	PX4	O5-C9-O6	3.98	113.56	123.59	13	4
4	A	315	PX4	O7-C7-C8	3.97	122.79	108.40	14	7
4	A	380	PX4	O1-P1-O3	3.97	89.29	107.75	7	4
4	A	354	PX4	O7-C23-O8	3.97	114.10	123.70	14	4
4	A	367	PX4	O5-C9-C10	3.97	124.38	111.91	11	7
4	A	411	PX4	C1-C2-N1	3.97	129.04	115.78	14	4
4	A	395	PX4	P1-O4-C6	3.97	98.39	121.68	4	10
4	A	426	PX4	C5-N1-C4	3.97	98.76	108.97	1	5
4	A	429	PX4	P1-O3-C1	3.97	102.05	121.59	10	12
4	A	381	PX4	O1-P1-O2	3.97	131.86	112.24	3	9
4	A	414	PX4	O7-C7-C6	3.97	122.77	108.40	9	5
4	A	313	PX4	O1-P1-O2	3.97	131.85	112.24	5	8
4	A	346	PX4	C4-N1-C3	3.96	98.78	108.97	6	5
4	A	382	PX4	O5-C9-C10	3.96	124.35	111.91	1	7
4	A	330	PX4	C7-O7-C23	3.96	127.55	117.79	5	4
4	A	399	PX4	O4-P1-O2	3.96	124.55	109.07	9	2
4	A	339	PX4	O5-C9-O6	3.96	113.59	123.59	13	8
4	A	372	PX4	O7-C7-C8	3.96	122.74	108.40	4	5
4	A	375	PX4	P1-O3-C1	3.96	102.09	121.59	1	10
4	A	407	PX4	P1-O3-C1	3.96	102.09	121.59	8	9
4	A	322	PX4	O7-C23-O8	3.96	114.14	123.70	7	5
4	A	395	PX4	C7-O7-C23	3.96	127.54	117.79	11	3
4	A	430	PX4	C7-O7-C23	3.96	108.04	117.79	5	5
4	A	421	PX4	O3-P1-O2	3.96	93.61	109.07	10	6
4	A	315	PX4	C7-O7-C23	3.95	108.06	117.79	14	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	C26-C25-C24	3.95	98.97	113.19	13	3
4	A	355	PX4	P1-O4-C6	3.95	98.49	121.68	14	7
4	A	425	PX4	O5-C8-C7	3.95	119.94	108.43	12	7
4	A	322	PX4	P1-O3-C1	3.95	102.13	121.59	6	11
4	A	402	PX4	O7-C7-C8	3.95	122.71	108.40	7	6
4	A	382	PX4	C8-C7-C6	3.95	102.44	111.79	12	10
4	A	325	PX4	O7-C23-C24	3.95	120.01	111.50	6	6
4	A	327	PX4	O7-C23-O8	3.95	114.16	123.70	9	6
4	A	392	PX4	C26-C25-C24	3.95	99.00	113.19	12	4
4	A	346	PX4	O5-C9-O6	3.95	113.63	123.59	13	2
4	A	371	PX4	C5-N1-C3	3.95	98.83	108.97	8	2
4	A	417	PX4	C1-C2-N1	3.95	128.95	115.78	3	5
4	A	310	PX4	O5-C9-C10	3.94	124.28	111.91	5	4
4	A	428	PX4	O7-C23-O8	3.94	114.17	123.70	1	6
4	A	339	PX4	O1-P1-O2	3.94	131.73	112.24	4	7
4	A	395	PX4	O7-C7-C6	3.94	122.67	108.40	2	6
4	A	331	PX4	O7-C23-O8	3.94	114.18	123.70	1	4
4	A	344	PX4	O7-C23-O8	3.94	114.18	123.70	12	6
4	A	369	PX4	O7-C7-C8	3.94	122.67	108.40	1	4
4	A	391	PX4	O4-P1-O2	3.94	124.47	109.07	9	4
4	A	389	PX4	C5-N1-C3	3.94	119.10	108.97	13	2
4	A	430	PX4	O5-C8-C7	3.94	119.90	108.43	5	9
4	A	372	PX4	C5-N1-C4	3.94	98.86	108.97	13	3
4	A	324	PX4	O7-C7-C6	3.93	122.64	108.40	11	7
4	A	405	PX4	O5-C8-C7	3.93	119.88	108.43	8	9
4	A	326	PX4	C8-C7-C6	3.93	102.49	111.79	5	8
4	A	327	PX4	C11-C10-C9	3.93	99.33	113.62	10	1
4	A	318	PX4	O5-C8-C7	3.93	119.87	108.43	4	7
4	A	414	PX4	P1-O4-C6	3.93	98.63	121.68	12	8
4	A	312	PX4	O7-C23-C24	3.93	119.96	111.50	2	6
4	A	359	PX4	O7-C23-C24	3.93	119.97	111.50	13	7
4	A	376	PX4	C5-N1-C3	3.93	119.07	108.97	4	3
4	A	398	PX4	O5-C9-O6	3.93	113.68	123.59	11	5
4	A	387	PX4	O5-C9-O6	3.92	113.69	123.59	13	3
4	A	367	PX4	P1-O4-C6	3.92	98.69	121.68	14	9
4	A	399	PX4	P1-O4-C6	3.92	98.71	121.68	6	11
4	A	383	PX4	C26-C25-C24	3.91	99.12	113.19	10	3
4	A	387	PX4	P1-O3-C1	3.91	102.32	121.59	11	7
4	A	426	PX4	O7-C7-C8	3.91	122.58	108.40	11	6
4	A	394	PX4	P1-O4-C6	3.91	98.74	121.68	2	12
4	A	363	PX4	C1-C2-N1	3.91	128.84	115.78	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	P1-O3-C1	3.91	102.33	121.59	2	12
4	A	368	PX4	O7-C7-C8	3.91	122.56	108.40	8	4
4	A	321	PX4	O1-P1-O2	3.91	131.56	112.24	7	6
4	A	308	PX4	O4-P1-O2	3.90	124.32	109.07	12	4
4	A	343	PX4	C5-N1-C4	3.90	98.93	108.97	10	3
4	A	359	PX4	O1-P1-O2	3.91	131.55	112.24	4	8
4	A	357	PX4	O7-C7-C8	3.90	122.53	108.40	12	7
4	A	348	PX4	P1-O3-C1	3.90	102.38	121.59	4	11
4	A	374	PX4	P1-O4-C6	3.90	98.80	121.68	1	12
4	A	386	PX4	O5-C8-C7	3.90	119.79	108.43	1	7
4	A	413	PX4	C4-N1-C3	3.90	98.94	108.97	8	4
4	A	324	PX4	O7-C23-C24	3.90	119.91	111.50	2	6
4	A	400	PX4	O7-C7-C6	3.90	122.52	108.40	2	8
4	A	318	PX4	O7-C7-C6	3.90	122.51	108.40	13	4
4	A	354	PX4	P1-O3-C1	3.90	102.40	121.59	9	10
4	A	358	PX4	C5-N1-C3	3.90	98.96	108.97	11	3
4	A	321	PX4	O3-P1-O2	3.89	93.85	109.07	6	7
4	A	413	PX4	P1-O4-C6	3.90	98.84	121.68	13	9
4	A	309	PX4	P1-O3-C1	3.89	102.42	121.59	13	11
4	A	325	PX4	O7-C7-C6	3.89	122.50	108.40	10	3
4	A	350	PX4	O7-C7-C8	3.89	122.50	108.40	14	5
4	A	364	PX4	P1-O3-C1	3.89	102.43	121.59	9	9
4	A	366	PX4	O1-P1-O2	3.89	131.49	112.24	2	11
4	A	405	PX4	P1-O4-C6	3.89	98.86	121.68	6	8
4	A	417	PX4	P1-O3-C1	3.89	102.43	121.59	4	13
4	A	349	PX4	C8-C7-C6	3.89	102.59	111.79	4	8
4	A	386	PX4	O5-C9-C10	3.89	124.11	111.91	4	2
4	A	328	PX4	O7-C23-C24	3.89	119.87	111.50	11	5
4	A	395	PX4	O1-P1-O2	3.88	131.44	112.24	5	8
4	A	401	PX4	C8-C7-C6	3.88	102.60	111.79	1	6
4	A	421	PX4	C5-N1-C4	3.88	98.99	108.97	5	4
4	A	313	PX4	P1-O3-C1	3.88	102.49	121.59	4	12
4	A	343	PX4	P1-O4-C6	3.88	98.93	121.68	9	11
4	A	393	PX4	C4-N1-C3	3.88	99.00	108.97	14	3
4	A	366	PX4	C7-O7-C23	3.88	127.34	117.79	10	6
4	A	406	PX4	O7-C23-O8	3.88	114.33	123.70	14	5
4	A	429	PX4	O5-C8-C7	3.88	119.72	108.43	10	7
4	A	362	PX4	C5-N1-C3	3.87	99.01	108.97	13	1
4	A	356	PX4	C7-O7-C23	3.87	127.33	117.79	11	3
4	A	381	PX4	O3-P1-O2	3.87	93.93	109.07	6	5
4	A	430	PX4	C1-C2-N1	3.87	128.70	115.78	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	310	PX4	O1-P1-O2	3.87	131.35	112.24	1	6
4	A	325	PX4	P1-O3-C1	3.87	102.56	121.59	5	7
4	A	389	PX4	P1-O4-C6	3.87	99.00	121.68	1	12
4	A	385	PX4	C5-N1-C3	3.87	99.04	108.97	13	5
4	A	354	PX4	O7-C7-C8	3.86	122.39	108.40	12	10
4	A	324	PX4	P1-O3-C1	3.86	102.61	121.59	9	11
4	A	349	PX4	C5-N1-C3	3.85	99.07	108.97	13	1
4	A	363	PX4	C20-C19-C18	3.85	94.86	114.42	5	2
4	A	385	PX4	P1-O3-C1	3.85	102.62	121.59	8	12
4	A	311	PX4	C7-O7-C23	3.85	127.27	117.79	14	5
4	A	382	PX4	P1-O3-C1	3.85	102.64	121.59	1	12
4	A	408	PX4	O7-C7-C8	3.85	122.33	108.40	7	4
4	A	325	PX4	O1-P1-O3	3.85	89.88	107.75	11	3
4	A	348	PX4	C5-N1-C3	3.85	118.86	108.97	8	1
4	A	337	PX4	O7-C23-C24	3.85	119.79	111.50	4	3
4	A	342	PX4	O5-C8-C7	3.84	119.62	108.43	4	7
4	A	358	PX4	P1-O4-C6	3.84	99.14	121.68	11	8
4	A	325	PX4	O1-P1-O4	3.84	125.59	107.75	8	1
4	A	397	PX4	C1-C2-N1	3.84	128.61	115.78	7	4
4	A	406	PX4	C1-C2-N1	3.84	128.61	115.78	14	6
4	A	345	PX4	P1-O4-C6	3.84	99.15	121.68	9	9
4	A	364	PX4	O1-P1-O3	3.84	89.91	107.75	6	2
4	A	389	PX4	O1-P1-O2	3.84	131.23	112.24	8	6
4	A	421	PX4	O1-P1-O4	3.84	125.58	107.75	13	2
4	A	425	PX4	O7-C7-C8	3.84	122.31	108.40	3	6
4	A	357	PX4	C20-C19-C18	3.84	94.94	114.42	8	2
4	A	411	PX4	P1-O4-C6	3.84	99.17	121.68	1	7
4	A	312	PX4	O4-P1-O2	3.84	94.08	109.07	9	2
4	A	368	PX4	O3-P1-O2	3.84	94.08	109.07	4	3
4	A	369	PX4	C5-N1-C4	3.84	99.11	108.97	12	5
4	A	378	PX4	C5-N1-C4	3.84	99.11	108.97	10	4
4	A	350	PX4	C8-C7-C6	3.83	102.72	111.79	13	7
4	A	430	PX4	O7-C7-C8	3.83	122.27	108.40	6	5
4	A	360	PX4	P1-O4-C6	3.83	99.23	121.68	7	7
4	A	384	PX4	P1-O4-C6	3.83	99.23	121.68	1	8
4	A	339	PX4	C34-C33-C32	3.82	95.01	114.42	2	1
4	A	357	PX4	O7-C23-O8	3.82	114.46	123.70	13	8
4	A	376	PX4	O1-P1-O3	3.82	89.98	107.75	13	3
4	A	356	PX4	O7-C7-C8	3.82	122.24	108.40	5	7
4	A	390	PX4	O5-C9-O6	3.82	113.94	123.59	12	6
4	A	415	PX4	O1-P1-O4	3.82	125.50	107.75	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	338	PX4	O7-C7-C8	3.82	122.22	108.40	5	4
4	A	376	PX4	O7-C23-C24	3.82	119.73	111.50	5	7
4	A	402	PX4	O7-C23-O8	3.82	114.48	123.70	5	4
4	A	320	PX4	C7-O7-C23	3.81	127.18	117.79	8	2
4	A	429	PX4	O5-C9-C10	3.81	123.88	111.91	9	3
4	A	401	PX4	C5-N1-C3	3.81	118.78	108.97	7	4
4	A	359	PX4	O7-C7-C8	3.81	122.20	108.40	6	5
4	A	318	PX4	O7-C23-O8	3.81	114.51	123.70	10	3
4	A	307	PX4	P1-O3-C1	3.80	102.86	121.59	10	8
4	A	424	PX4	O1-P1-O2	3.80	131.05	112.24	4	8
4	A	333	PX4	C7-O7-C23	3.80	108.43	117.79	10	6
4	A	307	PX4	P1-O4-C6	3.80	99.42	121.68	14	8
4	A	306	PX4	O7-C23-C24	3.79	119.68	111.50	9	8
4	A	388	PX4	C12-C11-C10	3.79	99.55	113.19	4	4
4	A	392	PX4	C5-N1-C3	3.79	118.73	108.97	3	4
4	A	333	PX4	O5-C9-O6	3.79	114.02	123.59	2	4
4	A	372	PX4	C5-N1-C3	3.79	99.22	108.97	11	1
4	A	377	PX4	C26-C25-C24	3.79	99.56	113.19	7	1
4	A	408	PX4	C11-C10-C9	3.79	99.83	113.62	13	3
4	A	316	PX4	P1-O3-C1	3.79	102.93	121.59	6	6
4	A	388	PX4	C7-O7-C23	3.79	127.12	117.79	7	3
4	A	407	PX4	O7-C23-O8	3.79	114.54	123.70	2	6
4	A	420	PX4	O7-C23-C24	3.79	119.67	111.50	9	9
4	A	325	PX4	O7-C23-O8	3.78	114.56	123.70	6	7
4	A	382	PX4	C26-C25-C24	3.78	99.59	113.19	4	3
4	A	404	PX4	P1-O4-C6	3.78	99.49	121.68	1	6
4	A	410	PX4	C5-N1-C3	3.78	99.25	108.97	1	3
4	A	308	PX4	O1-P1-O3	3.78	90.18	107.75	8	2
4	A	343	PX4	C4-N1-C3	3.78	118.70	108.97	4	3
4	A	389	PX4	C5-N1-C4	3.78	99.25	108.97	9	3
4	A	420	PX4	O5-C9-O6	3.78	114.05	123.59	14	2
4	A	413	PX4	O1-P1-O3	3.78	90.18	107.75	8	4
4	A	366	PX4	O7-C7-C8	3.78	122.08	108.40	3	7
4	A	392	PX4	O7-C7-C8	3.78	122.08	108.40	11	6
4	A	400	PX4	P1-O4-C6	3.78	99.52	121.68	6	12
4	A	392	PX4	C1-C2-N1	3.78	128.39	115.78	10	2
4	A	349	PX4	C7-O7-C23	3.77	127.08	117.79	1	7
4	A	361	PX4	C8-C7-C6	3.77	102.86	111.79	13	8
4	A	355	PX4	O4-P1-O2	3.77	123.80	109.07	2	2
4	A	382	PX4	O3-P1-O2	3.77	94.33	109.07	1	6
4	A	309	PX4	O7-C7-C6	3.77	122.05	108.40	9	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	355	PX4	P1-O3-C1	3.77	103.03	121.59	12	9
4	A	382	PX4	O1-P1-O2	3.77	130.88	112.24	6	7
4	A	311	PX4	O7-C23-C24	3.77	119.62	111.50	11	8
4	A	332	PX4	O7-C7-C8	3.77	122.03	108.40	9	10
4	A	344	PX4	C7-O7-C23	3.77	127.06	117.79	6	2
4	A	398	PX4	O5-C9-C10	3.77	123.73	111.91	2	6
4	A	425	PX4	C25-C24-C23	3.77	99.92	113.62	14	1
4	A	341	PX4	C12-C11-C10	3.76	99.66	113.19	8	2
4	A	354	PX4	P1-O4-C6	3.76	99.63	121.68	13	8
4	A	364	PX4	O7-C23-C24	3.76	119.61	111.50	13	7
4	A	415	PX4	C1-C2-N1	3.76	128.34	115.78	5	4
4	A	375	PX4	C1-C2-N1	3.76	128.33	115.78	2	6
4	A	320	PX4	O5-C8-C7	3.76	119.37	108.43	4	8
4	A	323	PX4	C5-N1-C4	3.76	99.31	108.97	1	4
4	A	423	PX4	C5-N1-C3	3.76	99.31	108.97	4	4
4	A	330	PX4	C8-C7-C6	3.76	102.90	111.79	1	7
4	A	390	PX4	O7-C23-O8	3.75	114.64	123.70	10	3
4	A	366	PX4	C11-C10-C9	3.75	99.99	113.62	7	4
4	A	417	PX4	O5-C8-C7	3.75	119.34	108.43	5	7
4	A	374	PX4	O5-C9-O6	3.75	114.14	123.59	3	1
4	A	387	PX4	O3-P1-O2	3.75	94.43	109.07	1	4
4	A	364	PX4	O3-P1-O2	3.74	94.44	109.07	2	4
4	A	416	PX4	O7-C23-O8	3.74	114.66	123.70	6	9
4	A	417	PX4	O3-P1-O2	3.74	94.44	109.07	7	4
4	A	360	PX4	C4-N1-C3	3.74	99.36	108.97	2	4
4	A	325	PX4	C5-N1-C4	3.74	99.36	108.97	4	4
4	A	339	PX4	O1-P1-O3	3.74	90.39	107.75	3	6
4	A	370	PX4	C4-N1-C3	3.74	99.36	108.97	13	4
4	A	380	PX4	O5-C9-C10	3.74	123.64	111.91	5	4
4	A	428	PX4	O3-P1-O2	3.74	94.46	109.07	5	5
4	A	308	PX4	P1-O3-C1	3.74	103.20	121.59	13	11
4	A	342	PX4	O5-C9-C10	3.74	123.63	111.91	6	3
4	A	418	PX4	O4-P1-O2	3.74	94.47	109.07	3	5
4	A	363	PX4	O7-C23-O8	3.73	114.68	123.70	11	7
4	A	368	PX4	C5-N1-C3	3.73	99.37	108.97	14	3
4	A	316	PX4	C4-N1-C3	3.73	118.57	108.97	3	2
4	A	344	PX4	O1-P1-O4	3.73	125.08	107.75	7	3
4	A	376	PX4	O5-C9-C10	3.73	123.62	111.91	5	5
4	A	347	PX4	P1-O3-C1	3.73	103.23	121.59	13	11
4	A	349	PX4	C5-N1-C4	3.73	99.39	108.97	12	4
4	A	416	PX4	O1-P1-O2	3.72	130.65	112.24	8	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	340	PX4	O7-C7-C6	3.72	121.88	108.40	1	3
4	A	417	PX4	O7-C23-C24	3.72	119.52	111.50	7	8
4	A	310	PX4	C7-O7-C23	3.72	126.95	117.79	7	3
4	A	317	PX4	C5-N1-C4	3.72	99.41	108.97	9	3
4	A	367	PX4	O7-C23-C24	3.72	119.51	111.50	2	6
4	A	382	PX4	C5-N1-C3	3.72	99.41	108.97	10	5
4	A	383	PX4	P1-O4-C6	3.72	99.88	121.68	14	9
4	A	416	PX4	C4-N1-C3	3.72	118.53	108.97	3	1
4	A	429	PX4	C8-C7-C6	3.72	102.99	111.79	3	9
4	A	388	PX4	O7-C7-C8	3.72	121.86	108.40	12	5
4	A	382	PX4	P1-O4-C6	3.71	99.90	121.68	2	7
4	A	425	PX4	P1-O3-C1	3.71	103.30	121.59	3	11
4	A	322	PX4	C5-N1-C4	3.71	99.43	108.97	13	4
4	A	352	PX4	O1-P1-O2	3.71	130.59	112.24	8	7
4	A	426	PX4	P1-O4-C6	3.71	99.91	121.68	14	8
4	A	310	PX4	C8-C7-C6	3.71	103.01	111.79	8	10
4	A	427	PX4	O7-C7-C8	3.71	121.84	108.40	10	6
4	A	376	PX4	C11-C10-C9	3.71	100.13	113.62	14	3
4	A	329	PX4	O7-C23-O8	3.71	114.74	123.70	11	6
4	A	400	PX4	C26-C25-C24	3.71	99.86	113.19	6	2
4	A	408	PX4	C7-O7-C23	3.71	126.92	117.79	6	5
4	A	408	PX4	O5-C8-C7	3.71	119.22	108.43	12	7
4	A	382	PX4	O7-C23-O8	3.70	114.75	123.70	2	5
4	A	337	PX4	O7-C7-C8	3.70	121.81	108.40	3	3
4	A	351	PX4	O7-C23-C24	3.70	119.48	111.50	6	4
4	A	425	PX4	C4-N1-C3	3.70	99.45	108.97	5	6
4	A	428	PX4	O5-C9-C10	3.70	123.53	111.91	1	5
4	A	382	PX4	O7-C7-C8	3.70	121.80	108.40	6	6
4	A	391	PX4	O1-P1-O2	3.70	130.54	112.24	10	11
4	A	319	PX4	P1-O3-C1	3.70	103.38	121.59	10	8
4	A	414	PX4	O8-C23-C24	3.70	109.30	123.73	7	1
4	A	421	PX4	C7-O7-C23	3.70	126.90	117.79	1	3
4	A	320	PX4	O1-P1-O2	3.70	130.52	112.24	10	10
4	A	379	PX4	C11-C10-C9	3.70	100.17	113.62	1	3
4	A	406	PX4	O7-C7-C8	3.70	121.79	108.40	4	3
4	A	382	PX4	C7-O7-C23	3.69	126.88	117.79	11	3
4	A	384	PX4	C1-C2-N1	3.69	128.11	115.78	8	3
4	A	319	PX4	O7-C23-C24	3.69	119.45	111.50	4	9
4	A	327	PX4	O5-C8-C7	3.69	119.17	108.43	11	9
4	A	349	PX4	O7-C7-C8	3.69	121.76	108.40	3	5
4	A	414	PX4	O3-P1-O2	3.69	94.65	109.07	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	333	PX4	C8-O5-C9	3.69	103.47	117.12	3	1
4	A	386	PX4	O1-P1-O2	3.69	130.46	112.24	13	7
4	A	398	PX4	C7-O7-C23	3.69	126.86	117.79	5	5
4	A	397	PX4	P1-O4-C6	3.68	100.08	121.68	1	5
4	A	309	PX4	O3-P1-O2	3.68	94.68	109.07	11	2
4	A	396	PX4	O7-C23-C24	3.68	119.44	111.50	6	6
4	A	334	PX4	O5-C9-C10	3.68	123.45	111.91	7	1
4	A	430	PX4	O4-P1-O2	3.68	123.44	109.07	14	2
4	A	368	PX4	C7-O7-C23	3.68	126.84	117.79	1	4
4	A	398	PX4	C12-C11-C10	3.68	99.97	113.19	14	1
4	A	345	PX4	O1-P1-O2	3.67	130.41	112.24	13	10
4	A	308	PX4	C12-C11-C10	3.67	99.99	113.19	5	1
4	A	340	PX4	C4-N1-C3	3.67	99.54	108.97	14	2
4	A	417	PX4	C25-C24-C23	3.67	100.28	113.62	13	3
4	A	315	PX4	O7-C23-O8	3.67	114.84	123.70	8	5
4	A	414	PX4	C5-N1-C4	3.67	99.55	108.97	7	3
4	A	416	PX4	O7-C7-C6	3.67	121.68	108.40	5	7
4	A	392	PX4	P1-O3-C1	3.67	103.54	121.59	10	9
4	A	310	PX4	C8-O5-C9	3.66	130.68	117.12	5	2
4	A	353	PX4	P1-O4-C6	3.66	100.20	121.68	12	7
4	A	405	PX4	O4-P1-O2	3.66	94.76	109.07	9	2
4	A	419	PX4	O7-C7-C6	3.66	121.67	108.40	7	6
4	A	321	PX4	O7-C23-O8	3.66	114.86	123.70	5	4
4	A	391	PX4	C5-N1-C3	3.66	99.57	108.97	11	2
4	A	359	PX4	O5-C8-C7	3.66	119.08	108.43	10	7
4	A	389	PX4	C4-N1-C3	3.66	99.57	108.97	12	5
4	A	403	PX4	P1-O4-C6	3.66	100.23	121.68	14	11
4	A	408	PX4	C5-N1-C4	3.65	99.58	108.97	13	2
4	A	355	PX4	O5-C8-C7	3.65	119.06	108.43	10	5
4	A	355	PX4	O3-P1-O2	3.65	94.80	109.07	10	3
4	A	403	PX4	O5-C8-C7	3.65	119.06	108.43	8	5
4	A	421	PX4	O4-P1-O2	3.65	123.33	109.07	11	4
4	A	414	PX4	P1-O3-C1	3.65	103.63	121.59	10	12
4	A	313	PX4	O4-P1-O2	3.65	123.32	109.07	10	3
4	A	392	PX4	O5-C9-O6	3.65	114.39	123.59	12	3
4	A	318	PX4	O7-C7-C8	3.65	121.60	108.40	8	4
4	A	426	PX4	O5-C9-C10	3.65	123.35	111.91	3	5
4	A	323	PX4	O5-C9-O6	3.64	114.40	123.59	8	4
4	A	409	PX4	P1-O4-C6	3.64	100.32	121.68	6	9
4	A	347	PX4	O5-C9-C10	3.64	123.33	111.91	14	5
4	A	338	PX4	P1-O4-C6	3.64	100.34	121.68	13	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	381	PX4	C5-N1-C4	3.64	118.33	108.97	8	5
4	A	386	PX4	O7-C7-C8	3.64	121.58	108.40	3	6
4	A	388	PX4	O7-C23-O8	3.64	114.90	123.70	3	5
4	A	423	PX4	O3-P1-O2	3.64	94.84	109.07	8	4
4	A	429	PX4	P1-O4-C6	3.64	100.33	121.68	12	9
4	A	313	PX4	P1-O4-C6	3.64	100.35	121.68	8	7
4	A	340	PX4	O5-C8-C7	3.64	119.02	108.43	9	7
4	A	354	PX4	C5-N1-C4	3.64	99.63	108.97	10	3
4	A	335	PX4	C26-C25-C24	3.63	100.13	113.19	11	2
4	A	398	PX4	O7-C23-O8	3.63	114.92	123.70	9	3
4	A	399	PX4	C5-N1-C4	3.63	118.32	108.97	13	4
4	A	370	PX4	C5-N1-C4	3.63	99.63	108.97	4	4
4	A	399	PX4	O7-C7-C6	3.63	121.56	108.40	3	8
4	A	420	PX4	C7-O7-C23	3.63	126.73	117.79	6	3
4	A	306	PX4	C15-C14-C13	3.62	96.04	114.42	1	2
4	A	395	PX4	O7-C23-C24	3.62	119.31	111.50	1	7
4	A	373	PX4	O3-P1-O2	3.62	94.92	109.07	8	4
4	A	425	PX4	C12-C11-C10	3.62	100.17	113.19	11	1
4	A	338	PX4	C1-C2-N1	3.62	127.87	115.78	5	4
4	A	363	PX4	O1-P1-O2	3.62	130.14	112.24	5	8
4	A	380	PX4	O7-C23-O8	3.62	114.95	123.70	13	5
4	A	408	PX4	O1-P1-O3	3.62	90.94	107.75	2	4
4	A	382	PX4	C4-N1-C3	3.62	118.28	108.97	3	3
4	A	374	PX4	O7-C23-O8	3.62	114.96	123.70	12	5
4	A	392	PX4	C8-C7-C6	3.61	103.24	111.79	10	9
4	A	379	PX4	O7-C23-C24	3.61	119.28	111.50	7	6
4	A	422	PX4	O7-C7-C6	3.61	121.47	108.40	4	6
4	A	341	PX4	O5-C9-O6	3.61	114.48	123.59	1	2
4	A	384	PX4	O1-P1-O2	3.61	130.08	112.24	3	5
4	A	414	PX4	O7-C23-O8	3.61	114.98	123.70	5	4
4	A	399	PX4	O5-C8-C7	3.61	118.93	108.43	5	6
4	A	429	PX4	O7-C7-C6	3.61	121.46	108.40	2	7
4	A	405	PX4	O7-C7-C6	3.61	121.46	108.40	12	3
4	A	368	PX4	P1-O3-C1	3.60	103.84	121.59	10	8
4	A	356	PX4	C11-C10-C9	3.60	100.52	113.62	9	2
4	A	372	PX4	P1-O3-C1	3.60	103.85	121.59	1	7
4	A	420	PX4	P1-O4-C6	3.60	100.55	121.68	3	7
4	A	427	PX4	O7-C23-O8	3.60	114.99	123.70	11	4
4	A	319	PX4	O5-C9-C10	3.60	123.21	111.91	11	3
4	A	357	PX4	O1-P1-O2	3.60	130.04	112.24	3	8
4	A	367	PX4	P1-O3-C1	3.60	103.86	121.59	14	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	O7-C23-O8	3.60	115.00	123.70	7	3
4	A	426	PX4	O4-P1-O2	3.60	123.13	109.07	13	4
4	A	340	PX4	P1-O4-C6	3.60	100.58	121.68	8	8
4	A	332	PX4	O4-P1-O2	3.60	123.12	109.07	7	7
4	A	387	PX4	C14-C13-C12	3.59	96.18	114.42	12	1
4	A	423	PX4	O7-C7-C6	3.59	121.42	108.40	13	6
4	A	336	PX4	C8-C7-C6	3.59	103.30	111.79	5	5
4	A	398	PX4	O1-P1-O4	3.59	124.42	107.75	7	4
4	A	379	PX4	O5-C8-C7	3.59	118.88	108.43	9	10
4	A	422	PX4	C4-N1-C3	3.59	99.74	108.97	12	5
4	A	355	PX4	C7-O7-C23	3.59	126.63	117.79	2	3
4	A	417	PX4	O7-C7-C6	3.59	121.40	108.40	3	6
4	A	355	PX4	C5-N1-C3	3.59	99.75	108.97	12	4
4	A	335	PX4	C7-O7-C23	3.59	126.62	117.79	13	4
4	A	308	PX4	O7-C7-C8	3.58	121.38	108.40	7	7
4	A	364	PX4	O7-C7-C6	3.58	121.38	108.40	12	6
4	A	366	PX4	O7-C23-O8	3.58	115.04	123.70	8	3
4	A	406	PX4	O5-C9-O6	3.58	114.55	123.59	4	3
4	A	410	PX4	O5-C8-C7	3.58	118.86	108.43	5	9
4	A	408	PX4	O7-C23-O8	3.58	115.05	123.70	5	3
4	A	333	PX4	O5-C9-C10	3.58	123.14	111.91	2	7
4	A	310	PX4	O5-C8-C7	3.58	118.85	108.43	5	6
4	A	348	PX4	O7-C7-C6	3.58	121.36	108.40	4	5
4	A	361	PX4	O4-P1-O2	3.58	123.06	109.07	14	6
4	A	322	PX4	C15-C14-C13	3.58	96.27	114.42	8	1
4	A	380	PX4	O1-P1-O2	3.58	129.92	112.24	3	9
4	A	412	PX4	P1-O4-C6	3.58	100.72	121.68	7	8
4	A	313	PX4	C5-N1-C3	3.57	118.16	108.97	1	4
4	A	318	PX4	O1-P1-O2	3.57	129.90	112.24	4	8
4	A	377	PX4	O3-P1-O2	3.57	95.11	109.07	10	5
4	A	306	PX4	C12-C11-C10	3.57	100.36	113.19	8	5
4	A	318	PX4	C26-C25-C24	3.57	100.36	113.19	2	3
4	A	369	PX4	C5-N1-C3	3.57	118.15	108.97	10	4
4	A	430	PX4	C4-N1-C3	3.57	99.79	108.97	7	4
4	A	341	PX4	C5-N1-C4	3.57	99.80	108.97	14	2
4	A	326	PX4	P1-O4-C6	3.57	100.76	121.68	7	9
4	A	388	PX4	P1-O4-C6	3.57	100.76	121.68	4	9
4	A	348	PX4	C13-C12-C11	3.56	96.33	114.42	13	3
4	A	415	PX4	O5-C8-C7	3.57	118.81	108.43	6	6
4	A	377	PX4	P1-O4-C6	3.56	100.78	121.68	9	11
4	A	358	PX4	O7-C7-C8	3.56	121.30	108.40	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	398	PX4	O1-P1-O2	3.56	129.85	112.24	4	7
4	A	350	PX4	O7-C23-O8	3.56	115.10	123.70	14	3
4	A	381	PX4	C5-N1-C3	3.56	99.82	108.97	8	5
4	A	420	PX4	O5-C9-C10	3.56	123.08	111.91	7	5
4	A	306	PX4	O7-C23-O8	3.56	115.10	123.70	9	8
4	A	317	PX4	C4-N1-C3	3.56	99.82	108.97	8	3
4	A	322	PX4	O3-P1-O2	3.56	95.16	109.07	14	5
4	A	388	PX4	C5-N1-C3	3.56	118.12	108.97	8	4
4	A	395	PX4	O5-C8-C7	3.56	118.80	108.43	14	5
4	A	409	PX4	O5-C9-O6	3.56	114.61	123.59	2	3
4	A	308	PX4	C26-C25-C24	3.56	100.41	113.19	5	4
4	A	325	PX4	C5-N1-C2	3.56	95.37	109.92	1	2
4	A	352	PX4	O7-C7-C8	3.56	121.28	108.40	3	5
4	A	398	PX4	P1-O4-C6	3.56	100.83	121.68	2	7
4	A	306	PX4	O7-C7-C8	3.55	121.26	108.40	2	6
4	A	353	PX4	C5-N1-C3	3.55	99.84	108.97	2	6
4	A	375	PX4	C26-C25-C24	3.55	100.43	113.19	14	5
4	A	399	PX4	C5-N1-C3	3.55	99.85	108.97	9	5
4	A	429	PX4	O4-P1-O2	3.55	122.94	109.07	3	5
4	A	430	PX4	P1-O3-C1	3.55	104.12	121.59	6	12
4	A	384	PX4	C8-O5-C9	3.55	103.99	117.12	3	1
4	A	416	PX4	C7-O7-C23	3.55	109.06	117.79	10	6
4	A	308	PX4	C5-N1-C3	3.54	99.86	108.97	12	3
4	A	375	PX4	C20-C19-C18	3.54	96.43	114.42	3	2
4	A	386	PX4	O7-C7-C6	3.54	121.23	108.40	12	5
4	A	388	PX4	P1-O3-C1	3.54	104.14	121.59	1	11
4	A	409	PX4	O7-C23-O8	3.55	115.13	123.70	3	6
4	A	308	PX4	O7-C23-O8	3.54	115.14	123.70	12	5
4	A	367	PX4	O5-C9-O6	3.54	114.65	123.59	7	6
4	A	409	PX4	O7-C23-C24	3.54	119.14	111.50	8	7
4	A	426	PX4	P1-O3-C1	3.54	104.15	121.59	6	12
4	A	315	PX4	O1-P1-O2	3.54	129.74	112.24	10	6
4	A	336	PX4	P1-O4-C6	3.54	100.93	121.68	14	7
4	A	318	PX4	C3-N1-C2	3.54	124.39	109.92	7	2
4	A	361	PX4	P1-O4-C6	3.54	100.94	121.68	13	9
4	A	393	PX4	O1-P1-O2	3.54	129.72	112.24	14	6
4	A	399	PX4	O1-P1-O2	3.54	129.72	112.24	5	7
4	A	311	PX4	O7-C7-C8	3.53	121.20	108.40	11	12
4	A	344	PX4	P1-O4-C6	3.53	100.95	121.68	3	9
4	A	378	PX4	O3-P1-O2	3.53	95.26	109.07	8	2
4	A	420	PX4	O3-P1-O2	3.53	95.26	109.07	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	O7-C23-C24	3.53	119.11	111.50	6	6
4	A	345	PX4	C4-N1-C3	3.53	99.90	108.97	8	3
4	A	349	PX4	C1-C2-N1	3.53	127.57	115.78	7	2
4	A	317	PX4	O7-C7-C8	3.53	121.18	108.40	11	7
4	A	359	PX4	O7-C23-O8	3.53	115.17	123.70	2	2
4	A	335	PX4	C1-C2-N1	3.53	127.56	115.78	7	5
4	A	419	PX4	C15-C14-C13	3.53	96.51	114.42	6	1
4	A	378	PX4	O1-P1-O2	3.53	129.67	112.24	7	9
4	A	406	PX4	O1-P1-O2	3.53	129.67	112.24	4	8
4	A	307	PX4	C19-C18-C17	3.53	96.53	114.42	7	1
4	A	425	PX4	C5-N1-C3	3.52	99.91	108.97	8	4
4	A	326	PX4	O5-C9-O6	3.52	114.70	123.59	9	6
4	A	348	PX4	C8-O5-C9	3.52	104.08	117.12	8	3
4	A	381	PX4	P1-O3-C1	3.52	104.25	121.59	12	12
4	A	319	PX4	O1-P1-O2	3.52	129.64	112.24	5	9
4	A	377	PX4	C4-N1-C3	3.52	99.92	108.97	6	6
4	A	318	PX4	C18-C17-C16	3.52	96.56	114.42	6	2
4	A	325	PX4	C34-C33-C32	3.52	96.57	114.42	13	2
4	A	358	PX4	O1-P1-O2	3.52	129.63	112.24	12	8
4	A	378	PX4	O5-C8-C7	3.52	118.67	108.43	12	8
4	A	320	PX4	C19-C18-C17	3.52	96.58	114.42	8	2
4	A	378	PX4	O5-C9-O6	3.52	114.72	123.59	2	5
4	A	391	PX4	C7-O7-C23	3.52	126.45	117.79	2	4
4	A	375	PX4	O5-C9-O6	3.51	114.72	123.59	4	5
4	A	407	PX4	P1-O4-C6	3.51	101.07	121.68	12	10
4	A	390	PX4	C4-N1-C3	3.51	99.95	108.97	1	5
4	A	420	PX4	O1-P1-O3	3.51	91.44	107.75	10	6
4	A	373	PX4	P1-O3-C1	3.51	104.31	121.59	12	10
4	A	320	PX4	O3-P1-O2	3.51	95.36	109.07	6	2
4	A	374	PX4	O7-C23-C24	3.51	119.06	111.50	7	5
4	A	387	PX4	C11-C10-C9	3.51	126.38	113.62	9	2
4	A	332	PX4	C11-C10-C9	3.50	100.88	113.62	13	1
4	A	340	PX4	C33-C32-C31	3.50	96.64	114.42	2	2
4	A	341	PX4	P1-O4-C6	3.50	101.14	121.68	9	8
4	A	307	PX4	C7-O7-C23	3.50	109.17	117.79	3	2
4	A	365	PX4	O1-P1-O2	3.50	129.55	112.24	14	7
4	A	395	PX4	C20-C19-C18	3.50	96.65	114.42	13	4
4	A	334	PX4	O7-C23-O8	3.50	115.25	123.70	2	4
4	A	360	PX4	O5-C9-O6	3.50	114.76	123.59	8	5
4	A	360	PX4	C5-N1-C3	3.50	99.98	108.97	14	1
4	A	421	PX4	O7-C7-C6	3.50	121.06	108.40	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	424	PX4	C4-N1-C3	3.50	117.96	108.97	14	3
4	A	342	PX4	C7-O7-C23	3.49	126.39	117.79	8	4
4	A	356	PX4	O5-C8-C7	3.49	118.60	108.43	6	7
4	A	381	PX4	O7-C7-C6	3.49	121.04	108.40	11	4
4	A	385	PX4	P1-O4-C6	3.49	101.21	121.68	12	11
4	A	403	PX4	O5-C9-C10	3.49	122.86	111.91	5	4
4	A	337	PX4	P1-O4-C6	3.49	101.22	121.68	3	9
4	A	357	PX4	P1-O4-C6	3.49	101.22	121.68	12	10
4	A	416	PX4	C12-C11-C10	3.49	100.64	113.19	11	3
4	A	332	PX4	P1-O4-C6	3.49	101.23	121.68	11	10
4	A	368	PX4	O1-P1-O4	3.48	123.92	107.75	11	3
4	A	373	PX4	O1-P1-O2	3.48	129.46	112.24	2	7
4	A	390	PX4	O5-C8-C7	3.48	118.57	108.43	3	9
4	A	421	PX4	O7-C7-C8	3.48	121.02	108.40	4	3
4	A	315	PX4	O7-C7-C6	3.48	121.01	108.40	7	6
4	A	323	PX4	C32-C31-C30	3.48	96.75	114.42	10	2
4	A	365	PX4	P1-O4-C6	3.48	101.26	121.68	5	10
4	A	367	PX4	O3-P1-O2	3.48	95.46	109.07	14	2
4	A	322	PX4	C26-C25-C24	3.48	100.68	113.19	8	3
4	A	422	PX4	O5-C9-C10	3.48	122.83	111.91	10	5
4	A	341	PX4	O5-C8-C7	3.48	118.56	108.43	11	6
4	A	430	PX4	C20-C19-C18	3.48	96.76	114.42	3	1
4	A	388	PX4	C4-N1-C3	3.48	100.03	108.97	2	3
4	A	402	PX4	C5-N1-C4	3.48	100.03	108.97	11	3
4	A	382	PX4	C11-C10-C9	3.47	126.26	113.62	2	2
4	A	430	PX4	P1-O4-C6	3.47	101.30	121.68	14	11
4	A	308	PX4	O1-P1-O4	3.47	123.86	107.75	2	5
4	A	309	PX4	O7-C23-O8	3.47	115.32	123.70	7	7
4	A	356	PX4	P1-O4-C6	3.47	101.34	121.68	6	11
4	A	415	PX4	P1-O4-C6	3.47	101.34	121.68	12	6
4	A	317	PX4	O3-P1-O2	3.47	95.52	109.07	3	2
4	A	334	PX4	C7-O7-C23	3.46	109.26	117.79	5	3
4	A	337	PX4	C1-C2-N1	3.46	127.34	115.78	8	4
4	A	338	PX4	C12-C11-C10	3.46	100.74	113.19	11	3
4	A	396	PX4	C1-C2-N1	3.46	127.35	115.78	14	1
4	A	335	PX4	O7-C7-C8	3.46	120.94	108.40	12	8
4	A	378	PX4	C12-C11-C10	3.46	100.74	113.19	2	2
4	A	396	PX4	C5-N1-C4	3.46	100.07	108.97	7	2
4	A	308	PX4	C5-N1-C4	3.46	100.08	108.97	10	4
4	A	319	PX4	C5-N1-C3	3.46	117.87	108.97	8	4
4	A	348	PX4	P1-O4-C6	3.46	101.38	121.68	13	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	350	PX4	P1-O3-C1	3.46	104.55	121.59	5	10
4	A	308	PX4	P1-O4-C6	3.46	101.40	121.68	7	9
4	A	324	PX4	C1-C2-N1	3.46	127.33	115.78	14	2
4	A	321	PX4	O3-C1-C2	3.46	127.34	109.16	5	1
4	A	416	PX4	O5-C9-C10	3.46	122.76	111.91	7	3
4	A	314	PX4	O7-C23-O8	3.46	115.35	123.70	1	3
4	A	334	PX4	C4-N1-C3	3.46	117.86	108.97	1	4
4	A	420	PX4	O1-P1-O2	3.46	129.32	112.24	9	10
4	A	324	PX4	P1-O4-C6	3.45	101.43	121.68	10	7
4	A	351	PX4	P1-O4-C6	3.45	101.43	121.68	12	6
4	A	321	PX4	O1-P1-O3	3.45	91.71	107.75	3	6
4	A	398	PX4	O4-P1-O2	3.45	95.58	109.07	1	4
4	A	352	PX4	C1-C2-N1	3.45	127.30	115.78	3	4
4	A	318	PX4	P1-O4-C6	3.45	101.46	121.68	1	7
4	A	370	PX4	O5-C9-C10	3.45	122.73	111.91	4	2
4	A	405	PX4	P1-O3-C1	3.45	104.61	121.59	9	8
4	A	409	PX4	O5-C9-C10	3.45	122.73	111.91	5	4
4	A	427	PX4	O4-P1-O2	3.45	122.53	109.07	5	2
4	A	330	PX4	O5-C9-C10	3.45	122.72	111.91	13	4
4	A	371	PX4	C7-O7-C23	3.44	126.27	117.79	8	5
4	A	323	PX4	C5-N1-C3	3.44	100.12	108.97	5	5
4	A	351	PX4	O3-P1-O2	3.44	95.62	109.07	8	3
4	A	354	PX4	O1-P1-O4	3.44	123.74	107.75	3	3
4	A	406	PX4	P1-O4-C6	3.44	101.49	121.68	13	8
4	A	381	PX4	C12-C11-C10	3.44	100.82	113.19	12	3
4	A	383	PX4	O7-C7-C8	3.44	120.86	108.40	13	4
4	A	396	PX4	P1-O3-C1	3.44	104.64	121.59	14	11
4	A	430	PX4	O7-C7-C6	3.44	120.87	108.40	11	4
4	A	325	PX4	C8-O5-C9	3.44	104.38	117.12	10	3
4	A	339	PX4	O7-C23-O8	3.44	115.39	123.70	11	5
4	A	344	PX4	O5-C9-O6	3.44	114.92	123.59	10	4
4	A	377	PX4	C5-N1-C3	3.44	100.14	108.97	10	5
4	A	366	PX4	C4-N1-C3	3.44	100.14	108.97	2	5
4	A	325	PX4	O1-P1-O2	3.43	129.22	112.24	14	7
4	A	355	PX4	C12-C11-C10	3.43	100.85	113.19	8	1
4	A	419	PX4	C1-C2-N1	3.43	127.25	115.78	10	3
4	A	322	PX4	O1-P1-O2	3.43	129.20	112.24	12	6
4	A	314	PX4	C28-C27-C26	3.43	97.01	114.42	12	1
4	A	331	PX4	O1-P1-O2	3.43	129.20	112.24	9	7
4	A	332	PX4	O7-C23-O8	3.43	115.41	123.70	13	7
4	A	351	PX4	C7-O7-C23	3.43	126.23	117.79	6	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	315	PX4	C4-N1-C3	3.43	100.16	108.97	8	4
4	A	355	PX4	C5-N1-C2	3.43	123.94	109.92	12	3
4	A	379	PX4	C4-N1-C3	3.43	100.16	108.97	9	3
4	A	332	PX4	C32-C31-C30	3.42	97.04	114.42	13	2
4	A	388	PX4	O5-C9-O6	3.42	114.95	123.59	8	4
4	A	424	PX4	O8-C23-C24	3.42	110.37	123.73	10	3
4	A	345	PX4	O5-C8-C7	3.42	118.39	108.43	3	4
4	A	316	PX4	C32-C31-C30	3.42	97.06	114.42	2	2
4	A	378	PX4	P1-O4-C6	3.42	101.62	121.68	7	9
4	A	306	PX4	O3-P1-O2	3.42	95.71	109.07	8	2
4	A	364	PX4	C7-O7-C23	3.42	109.38	117.79	11	3
4	A	398	PX4	O5-C8-C7	3.42	118.39	108.43	4	7
4	A	403	PX4	C1-C2-N1	3.42	127.19	115.78	3	2
4	A	403	PX4	C5-N1-C2	3.42	123.91	109.92	3	2
4	A	421	PX4	C11-C10-C9	3.42	101.19	113.62	9	3
4	A	373	PX4	C1-C2-N1	3.42	127.19	115.78	3	3
4	A	340	PX4	O5-C9-O6	3.42	114.97	123.59	4	7
4	A	382	PX4	O5-C9-O6	3.42	114.97	123.59	14	4
4	A	392	PX4	C30-C29-C28	3.42	97.09	114.42	11	1
4	A	393	PX4	O3-P1-O2	3.42	95.72	109.07	8	4
4	A	362	PX4	P1-O3-C1	3.41	104.78	121.59	7	7
4	A	381	PX4	O1-P1-O3	3.41	91.89	107.75	5	4
4	A	424	PX4	O5-C9-C10	3.41	122.62	111.91	11	1
4	A	405	PX4	C5-N1-C4	3.41	100.20	108.97	3	3
4	A	415	PX4	O5-C9-O6	3.41	114.99	123.59	12	2
4	A	343	PX4	C26-C25-C24	3.41	125.44	113.19	10	3
4	A	412	PX4	C5-N1-C3	3.41	117.74	108.97	10	3
4	A	310	PX4	C33-C32-C31	3.41	97.13	114.42	1	2
4	A	313	PX4	C19-C18-C17	3.40	97.14	114.42	4	2
4	A	329	PX4	O1-P1-O2	3.41	129.08	112.24	13	5
4	A	400	PX4	C25-C24-C23	3.40	101.25	113.62	11	2
4	A	306	PX4	P1-O4-C6	3.40	101.74	121.68	7	9
4	A	308	PX4	O1-P1-O2	3.40	129.05	112.24	8	8
4	A	310	PX4	C5-N1-C4	3.40	100.23	108.97	11	2
4	A	329	PX4	C11-C10-C9	3.40	101.26	113.62	4	2
4	A	363	PX4	O3-P1-O2	3.40	95.78	109.07	8	5
4	A	387	PX4	O4-P1-O2	3.40	122.35	109.07	2	6
4	A	388	PX4	O7-C7-C6	3.40	120.71	108.40	9	4
4	A	311	PX4	O5-C9-C10	3.40	122.57	111.91	2	5
4	A	326	PX4	O7-C7-C8	3.40	120.70	108.40	7	4
4	A	359	PX4	C13-C12-C11	3.40	97.18	114.42	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PX4	C8-O5-C9	3.40	104.55	117.12	11	3
4	A	423	PX4	C25-C24-C23	3.40	101.27	113.62	14	3
4	A	370	PX4	O7-C23-O8	3.39	115.50	123.70	6	1
4	A	373	PX4	O1-P1-O4	3.39	123.51	107.75	1	2
4	A	334	PX4	C5-N1-C4	3.39	100.26	108.97	3	4
4	A	373	PX4	C33-C32-C31	3.39	97.22	114.42	3	1
4	A	311	PX4	C26-C25-C24	3.39	125.37	113.19	13	3
4	A	338	PX4	C5-N1-C4	3.39	100.26	108.97	13	5
4	A	319	PX4	P1-O4-C6	3.39	101.82	121.68	14	8
4	A	346	PX4	O7-C23-O8	3.39	115.52	123.70	1	7
4	A	353	PX4	C17-C16-C15	3.39	97.24	114.42	12	3
4	A	425	PX4	O5-C9-C10	3.39	122.53	111.91	10	3
4	A	355	PX4	O7-C7-C8	3.38	120.65	108.40	1	7
4	A	406	PX4	P1-O3-C1	3.38	104.93	121.59	4	10
4	A	306	PX4	O1-P1-O2	3.38	128.96	112.24	13	7
4	A	311	PX4	O3-P1-O2	3.38	95.85	109.07	1	2
4	A	332	PX4	C1-C2-N1	3.38	127.07	115.78	14	7
4	A	334	PX4	P1-O3-C1	3.38	104.95	121.59	13	11
4	A	345	PX4	O5-C9-O6	3.38	115.06	123.59	5	3
4	A	363	PX4	P1-O4-C6	3.38	101.86	121.68	8	9
4	A	417	PX4	O5-C9-O6	3.38	115.06	123.59	7	4
4	A	367	PX4	C1-C2-N1	3.38	127.06	115.78	7	2
4	A	313	PX4	O7-C7-C6	3.38	120.63	108.40	1	6
4	A	363	PX4	P1-O3-C1	3.38	104.97	121.59	8	12
4	A	374	PX4	C25-C24-C23	3.38	101.34	113.62	5	1
4	A	386	PX4	C25-C24-C23	3.38	101.34	113.62	7	3
4	A	379	PX4	O5-C9-C10	3.38	122.50	111.91	5	5
4	A	343	PX4	O7-C7-C8	3.37	120.62	108.40	7	8
4	A	350	PX4	O7-C7-C6	3.37	120.62	108.40	7	9
4	A	329	PX4	C4-N1-C2	3.37	96.12	109.92	14	1
4	A	390	PX4	O1-P1-O2	3.37	128.91	112.24	14	3
4	A	356	PX4	O1-P1-O2	3.37	128.91	112.24	1	6
4	A	373	PX4	C25-C24-C23	3.37	101.36	113.62	2	4
4	A	407	PX4	O1-P1-O2	3.37	128.90	112.24	11	9
4	A	427	PX4	O7-C7-C6	3.37	120.60	108.40	1	2
4	A	360	PX4	C25-C24-C23	3.37	101.37	113.62	13	4
4	A	386	PX4	C1-C2-N1	3.37	127.03	115.78	11	4
4	A	418	PX4	C5-N1-C2	3.37	123.70	109.92	2	2
4	A	352	PX4	C31-C30-C29	3.37	97.33	114.42	11	2
4	A	412	PX4	C5-N1-C4	3.37	100.32	108.97	4	3
4	A	323	PX4	O7-C7-C8	3.36	120.58	108.40	7	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	325	PX4	C3-N1-C2	3.36	123.68	109.92	2	3
4	A	387	PX4	C4-N1-C3	3.36	100.33	108.97	14	2
4	A	323	PX4	O7-C23-O8	3.36	115.58	123.70	10	4
4	A	359	PX4	O3-P1-O2	3.36	95.93	109.07	8	3
4	A	408	PX4	O1-P1-O2	3.36	128.87	112.24	11	8
4	A	366	PX4	P1-O4-C6	3.36	101.97	121.68	9	5
4	A	383	PX4	C11-C10-C9	3.36	101.40	113.62	1	1
4	A	417	PX4	C7-O7-C23	3.36	126.07	117.79	14	5
4	A	306	PX4	O5-C8-C7	3.36	118.21	108.43	3	6
4	A	384	PX4	C26-C25-C24	3.36	101.12	113.19	5	5
4	A	330	PX4	C11-C10-C9	3.36	101.41	113.62	8	3
4	A	342	PX4	O7-C7-C8	3.36	120.56	108.40	10	5
4	A	362	PX4	O5-C9-C10	3.36	122.44	111.91	5	3
4	A	400	PX4	O7-C23-C24	3.36	118.74	111.50	14	5
4	A	349	PX4	O1-P1-O2	3.36	128.83	112.24	11	6
4	A	397	PX4	O5-C9-C10	3.36	122.44	111.91	10	4
4	A	418	PX4	O1-P1-O3	3.35	123.32	107.75	11	1
4	A	328	PX4	C7-O7-C23	3.35	126.05	117.79	12	3
4	A	306	PX4	O7-C7-C6	3.35	120.54	108.40	6	4
4	A	421	PX4	O1-P1-O3	3.35	92.18	107.75	8	3
4	A	336	PX4	P1-O3-C1	3.35	105.11	121.59	14	9
4	A	337	PX4	P1-O3-C1	3.35	105.12	121.59	14	10
4	A	401	PX4	C18-C17-C16	3.35	97.44	114.42	1	1
4	A	312	PX4	O1-P1-O2	3.34	128.77	112.24	5	9
4	A	319	PX4	C4-N1-C2	3.34	123.60	109.92	14	1
4	A	361	PX4	O7-C23-O8	3.34	115.62	123.70	5	4
4	A	403	PX4	O1-P1-O2	3.34	128.77	112.24	3	10
4	A	424	PX4	O7-C7-C8	3.34	120.51	108.40	4	6
4	A	317	PX4	C12-C11-C10	3.34	101.18	113.19	14	1
4	A	364	PX4	O1-P1-O2	3.34	128.76	112.24	1	6
4	A	364	PX4	O1-P1-O4	3.34	123.27	107.75	7	1
4	A	381	PX4	P1-O4-C6	3.34	102.08	121.68	3	8
4	A	318	PX4	P1-O3-C1	3.34	105.14	121.59	12	8
4	A	401	PX4	C5-N1-C4	3.34	117.56	108.97	14	4
4	A	407	PX4	C4-N1-C3	3.34	100.39	108.97	4	5
4	A	408	PX4	O4-P1-O2	3.34	122.12	109.07	8	4
4	A	412	PX4	C7-O7-C23	3.34	126.02	117.79	5	5
4	A	346	PX4	O7-C7-C8	3.34	120.49	108.40	10	9
4	A	379	PX4	C5-N1-C4	3.34	100.39	108.97	14	2
4	A	410	PX4	O5-C9-C10	3.34	122.38	111.91	13	2
4	A	310	PX4	C5-N1-C3	3.34	100.40	108.97	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PX4	O4-P1-O2	3.33	122.10	109.07	4	2
4	A	380	PX4	O7-C7-C8	3.33	120.47	108.40	5	5
4	A	404	PX4	O7-C7-C6	3.33	120.46	108.40	11	1
4	A	386	PX4	C4-N1-C3	3.33	117.53	108.97	6	3
4	A	341	PX4	C8-C7-C6	3.33	103.92	111.79	3	3
4	A	327	PX4	C5-N1-C3	3.33	100.42	108.97	14	4
4	A	359	PX4	C5-N1-C4	3.32	117.52	108.97	7	3
4	A	360	PX4	O7-C7-C8	3.33	120.44	108.40	11	5
4	A	386	PX4	C11-C10-C9	3.33	101.53	113.62	13	3
4	A	397	PX4	C34-C33-C32	3.33	97.54	114.42	7	1
4	A	421	PX4	O5-C9-C10	3.33	122.35	111.91	7	5
4	A	380	PX4	O3-P1-O2	3.32	96.08	109.07	8	7
4	A	380	PX4	O4-P1-O2	3.32	122.05	109.07	4	1
4	A	351	PX4	O7-C7-C6	3.32	120.43	108.40	9	3
4	A	366	PX4	O3-P1-O2	3.32	96.09	109.07	12	3
4	A	338	PX4	O7-C23-O8	3.32	115.68	123.70	2	7
4	A	387	PX4	C1-C2-N1	3.32	126.86	115.78	11	5
4	A	397	PX4	O1-P1-O2	3.32	128.65	112.24	3	6
4	A	342	PX4	O7-C7-C6	3.32	120.41	108.40	12	6
4	A	357	PX4	O5-C9-O6	3.32	115.22	123.59	1	2
4	A	428	PX4	C12-C11-C10	3.32	101.27	113.19	2	2
4	A	352	PX4	O3-P1-O2	3.31	96.12	109.07	6	5
4	A	342	PX4	P1-O4-C6	3.31	102.25	121.68	2	8
4	A	364	PX4	P1-O4-C6	3.31	102.25	121.68	5	5
4	A	370	PX4	C1-C2-N1	3.31	126.85	115.78	6	5
4	A	380	PX4	C33-C32-C31	3.31	97.60	114.42	11	2
4	A	393	PX4	C5-N1-C4	3.31	100.45	108.97	12	5
4	A	393	PX4	O7-C7-C8	3.31	120.40	108.40	11	3
4	A	429	PX4	O3-P1-O2	3.31	96.12	109.07	7	4
4	A	422	PX4	C12-C11-C10	3.31	101.28	113.19	10	1
4	A	313	PX4	C25-C24-C23	3.31	101.58	113.62	5	2
4	A	329	PX4	C30-C29-C28	3.31	97.62	114.42	3	1
4	A	378	PX4	O5-C9-C10	3.31	122.30	111.91	13	6
4	A	379	PX4	P1-O4-C6	3.31	102.27	121.68	6	10
4	A	322	PX4	C7-O7-C23	3.31	125.94	117.79	11	5
4	A	368	PX4	P1-O4-C6	3.31	102.28	121.68	9	8
4	A	311	PX4	C4-N1-C3	3.31	100.47	108.97	9	5
4	A	330	PX4	O5-C9-O6	3.31	115.24	123.59	14	5
4	A	342	PX4	C5-N1-C3	3.31	100.47	108.97	9	3
4	A	347	PX4	C12-C11-C10	3.31	101.30	113.19	14	5
4	A	371	PX4	O7-C23-O8	3.31	115.71	123.70	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	309	PX4	O5-C9-C10	3.31	122.28	111.91	8	3
4	A	333	PX4	O7-C7-C6	3.31	120.38	108.40	1	6
4	A	371	PX4	O5-C9-C10	3.31	122.29	111.91	10	4
4	A	321	PX4	C27-C26-C25	3.30	97.65	114.42	7	3
4	A	353	PX4	O1-P1-O2	3.30	128.58	112.24	1	9
4	A	377	PX4	C5-N1-C4	3.30	117.47	108.97	4	4
4	A	391	PX4	P1-O4-C6	3.30	102.30	121.68	2	8
4	A	312	PX4	P1-O4-C6	3.30	102.31	121.68	1	10
4	A	322	PX4	O7-C7-C6	3.30	120.34	108.40	14	9
4	A	337	PX4	O7-C7-C6	3.30	120.35	108.40	2	5
4	A	409	PX4	O1-P1-O4	3.30	123.07	107.75	7	2
4	A	427	PX4	C34-C33-C32	3.30	97.69	114.42	5	1
4	A	354	PX4	O3-P1-O2	3.30	96.19	109.07	2	3
4	A	333	PX4	C4-N1-C3	3.29	100.51	108.97	14	4
4	A	386	PX4	C5-N1-C2	3.29	96.44	109.92	6	2
4	A	376	PX4	C5-N1-C4	3.29	100.51	108.97	3	4
4	A	330	PX4	C29-C28-C27	3.29	97.72	114.42	3	2
4	A	383	PX4	O5-C9-O6	3.29	115.28	123.59	8	3
4	A	398	PX4	C1-C2-N1	3.29	126.77	115.78	10	1
4	A	391	PX4	C4-N1-C3	3.29	117.43	108.97	5	4
4	A	398	PX4	O1-P1-O3	3.29	92.47	107.75	12	3
4	A	423	PX4	P1-O4-C6	3.29	102.39	121.68	14	5
4	A	362	PX4	O7-C7-C6	3.29	120.31	108.40	7	5
4	A	415	PX4	O4-P1-O2	3.29	121.92	109.07	14	3
4	A	372	PX4	C11-C10-C9	3.29	101.67	113.62	10	2
4	A	344	PX4	O1-P1-O2	3.28	128.48	112.24	12	6
4	A	397	PX4	C7-O7-C23	3.29	125.88	117.79	11	2
4	A	403	PX4	C8-O5-C9	3.29	104.95	117.12	2	1
4	A	402	PX4	C7-O7-C23	3.28	125.88	117.79	2	3
4	A	411	PX4	C33-C32-C31	3.28	97.75	114.42	9	1
4	A	393	PX4	C27-C26-C25	3.28	97.75	114.42	14	2
4	A	320	PX4	O8-C23-C24	3.28	110.93	123.73	3	1
4	A	353	PX4	C4-N1-C3	3.28	100.54	108.97	3	3
4	A	384	PX4	C12-C11-C10	3.28	101.39	113.19	6	4
4	A	423	PX4	C26-C25-C24	3.28	101.39	113.19	8	3
4	A	316	PX4	P1-O4-C6	3.28	102.46	121.68	2	10
4	A	327	PX4	C4-N1-C3	3.28	117.40	108.97	8	3
4	A	327	PX4	C31-C30-C29	3.28	97.79	114.42	2	1
4	A	363	PX4	C5-N1-C4	3.28	100.55	108.97	1	6
4	A	384	PX4	C5-N1-C3	3.28	100.55	108.97	6	5
4	A	385	PX4	C12-C11-C10	3.28	101.41	113.19	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	P1-O4-C6	3.28	102.47	121.68	7	10
4	A	406	PX4	C4-N1-C3	3.28	100.55	108.97	8	3
4	A	388	PX4	C28-C27-C26	3.27	97.80	114.42	2	3
4	A	409	PX4	C5-N1-C4	3.27	100.56	108.97	14	3
4	A	424	PX4	O3-P1-O2	3.28	96.27	109.07	14	2
4	A	315	PX4	P1-O4-C6	3.27	102.49	121.68	9	9
4	A	336	PX4	O1-P1-O2	3.27	128.42	112.24	4	8
4	A	354	PX4	O1-P1-O2	3.27	128.42	112.24	12	12
4	A	309	PX4	O1-P1-O2	3.27	128.40	112.24	11	9
4	A	310	PX4	C12-C11-C10	3.27	101.44	113.19	5	1
4	A	409	PX4	O3-P1-O2	3.27	96.29	109.07	7	2
4	A	316	PX4	C31-C30-C29	3.27	97.84	114.42	4	1
4	A	372	PX4	C12-C11-C10	3.27	101.45	113.19	13	4
4	A	385	PX4	C3-N1-C2	3.27	96.55	109.92	8	1
4	A	388	PX4	O1-P1-O2	3.27	128.39	112.24	3	7
4	A	409	PX4	C7-O7-C23	3.27	125.83	117.79	8	3
4	A	338	PX4	O5-C9-O6	3.26	115.36	123.59	1	4
4	A	368	PX4	O7-C23-C24	3.26	118.53	111.50	10	3
4	A	373	PX4	O4-P1-O2	3.26	121.81	109.07	11	2
4	A	387	PX4	C7-O7-C23	3.26	125.82	117.79	3	9
4	A	395	PX4	C34-C33-C32	3.26	97.86	114.42	5	1
4	A	307	PX4	C1-C2-N1	3.26	126.67	115.78	8	4
4	A	314	PX4	O7-C7-C6	3.26	120.21	108.40	6	5
4	A	360	PX4	O1-P1-O2	3.26	128.36	112.24	14	7
4	A	360	PX4	O7-C7-C6	3.26	120.21	108.40	13	2
4	A	311	PX4	P1-O4-C6	3.26	102.57	121.68	14	5
4	A	317	PX4	O7-C7-C6	3.26	120.20	108.40	9	2
4	A	353	PX4	C28-C27-C26	3.26	97.88	114.42	9	4
4	A	355	PX4	O7-C23-O8	3.26	115.83	123.70	8	3
4	A	387	PX4	C29-C28-C27	3.26	97.89	114.42	1	2
4	A	387	PX4	C13-C12-C11	3.26	97.89	114.42	14	2
4	A	321	PX4	O7-C7-C8	3.26	120.19	108.40	5	7
4	A	369	PX4	C1-C2-N1	3.25	126.65	115.78	8	2
4	A	373	PX4	C12-C11-C10	3.26	101.49	113.19	11	3
4	A	422	PX4	C7-O7-C23	3.25	125.80	117.79	13	8
4	A	415	PX4	C7-O7-C23	3.25	125.80	117.79	12	1
4	A	357	PX4	C25-C24-C23	3.25	101.80	113.62	12	1
4	A	427	PX4	C5-N1-C4	3.25	100.61	108.97	13	4
4	A	311	PX4	O5-C9-O6	3.25	115.39	123.59	2	4
4	A	363	PX4	C30-C29-C28	3.25	97.93	114.42	7	2
4	A	376	PX4	O5-C9-O6	3.25	115.39	123.59	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PX4	C13-C12-C11	3.25	97.93	114.42	9	2
4	A	327	PX4	O5-C9-O6	3.25	115.40	123.59	10	5
4	A	365	PX4	O3-P1-O2	3.25	96.38	109.07	5	4
4	A	362	PX4	O3-P1-O2	3.25	96.39	109.07	11	7
4	A	319	PX4	O4-P1-O2	3.24	121.74	109.07	7	1
4	A	337	PX4	C25-C24-C23	3.24	101.82	113.62	9	2
4	A	356	PX4	C26-C25-C24	3.24	101.54	113.19	14	5
4	A	343	PX4	O7-C7-C6	3.24	120.13	108.40	14	5
4	A	391	PX4	O1-P1-O3	3.24	92.71	107.75	5	4
4	A	370	PX4	P1-O4-C6	3.24	102.70	121.68	2	9
4	A	325	PX4	C7-O7-C23	3.23	109.83	117.79	14	4
4	A	336	PX4	O1-P1-O3	3.24	92.72	107.75	7	3
4	A	363	PX4	C14-C13-C12	3.24	98.00	114.42	4	4
4	A	375	PX4	O7-C7-C6	3.24	120.12	108.40	8	4
4	A	430	PX4	C3-N1-C2	3.24	123.16	109.92	12	1
4	A	385	PX4	C11-C10-C9	3.23	101.86	113.62	5	1
4	A	413	PX4	O1-P1-O2	3.23	128.23	112.24	2	7
4	A	332	PX4	O5-C9-O6	3.23	115.43	123.59	2	2
4	A	427	PX4	O1-P1-O2	3.23	128.23	112.24	2	10
4	A	401	PX4	C33-C32-C31	3.23	98.01	114.42	6	1
4	A	333	PX4	C5-N1-C3	3.23	100.66	108.97	10	3
4	A	409	PX4	P1-O3-C1	3.23	105.67	121.59	3	11
4	A	396	PX4	C3-N1-C2	3.23	123.14	109.92	5	1
4	A	409	PX4	C17-C16-C15	3.23	98.02	114.42	6	2
4	A	346	PX4	C5-N1-C3	3.23	100.67	108.97	14	4
4	A	391	PX4	C25-C24-C23	3.23	101.87	113.62	12	1
4	A	395	PX4	C19-C18-C17	3.23	98.03	114.42	3	2
4	A	409	PX4	C11-C10-C9	3.23	101.88	113.62	1	1
4	A	352	PX4	O5-C9-O6	3.23	115.45	123.59	7	4
4	A	402	PX4	O1-P1-O2	3.23	128.19	112.24	2	6
4	A	411	PX4	O1-P1-O3	3.23	92.76	107.75	6	4
4	A	412	PX4	O1-P1-O2	3.23	128.19	112.24	5	11
4	A	374	PX4	C34-C33-C32	3.23	98.05	114.42	6	3
4	A	349	PX4	O7-C7-C6	3.22	120.07	108.40	10	5
4	A	394	PX4	O4-P1-O2	3.22	121.66	109.07	6	1
4	A	328	PX4	P1-O4-C6	3.22	102.78	121.68	8	10
4	A	336	PX4	O5-C9-O6	3.22	115.46	123.59	2	2
4	A	369	PX4	C16-C15-C14	3.22	98.08	114.42	7	2
4	A	393	PX4	C7-O7-C23	3.22	125.72	117.79	7	4
4	A	407	PX4	O7-C7-C6	3.22	120.06	108.40	13	9
4	A	335	PX4	O1-P1-O2	3.22	128.15	112.24	13	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	395	PX4	C1-C2-N1	3.22	126.53	115.78	4	5
4	A	414	PX4	C16-C15-C14	3.22	98.09	114.42	2	2
4	A	417	PX4	C15-C14-C13	3.22	98.09	114.42	14	1
4	A	426	PX4	O7-C7-C6	3.22	120.05	108.40	9	6
4	A	383	PX4	P1-O3-C1	3.21	105.76	121.59	10	10
4	A	408	PX4	O1-P1-O4	3.21	122.68	107.75	2	5
4	A	413	PX4	C5-N1-C4	3.22	100.71	108.97	2	2
4	A	347	PX4	O1-P1-O2	3.21	128.12	112.24	4	5
4	A	349	PX4	C11-C10-C9	3.21	101.94	113.62	8	2
4	A	410	PX4	C4-N1-C2	3.21	96.77	109.92	14	1
4	A	369	PX4	O5-C9-C10	3.21	121.99	111.91	6	4
4	A	377	PX4	C8-O5-C9	3.21	105.22	117.12	5	1
4	A	306	PX4	O5-C9-C10	3.21	121.98	111.91	8	2
4	A	320	PX4	C4-N1-C2	3.21	123.06	109.92	2	4
4	A	386	PX4	C3-N1-C2	3.21	96.77	109.92	2	1
4	A	391	PX4	C13-C12-C11	3.21	98.12	114.42	3	1
4	A	430	PX4	O7-C23-O8	3.21	115.94	123.70	3	5
4	A	331	PX4	P1-O4-C6	3.21	102.85	121.68	11	8
4	A	423	PX4	O5-C9-O6	3.21	115.49	123.59	13	5
4	A	427	PX4	O3-P1-O2	3.21	96.53	109.07	5	4
4	A	311	PX4	C15-C14-C13	3.21	98.14	114.42	13	1
4	A	321	PX4	O5-C9-C10	3.21	121.97	111.91	11	5
4	A	364	PX4	C4-N1-C3	3.21	100.73	108.97	8	7
4	A	373	PX4	O7-C23-O8	3.21	115.95	123.70	9	6
4	A	314	PX4	C5-N1-C4	3.20	100.74	108.97	2	6
4	A	329	PX4	O3-P1-O2	3.20	96.55	109.07	8	3
4	A	343	PX4	O5-C9-O6	3.20	115.51	123.59	7	4
4	A	375	PX4	C7-O7-C23	3.20	125.68	117.79	13	5
4	A	336	PX4	C5-N1-C4	3.20	100.74	108.97	5	2
4	A	349	PX4	C4-N1-C2	3.20	123.01	109.92	12	3
4	A	370	PX4	O3-P1-O2	3.20	96.56	109.07	12	1
4	A	309	PX4	C30-C29-C28	3.20	98.18	114.42	8	3
4	A	318	PX4	O5-C9-C10	3.20	121.95	111.91	3	3
4	A	326	PX4	C12-C11-C10	3.20	101.69	113.19	3	4
4	A	332	PX4	C7-O7-C23	3.20	109.92	117.79	4	4
4	A	372	PX4	C4-N1-C3	3.20	100.75	108.97	4	4
4	A	333	PX4	O7-C23-O8	3.20	115.97	123.70	7	4
4	A	373	PX4	O5-C9-O6	3.20	115.52	123.59	12	6
4	A	373	PX4	O7-C7-C6	3.20	119.98	108.40	6	6
4	A	419	PX4	P1-O4-C6	3.20	102.93	121.68	10	8
4	A	421	PX4	C27-C26-C25	3.20	98.19	114.42	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	423	PX4	O1-P1-O2	3.20	128.04	112.24	12	4
4	A	321	PX4	C5-N1-C4	3.20	100.76	108.97	13	3
4	A	375	PX4	C12-C11-C10	3.19	101.71	113.19	1	3
4	A	397	PX4	C11-C10-C9	3.19	102.00	113.62	13	3
4	A	417	PX4	O7-C23-O8	3.20	115.98	123.70	1	5
4	A	328	PX4	C11-C10-C9	3.19	125.23	113.62	4	2
4	A	344	PX4	C5-N1-C3	3.19	100.76	108.97	8	3
4	A	325	PX4	C4-N1-C2	3.19	96.86	109.92	13	1
4	A	329	PX4	P1-O4-C6	3.19	102.97	121.68	10	8
4	A	322	PX4	O7-C7-C8	3.19	119.95	108.40	9	5
4	A	349	PX4	P1-O4-C6	3.19	102.97	121.68	7	10
4	A	351	PX4	O1-P1-O4	3.19	122.56	107.75	8	2
4	A	390	PX4	O1-P1-O4	3.19	122.56	107.75	5	4
4	A	311	PX4	C12-C11-C10	3.19	101.73	113.19	4	2
4	A	348	PX4	C1-C2-N1	3.19	126.43	115.78	3	3
4	A	409	PX4	O1-P1-O2	3.19	128.01	112.24	13	7
4	A	378	PX4	C26-C25-C24	3.19	101.73	113.19	12	4
4	A	414	PX4	O5-C9-C10	3.19	121.92	111.91	7	5
4	A	366	PX4	C26-C25-C24	3.19	101.73	113.19	9	3
4	A	349	PX4	O5-C8-C7	3.19	117.71	108.43	7	9
4	A	401	PX4	C7-O7-C23	3.19	125.63	117.79	12	2
4	A	415	PX4	O7-C7-C6	3.19	119.94	108.40	2	7
4	A	320	PX4	C26-C25-C24	3.18	101.75	113.19	11	2
4	A	375	PX4	O1-P1-O2	3.18	127.98	112.24	8	10
4	A	319	PX4	O5-C9-O6	3.18	115.56	123.59	13	3
4	A	384	PX4	O7-C23-O8	3.18	116.01	123.70	8	4
4	A	399	PX4	O3-P1-O2	3.18	96.63	109.07	9	1
4	A	372	PX4	C7-O7-C23	3.18	109.97	117.79	6	4
4	A	402	PX4	C26-C25-C24	3.18	101.76	113.19	11	2
4	A	368	PX4	O7-C7-C6	3.18	119.91	108.40	5	5
4	A	429	PX4	C4-N1-C3	3.18	117.14	108.97	12	3
4	A	420	PX4	C5-N1-C2	3.17	122.90	109.92	14	3
4	A	425	PX4	C5-N1-C4	3.17	100.81	108.97	3	6
4	A	428	PX4	C4-N1-C2	3.17	96.93	109.92	12	2
4	A	367	PX4	O7-C7-C6	3.17	119.89	108.40	10	3
4	A	371	PX4	O5-C8-C7	3.17	117.67	108.43	4	6
4	A	328	PX4	C5-N1-C4	3.17	117.13	108.97	2	2
4	A	330	PX4	C5-N1-C3	3.17	100.82	108.97	13	3
4	A	385	PX4	C27-C26-C25	3.17	98.33	114.42	13	3
4	A	415	PX4	C29-C28-C27	3.17	98.33	114.42	13	2
4	A	375	PX4	P1-O4-C6	3.17	103.09	121.68	14	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	371	PX4	P1-O4-C6	3.17	103.10	121.68	9	4
4	A	374	PX4	O1-P1-O2	3.17	127.91	112.24	3	5
4	A	385	PX4	O3-P1-O2	3.17	96.69	109.07	12	2
4	A	389	PX4	C4-N1-C2	3.17	122.88	109.92	9	2
4	A	334	PX4	O7-C7-C8	3.17	119.86	108.40	14	5
4	A	356	PX4	O7-C7-C6	3.17	119.86	108.40	8	4
4	A	393	PX4	O4-P1-O2	3.17	121.44	109.07	5	4
4	A	420	PX4	O7-C23-O8	3.17	116.05	123.70	13	6
4	A	347	PX4	O7-C23-O8	3.16	116.06	123.70	6	6
4	A	353	PX4	P1-O3-C1	3.16	106.02	121.59	11	8
4	A	363	PX4	C8-O5-C9	3.16	105.40	117.12	13	1
4	A	384	PX4	C7-O7-C23	3.16	125.57	117.79	10	2
4	A	392	PX4	O7-C23-O8	3.16	116.07	123.70	11	5
4	A	393	PX4	P1-O4-C6	3.16	103.15	121.68	9	8
4	A	427	PX4	O5-C9-C10	3.16	121.83	111.91	3	1
4	A	408	PX4	O7-C7-C6	3.16	119.84	108.40	9	6
4	A	427	PX4	C4-N1-C3	3.16	100.85	108.97	3	3
4	A	415	PX4	C5-N1-C4	3.16	100.85	108.97	8	3
4	A	335	PX4	C4-N1-C3	3.16	100.86	108.97	14	5
4	A	343	PX4	C5-N1-C3	3.16	100.86	108.97	4	5
4	A	352	PX4	C5-N1-C3	3.16	100.86	108.97	6	4
4	A	380	PX4	C12-C11-C10	3.16	101.84	113.19	10	3
4	A	385	PX4	O7-C7-C8	3.16	119.83	108.40	5	5
4	A	337	PX4	C7-O7-C23	3.15	125.56	117.79	8	3
4	A	373	PX4	P1-O4-C6	3.15	103.19	121.68	14	11
4	A	361	PX4	P1-O3-C1	3.15	106.07	121.59	6	8
4	A	377	PX4	O7-C23-O8	3.15	116.08	123.70	11	1
4	A	387	PX4	O7-C23-C24	3.15	118.30	111.50	3	6
4	A	372	PX4	O4-P1-O2	3.15	121.38	109.07	3	2
4	A	381	PX4	C4-N1-C3	3.15	100.88	108.97	5	2
4	A	381	PX4	C7-O7-C23	3.15	125.54	117.79	3	4
4	A	399	PX4	C11-C10-C9	3.15	102.17	113.62	2	3
4	A	402	PX4	P1-O4-C6	3.15	103.23	121.68	13	8
4	A	402	PX4	C12-C11-C10	3.15	101.88	113.19	6	3
4	A	413	PX4	O4-P1-O2	3.15	121.37	109.07	6	5
4	A	424	PX4	O5-C9-O6	3.15	115.65	123.59	10	7
4	A	424	PX4	C5-N1-C3	3.15	117.07	108.97	12	2
4	A	335	PX4	P1-O4-C6	3.15	103.23	121.68	12	11
4	A	347	PX4	O3-P1-O2	3.15	96.77	109.07	11	2
4	A	383	PX4	O7-C23-O8	3.15	116.10	123.70	11	4
4	A	374	PX4	O7-C7-C8	3.14	119.79	108.40	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	377	PX4	C4-N1-C2	3.15	122.78	109.92	11	2
4	A	419	PX4	C4-N1-C3	3.14	100.89	108.97	13	2
4	A	426	PX4	C1-C2-N1	3.15	126.28	115.78	11	2
4	A	379	PX4	C1-C2-N1	3.14	126.28	115.78	6	4
4	A	378	PX4	O7-C7-C6	3.14	119.78	108.40	2	4
4	A	387	PX4	O1-P1-O2	3.14	127.78	112.24	13	6
4	A	314	PX4	C33-C32-C31	3.14	98.48	114.42	8	1
4	A	331	PX4	C1-C2-N1	3.14	126.27	115.78	9	2
4	A	351	PX4	O5-C9-C10	3.14	121.77	111.91	13	8
4	A	367	PX4	C4-N1-C3	3.14	100.89	108.97	10	4
4	A	388	PX4	C8-O5-C9	3.14	105.49	117.12	6	3
4	A	393	PX4	O7-C23-O8	3.14	116.11	123.70	3	1
4	A	394	PX4	C7-O7-C23	3.14	110.06	117.79	6	3
4	A	396	PX4	O1-P1-O2	3.14	127.77	112.24	5	7
4	A	402	PX4	O5-C9-C10	3.14	121.76	111.91	6	3
4	A	406	PX4	O7-C23-C24	3.14	118.27	111.50	8	3
4	A	335	PX4	O7-C7-C6	3.14	119.77	108.40	7	6
4	A	411	PX4	C34-C33-C32	3.14	98.48	114.42	12	2
4	A	427	PX4	C25-C24-C23	3.14	102.20	113.62	1	2
4	A	314	PX4	C20-C19-C18	3.14	98.51	114.42	2	2
4	A	328	PX4	C5-N1-C3	3.14	100.91	108.97	4	3
4	A	333	PX4	P1-O3-C1	3.13	106.16	121.59	2	8
4	A	411	PX4	O1-P1-O2	3.14	127.74	112.24	10	9
4	A	382	PX4	O4-P1-O2	3.13	121.31	109.07	7	2
4	A	400	PX4	O1-P1-O2	3.13	127.72	112.24	14	6
4	A	383	PX4	O5-C9-C10	3.13	121.73	111.91	8	3
4	A	403	PX4	O3-C1-C2	3.13	125.63	109.16	14	3
4	A	329	PX4	O5-C9-O6	3.13	115.69	123.59	7	5
4	A	345	PX4	C7-O7-C23	3.13	125.50	117.79	12	4
4	A	366	PX4	C28-C27-C26	3.13	98.54	114.42	11	2
4	A	314	PX4	O1-P1-O2	3.13	127.69	112.24	10	3
4	A	323	PX4	C1-C2-N1	3.13	126.21	115.78	2	3
4	A	351	PX4	O5-C9-O6	3.12	115.71	123.59	2	5
4	A	359	PX4	P1-O4-C6	3.12	103.36	121.68	9	8
4	A	328	PX4	C1-C2-N1	3.12	126.20	115.78	6	2
4	A	384	PX4	O1-P1-O4	3.12	122.25	107.75	7	3
4	A	311	PX4	C5-N1-C4	3.12	117.00	108.97	10	2
4	A	344	PX4	O7-C7-C6	3.12	119.70	108.40	14	5
4	A	394	PX4	O5-C9-O6	3.12	115.72	123.59	7	2
4	A	402	PX4	C3-N1-C2	3.12	97.15	109.92	1	3
4	A	345	PX4	O7-C7-C6	3.12	119.69	108.40	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	424	PX4	C7-O7-C23	3.12	125.47	117.79	7	2
4	A	429	PX4	O1-P1-O2	3.12	127.66	112.24	7	7
4	A	343	PX4	O7-C23-O8	3.12	116.17	123.70	3	6
4	A	314	PX4	C5-N1-C3	3.12	116.98	108.97	8	2
4	A	356	PX4	O3-P1-O2	3.12	96.89	109.07	3	2
4	A	364	PX4	O7-C23-O8	3.12	116.17	123.70	12	6
4	A	397	PX4	O7-C7-C8	3.12	119.68	108.40	14	8
4	A	403	PX4	C32-C31-C30	3.11	98.61	114.42	3	1
4	A	410	PX4	P1-O4-C6	3.11	103.42	121.68	13	6
4	A	428	PX4	C15-C14-C13	3.11	98.62	114.42	5	1
4	A	317	PX4	C8-O5-C9	3.11	105.60	117.12	3	3
4	A	327	PX4	C30-C29-C28	3.11	98.63	114.42	14	4
4	A	397	PX4	C4-N1-C3	3.11	100.98	108.97	6	2
4	A	314	PX4	C18-C17-C16	3.11	98.64	114.42	1	1
4	A	346	PX4	C26-C25-C24	3.11	102.02	113.19	4	3
4	A	312	PX4	C1-C2-N1	3.11	126.16	115.78	9	2
4	A	312	PX4	O7-C23-O8	3.11	116.19	123.70	3	4
4	A	324	PX4	C5-N1-C3	3.11	116.96	108.97	1	2
4	A	403	PX4	C4-N1-C3	3.11	100.98	108.97	3	4
4	A	403	PX4	C25-C24-C23	3.11	102.32	113.62	5	4
4	A	378	PX4	C4-N1-C3	3.11	100.99	108.97	12	3
4	A	395	PX4	C12-C11-C10	3.11	124.36	113.19	9	1
4	A	319	PX4	C26-C25-C24	3.10	102.03	113.19	2	2
4	A	386	PX4	P1-O4-C6	3.10	103.48	121.68	1	9
4	A	341	PX4	O1-P1-O2	3.10	127.58	112.24	10	6
4	A	430	PX4	O3-P1-O2	3.10	96.94	109.07	3	4
4	A	397	PX4	C12-C11-C10	3.10	102.04	113.19	9	3
4	A	344	PX4	C8-O5-C9	3.10	105.64	117.12	14	2
4	A	326	PX4	C5-N1-C3	3.10	116.94	108.97	13	3
4	A	368	PX4	C11-C10-C9	3.10	102.35	113.62	8	2
4	A	384	PX4	C11-C10-C9	3.10	102.35	113.62	10	2
4	A	390	PX4	O5-C9-C10	3.10	121.63	111.91	10	6
4	A	424	PX4	P1-O4-C6	3.10	103.51	121.68	13	10
4	A	426	PX4	O1-P1-O2	3.10	127.56	112.24	8	11
4	A	332	PX4	O1-P1-O2	3.10	127.55	112.24	13	10
4	A	319	PX4	O1-P1-O3	3.10	93.37	107.75	1	2
4	A	345	PX4	C1-C2-N1	3.10	126.12	115.78	11	3
4	A	425	PX4	C30-C29-C28	3.10	98.70	114.42	8	1
4	A	369	PX4	P1-O4-C6	3.10	103.52	121.68	8	7
4	A	377	PX4	O3-C1-C2	3.10	125.44	109.16	3	3
4	A	423	PX4	O1-P1-O3	3.09	93.37	107.75	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	316	PX4	O5-C9-C10	3.09	121.61	111.91	12	4
4	A	342	PX4	O5-C9-O6	3.09	131.40	123.59	7	3
4	A	425	PX4	C26-C25-C24	3.09	124.31	113.19	4	3
4	A	430	PX4	C27-C26-C25	3.09	98.72	114.42	3	2
4	A	363	PX4	C5-N1-C3	3.09	116.92	108.97	2	4
4	A	342	PX4	C1-C2-N1	3.09	126.10	115.78	3	4
4	A	380	PX4	P1-O4-C6	3.09	103.55	121.68	9	11
4	A	418	PX4	P1-O4-C6	3.09	103.55	121.68	11	12
4	A	310	PX4	O7-C7-C6	3.09	119.59	108.40	8	5
4	A	326	PX4	C4-N1-C3	3.09	101.03	108.97	3	5
4	A	418	PX4	O7-C7-C8	3.09	119.59	108.40	12	3
4	A	396	PX4	O5-C9-O6	3.09	115.80	123.59	4	3
4	A	336	PX4	O7-C7-C8	3.09	119.58	108.40	2	3
4	A	339	PX4	P1-O4-C6	3.09	103.58	121.68	12	9
4	A	383	PX4	C7-O7-C23	3.09	125.39	117.79	10	2
4	A	394	PX4	O7-C7-C6	3.09	119.58	108.40	11	4
4	A	312	PX4	C7-O7-C23	3.08	125.38	117.79	12	5
4	A	356	PX4	C5-N1-C4	3.09	116.91	108.97	13	2
4	A	351	PX4	C4-N1-C3	3.08	101.05	108.97	11	4
4	A	370	PX4	O1-P1-O2	3.08	127.49	112.24	11	9
4	A	394	PX4	C26-C25-C24	3.08	102.11	113.19	6	3
4	A	416	PX4	O5-C9-O6	3.08	115.81	123.59	7	4
4	A	327	PX4	P1-O4-C6	3.08	103.61	121.68	5	7
4	A	331	PX4	C25-C24-C23	3.08	102.42	113.62	3	2
4	A	385	PX4	O1-P1-O2	3.08	127.47	112.24	8	8
4	A	394	PX4	C20-C19-C18	3.08	98.79	114.42	3	4
4	A	422	PX4	O7-C7-C8	3.08	119.55	108.40	4	9
4	A	343	PX4	C28-C27-C26	3.08	98.80	114.42	4	2
4	A	422	PX4	O7-C23-O8	3.08	116.27	123.70	12	2
4	A	362	PX4	C11-C10-C9	3.08	102.44	113.62	10	3
4	A	360	PX4	O1-P1-O3	3.07	93.47	107.75	14	5
4	A	318	PX4	C15-C14-C13	3.07	98.82	114.42	3	4
4	A	328	PX4	O1-P1-O2	3.07	127.44	112.24	14	8
4	A	386	PX4	C12-C11-C10	3.07	102.14	113.19	7	4
4	A	316	PX4	C5-N1-C4	3.07	101.08	108.97	3	3
4	A	332	PX4	C4-N1-C2	3.07	97.36	109.92	12	1
4	A	376	PX4	O7-C7-C8	3.07	119.52	108.40	12	7
4	A	316	PX4	O1-P1-O2	3.07	127.41	112.24	3	6
4	A	342	PX4	C28-C27-C26	3.07	98.85	114.42	14	2
4	A	364	PX4	O7-C7-C8	3.07	119.51	108.40	5	4
4	A	372	PX4	C25-C24-C23	3.07	102.46	113.62	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	372	PX4	O3-P1-O2	3.07	97.07	109.07	13	2
4	A	378	PX4	C19-C18-C17	3.07	98.84	114.42	4	2
4	A	315	PX4	C5-N1-C4	3.07	101.09	108.97	14	4
4	A	357	PX4	C5-N1-C3	3.07	101.09	108.97	1	3
4	A	415	PX4	C8-O5-C9	3.07	105.77	117.12	8	1
4	A	421	PX4	C30-C29-C28	3.06	98.87	114.42	13	2
4	A	364	PX4	C5-N1-C3	3.06	101.10	108.97	5	3
4	A	428	PX4	O5-C9-O6	3.06	115.86	123.59	11	3
4	A	361	PX4	O1-P1-O2	3.06	127.37	112.24	3	10
4	A	369	PX4	O5-C9-O6	3.06	115.86	123.59	5	5
4	A	330	PX4	C19-C18-C17	3.06	98.89	114.42	8	2
4	A	409	PX4	C15-C14-C13	3.06	98.89	114.42	3	1
4	A	338	PX4	C11-C10-C9	3.06	124.74	113.62	12	4
4	A	400	PX4	O7-C7-C8	3.06	119.47	108.40	3	5
4	A	394	PX4	C4-N1-C3	3.05	101.12	108.97	3	3
4	A	422	PX4	C1-C2-N1	3.05	125.98	115.78	13	2
4	A	401	PX4	C12-C11-C10	3.05	102.21	113.19	3	1
4	A	377	PX4	O5-C9-C10	3.05	121.49	111.91	8	1
4	A	387	PX4	O7-C23-O8	3.05	116.33	123.70	12	2
4	A	387	PX4	C5-N1-C4	3.05	101.13	108.97	14	1
4	A	331	PX4	C5-N1-C3	3.05	116.82	108.97	5	3
4	A	359	PX4	O7-C7-C6	3.05	119.45	108.40	14	8
4	A	366	PX4	C5-N1-C3	3.05	101.13	108.97	5	4
4	A	371	PX4	O1-P1-O3	3.05	93.58	107.75	3	3
4	A	339	PX4	O5-C9-C10	3.05	121.47	111.91	1	5
4	A	328	PX4	C26-C25-C24	3.05	102.24	113.19	9	3
4	A	403	PX4	C5-N1-C4	3.05	101.14	108.97	4	4
4	A	318	PX4	O5-C9-O6	3.04	115.91	123.59	3	2
4	A	341	PX4	C4-N1-C3	3.04	116.80	108.97	1	3
4	A	353	PX4	C31-C30-C29	3.05	98.97	114.42	11	1
4	A	385	PX4	C8-O5-C9	3.05	128.40	117.12	8	2
4	A	389	PX4	C25-C24-C23	3.05	124.70	113.62	2	4
4	A	391	PX4	C12-C11-C10	3.05	102.24	113.19	10	3
4	A	390	PX4	C12-C11-C10	3.04	102.25	113.19	4	2
4	A	413	PX4	O3-P1-O2	3.05	97.17	109.07	13	6
4	A	419	PX4	O7-C23-O8	3.05	116.34	123.70	5	3
4	A	340	PX4	C8-O5-C9	3.04	128.39	117.12	9	1
4	A	384	PX4	O5-C9-C10	3.04	121.46	111.91	12	3
4	A	310	PX4	O7-C7-C8	3.04	119.41	108.40	7	4
4	A	396	PX4	C4-N1-C3	3.04	101.15	108.97	5	1
4	A	363	PX4	C12-C11-C10	3.04	102.26	113.19	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	C12-C11-C10	3.04	102.26	113.19	11	2
4	A	327	PX4	O8-C23-C24	3.04	111.87	123.73	1	2
4	A	393	PX4	O1-P1-O3	3.04	93.62	107.75	14	4
4	A	395	PX4	O5-C9-C10	3.04	121.45	111.91	4	4
4	A	420	PX4	O1-P1-O4	3.04	121.87	107.75	13	7
4	A	316	PX4	C26-C25-C24	3.04	102.27	113.19	4	3
4	A	350	PX4	O5-C9-O6	3.04	115.93	123.59	13	3
4	A	360	PX4	C1-C2-N1	3.04	125.92	115.78	2	3
4	A	399	PX4	C33-C32-C31	3.04	99.01	114.42	5	1
4	A	402	PX4	O5-C9-O6	3.04	115.93	123.59	1	3
4	A	316	PX4	C27-C26-C25	3.03	99.02	114.42	1	1
4	A	322	PX4	O5-C9-O6	3.03	115.94	123.59	6	4
4	A	363	PX4	O5-C9-O6	3.03	115.93	123.59	10	2
4	A	371	PX4	C27-C26-C25	3.03	99.02	114.42	5	3
4	A	382	PX4	O1-P1-O3	3.03	93.66	107.75	2	3
4	A	420	PX4	C11-C10-C9	3.03	102.59	113.62	11	3
4	A	426	PX4	C12-C11-C10	3.03	102.29	113.19	8	1
4	A	364	PX4	O5-C9-O6	3.03	115.94	123.59	7	4
4	A	313	PX4	O5-C9-C10	3.03	121.42	111.91	12	5
4	A	322	PX4	P1-O4-C6	3.03	103.90	121.68	5	10
4	A	390	PX4	O3-P1-O2	3.03	97.23	109.07	1	2
4	A	405	PX4	C29-C28-C27	3.03	99.05	114.42	6	2
4	A	309	PX4	C1-C2-N1	3.03	125.89	115.78	4	9
4	A	312	PX4	O3-C1-C2	3.03	125.08	109.16	9	3
4	A	351	PX4	C12-C11-C10	3.03	102.31	113.19	4	5
4	A	306	PX4	O5-C9-O6	3.02	115.96	123.59	5	3
4	A	374	PX4	C1-C2-N1	3.02	125.88	115.78	9	2
4	A	377	PX4	C12-C11-C10	3.02	102.32	113.19	6	4
4	A	315	PX4	O5-C8-C7	3.02	117.23	108.43	13	3
4	A	346	PX4	O3-P1-O2	3.02	97.25	109.07	12	1
4	A	378	PX4	C13-C12-C11	3.02	99.07	114.42	13	2
4	A	337	PX4	C8-O5-C9	3.02	105.93	117.12	14	3
4	A	353	PX4	C29-C28-C27	3.02	99.08	114.42	11	2
4	A	380	PX4	C17-C16-C15	3.02	99.07	114.42	8	5
4	A	399	PX4	O5-C9-C10	3.02	121.39	111.91	5	2
4	A	411	PX4	C12-C11-C10	3.02	102.33	113.19	6	1
4	A	345	PX4	C12-C11-C10	3.02	124.05	113.19	7	3
4	A	354	PX4	O7-C7-C6	3.02	119.34	108.40	11	10
4	A	417	PX4	C3-N1-C2	3.02	97.56	109.92	9	1
4	A	310	PX4	O7-C23-O8	3.02	116.41	123.70	8	5
4	A	318	PX4	C28-C27-C26	3.02	99.11	114.42	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	369	PX4	O7-C23-O8	3.02	116.42	123.70	2	3
4	A	314	PX4	O5-C9-C10	3.01	121.37	111.91	14	3
4	A	326	PX4	C7-O7-C23	3.02	125.21	117.79	3	4
4	A	379	PX4	O1-P1-O4	3.01	121.75	107.75	3	3
4	A	394	PX4	O7-C23-O8	3.02	116.42	123.70	7	3
4	A	411	PX4	O7-C7-C6	3.02	119.32	108.40	1	6
4	A	329	PX4	C26-C25-C24	3.01	102.36	113.19	9	3
4	A	379	PX4	O5-C9-O6	3.01	115.99	123.59	5	5
4	A	403	PX4	O7-C7-C8	3.01	119.31	108.40	11	3
4	A	425	PX4	O1-P1-O4	3.01	121.74	107.75	2	3
4	A	347	PX4	P1-O4-C6	3.01	104.02	121.68	2	7
4	A	417	PX4	C29-C28-C27	3.01	99.13	114.42	11	3
4	A	321	PX4	O4-P1-O2	3.01	120.83	109.07	14	4
4	A	309	PX4	C5-N1-C3	3.01	116.71	108.97	2	2
4	A	315	PX4	C1-C2-N1	3.01	125.83	115.78	5	3
4	A	324	PX4	O1-P1-O2	3.01	127.12	112.24	8	7
4	A	336	PX4	O1-P1-O4	3.01	121.73	107.75	12	4
4	A	404	PX4	O7-C7-C8	3.01	119.30	108.40	4	3
4	A	418	PX4	C8-O5-C9	3.01	105.97	117.12	5	2
4	A	316	PX4	O5-C9-O6	3.01	116.00	123.59	12	2
4	A	332	PX4	O5-C9-C10	3.01	121.35	111.91	5	3
4	A	333	PX4	C30-C29-C28	3.01	99.15	114.42	14	3
4	A	396	PX4	C26-C25-C24	3.01	102.38	113.19	1	1
4	A	413	PX4	O7-C7-C6	3.01	119.30	108.40	4	4
4	A	418	PX4	C25-C24-C23	3.01	102.68	113.62	8	3
4	A	308	PX4	C34-C33-C32	3.01	99.16	114.42	2	3
4	A	325	PX4	O7-C7-C8	3.01	119.29	108.40	9	2
4	A	347	PX4	C18-C17-C16	3.01	99.16	114.42	12	2
4	A	366	PX4	C12-C11-C10	3.01	102.38	113.19	10	2
4	A	322	PX4	C5-N1-C3	3.00	101.25	108.97	9	4
4	A	354	PX4	C29-C28-C27	3.01	99.17	114.42	13	2
4	A	362	PX4	O1-P1-O2	3.01	127.10	112.24	4	2
4	A	412	PX4	O5-C9-O6	3.01	131.18	123.59	11	1
4	A	421	PX4	O1-P1-O2	3.01	127.10	112.24	8	7
4	A	428	PX4	C20-C19-C18	3.01	99.17	114.42	13	2
4	A	333	PX4	C33-C32-C31	3.00	99.18	114.42	12	1
4	A	358	PX4	O5-C9-C10	3.00	121.33	111.91	3	5
4	A	368	PX4	O5-C9-O6	3.00	116.01	123.59	4	5
4	A	427	PX4	C5-N1-C2	3.00	122.21	109.92	11	1
4	A	430	PX4	C8-O5-C9	3.00	106.00	117.12	2	2
4	A	395	PX4	C33-C32-C31	3.00	99.18	114.42	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	395	PX4	C4-N1-C3	3.00	101.25	108.97	8	1
4	A	313	PX4	C7-O7-C23	3.00	110.40	117.79	2	6
4	A	328	PX4	O7-C23-O8	3.00	116.45	123.70	11	1
4	A	330	PX4	O7-C7-C6	3.00	119.26	108.40	10	2
4	A	417	PX4	C17-C16-C15	3.00	99.20	114.42	6	2
4	A	317	PX4	O1-P1-O2	3.00	127.06	112.24	6	8
4	A	316	PX4	O3-P1-O2	3.00	97.36	109.07	3	3
4	A	351	PX4	C11-C10-C9	3.00	102.72	113.62	8	5
4	A	354	PX4	C26-C25-C24	3.00	102.41	113.19	4	3
4	A	359	PX4	C12-C11-C10	3.00	102.41	113.19	11	1
4	A	375	PX4	C5-N1-C3	3.00	116.68	108.97	7	3
4	A	407	PX4	O4-P1-O2	3.00	120.78	109.07	13	4
4	A	417	PX4	P1-O4-C6	3.00	104.11	121.68	5	10
4	A	380	PX4	C11-C10-C9	3.00	102.73	113.62	8	3
4	A	341	PX4	O7-C7-C6	2.99	119.24	108.40	9	4
4	A	350	PX4	C7-O7-C23	2.99	125.16	117.79	12	4
4	A	429	PX4	O7-C23-O8	2.99	116.47	123.70	6	5
4	A	323	PX4	P1-O4-C6	2.99	104.14	121.68	1	9
4	A	367	PX4	O7-C23-O8	2.99	130.93	123.70	9	4
4	A	384	PX4	O3-P1-O2	2.99	97.38	109.07	3	2
4	A	399	PX4	O7-C23-O8	2.99	116.47	123.70	8	3
4	A	411	PX4	C25-C24-C23	2.99	102.74	113.62	5	2
4	A	419	PX4	O1-P1-O2	2.99	127.03	112.24	11	7
4	A	331	PX4	C32-C31-C30	2.99	99.26	114.42	8	1
4	A	399	PX4	O7-C7-C8	2.99	119.22	108.40	6	3
4	A	361	PX4	C5-N1-C4	2.99	116.65	108.97	14	3
4	A	374	PX4	C8-O5-C9	2.98	106.07	117.12	13	2
4	A	378	PX4	C11-C10-C9	2.99	102.76	113.62	8	1
4	A	393	PX4	C1-C2-N1	2.98	125.75	115.78	8	5
4	A	408	PX4	O5-C9-C10	2.99	121.28	111.91	1	2
4	A	388	PX4	C5-N1-C4	2.98	101.30	108.97	5	4
4	A	400	PX4	C8-O5-C9	2.98	106.07	117.12	9	3
4	A	421	PX4	C32-C31-C30	2.99	99.27	114.42	7	1
4	A	327	PX4	O1-P1-O2	2.98	126.99	112.24	1	7
4	A	329	PX4	O7-C7-C6	2.98	119.20	108.40	6	3
4	A	334	PX4	P1-O4-C6	2.98	104.19	121.68	2	9
4	A	353	PX4	C26-C25-C24	2.98	102.48	113.19	7	1
4	A	361	PX4	C3-N1-C2	2.98	122.11	109.92	9	3
4	A	366	PX4	C18-C17-C16	2.98	99.30	114.42	9	1
4	A	385	PX4	C26-C25-C24	2.98	102.48	113.19	2	2
4	A	308	PX4	C30-C29-C28	2.98	99.30	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	333	PX4	O3-P1-O2	2.98	97.44	109.07	9	5
4	A	326	PX4	O7-C7-C6	2.98	119.17	108.40	12	2
4	A	356	PX4	C1-C2-N1	2.98	125.72	115.78	8	4
4	A	398	PX4	O7-C7-C6	2.98	119.18	108.40	7	1
4	A	370	PX4	C3-N1-C2	2.97	122.09	109.92	6	3
4	A	423	PX4	O1-P1-O4	2.98	121.56	107.75	10	3
4	A	333	PX4	O7-C7-C8	2.97	119.17	108.40	1	3
4	A	310	PX4	C26-C25-C24	2.97	102.51	113.19	3	2
4	A	336	PX4	C5-N1-C2	2.97	122.08	109.92	7	2
4	A	336	PX4	C26-C25-C24	2.97	102.50	113.19	12	1
4	A	380	PX4	O7-C7-C6	2.97	119.17	108.40	1	3
4	A	410	PX4	O4-P1-O2	2.97	120.68	109.07	2	2
4	A	416	PX4	O7-C7-C8	2.97	119.17	108.40	3	5
4	A	361	PX4	C30-C29-C28	2.97	99.34	114.42	7	1
4	A	363	PX4	O7-C7-C6	2.97	119.16	108.40	8	4
4	A	392	PX4	O5-C9-C10	2.97	121.23	111.91	14	3
4	A	319	PX4	C12-C11-C10	2.97	123.86	113.19	13	1
4	A	325	PX4	C11-C10-C9	2.97	102.82	113.62	1	4
4	A	408	PX4	C4-N1-C3	2.97	101.34	108.97	9	3
4	A	332	PX4	C26-C25-C24	2.97	102.53	113.19	12	3
4	A	425	PX4	C29-C28-C27	2.97	99.37	114.42	3	1
4	A	427	PX4	C12-C11-C10	2.97	102.53	113.19	8	3
4	A	407	PX4	C1-C2-N1	2.96	125.68	115.78	13	4
4	A	370	PX4	C14-C13-C12	2.96	99.38	114.42	7	4
4	A	312	PX4	C26-C25-C24	2.96	123.84	113.19	8	3
4	A	335	PX4	O1-P1-O4	2.96	121.51	107.75	10	2
4	A	381	PX4	C1-C2-N1	2.96	125.67	115.78	2	3
4	A	333	PX4	C1-C2-N1	2.96	125.67	115.78	5	3
4	A	349	PX4	C4-N1-C3	2.96	101.36	108.97	4	2
4	A	418	PX4	O1-P1-O2	2.96	126.88	112.24	4	5
4	A	341	PX4	C5-N1-C3	2.96	101.36	108.97	5	3
4	A	354	PX4	C25-C24-C23	2.96	102.86	113.62	7	3
4	A	357	PX4	C1-C2-N1	2.96	125.66	115.78	12	5
4	A	383	PX4	C16-C15-C14	2.96	99.40	114.42	9	2
4	A	406	PX4	C11-C10-C9	2.96	102.86	113.62	7	1
4	A	331	PX4	C28-C27-C26	2.96	99.41	114.42	3	1
4	A	336	PX4	C7-O7-C23	2.96	125.07	117.79	10	2
4	A	349	PX4	C12-C11-C10	2.96	102.56	113.19	1	3
4	A	415	PX4	C12-C11-C10	2.96	123.82	113.19	13	2
4	A	424	PX4	C14-C13-C12	2.96	99.41	114.42	8	1
4	A	327	PX4	C28-C27-C26	2.96	99.42	114.42	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	311	PX4	O7-C7-C6	2.95	119.09	108.40	13	5
4	A	395	PX4	C25-C24-C23	2.95	102.88	113.62	6	3
4	A	424	PX4	O1-P1-O3	2.95	94.03	107.75	4	2
4	A	401	PX4	C5-N1-C2	2.95	121.99	109.92	11	2
4	A	408	PX4	P1-O4-C6	2.95	104.37	121.68	5	7
4	A	425	PX4	O1-P1-O2	2.95	126.83	112.24	11	5
4	A	425	PX4	O7-C23-O8	2.95	116.57	123.70	2	3
4	A	338	PX4	C4-N1-C3	2.95	101.39	108.97	13	2
4	A	336	PX4	C4-N1-C3	2.95	101.39	108.97	13	4
4	A	379	PX4	C19-C18-C17	2.95	99.45	114.42	7	2
4	A	336	PX4	C15-C14-C13	2.95	99.47	114.42	9	2
4	A	367	PX4	C11-C10-C9	2.95	102.90	113.62	3	4
4	A	402	PX4	C16-C15-C14	2.95	99.46	114.42	6	1
4	A	404	PX4	C19-C18-C17	2.95	99.46	114.42	3	1
4	A	346	PX4	O1-P1-O2	2.94	126.80	112.24	13	5
4	A	364	PX4	C27-C26-C25	2.95	99.47	114.42	7	2
4	A	371	PX4	O7-C7-C8	2.95	119.07	108.40	6	5
4	A	429	PX4	C25-C24-C23	2.95	102.91	113.62	12	1
4	A	422	PX4	P1-O4-C6	2.95	104.41	121.68	5	7
4	A	315	PX4	C26-C25-C24	2.94	102.61	113.19	2	1
4	A	355	PX4	O7-C7-C6	2.94	119.06	108.40	11	4
4	A	410	PX4	O1-P1-O2	2.94	126.79	112.24	7	12
4	A	406	PX4	O7-C7-C6	2.94	119.05	108.40	11	6
4	A	413	PX4	C25-C24-C23	2.94	102.92	113.62	11	3
4	A	405	PX4	C19-C18-C17	2.94	99.50	114.42	6	2
4	A	430	PX4	C12-C11-C10	2.94	102.62	113.19	5	1
4	A	335	PX4	C8-O5-C9	2.94	106.24	117.12	10	2
4	A	371	PX4	C16-C15-C14	2.94	99.50	114.42	1	3
4	A	318	PX4	C8-O5-C9	2.94	106.24	117.12	11	2
4	A	375	PX4	O4-P1-O2	2.94	120.55	109.07	4	5
4	A	366	PX4	C30-C29-C28	2.94	99.51	114.42	11	1
4	A	386	PX4	C33-C32-C31	2.94	99.51	114.42	3	5
4	A	413	PX4	O7-C23-O8	2.94	116.60	123.70	12	4
4	A	395	PX4	O7-C7-C8	2.94	119.03	108.40	14	6
4	A	405	PX4	C3-N1-C2	2.94	121.93	109.92	13	1
4	A	412	PX4	C12-C11-C10	2.94	102.64	113.19	5	3
4	A	418	PX4	C1-C2-N1	2.94	125.58	115.78	10	4
4	A	326	PX4	C30-C29-C28	2.93	99.53	114.42	2	1
4	A	398	PX4	C29-C28-C27	2.93	99.53	114.42	1	2
4	A	419	PX4	O7-C7-C8	2.94	119.03	108.40	12	7
4	A	341	PX4	C1-C2-N1	2.93	125.57	115.78	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	C4-N1-C3	2.93	101.43	108.97	12	4
4	A	409	PX4	C18-C17-C16	2.93	99.53	114.42	3	1
4	A	341	PX4	C34-C33-C32	2.93	99.54	114.42	1	1
4	A	343	PX4	O5-C9-C10	2.93	121.11	111.91	9	4
4	A	418	PX4	O3-P1-O2	2.93	97.61	109.07	1	1
4	A	430	PX4	C25-C24-C23	2.93	102.95	113.62	7	1
4	A	385	PX4	C32-C31-C30	2.93	99.54	114.42	2	2
4	A	313	PX4	C5-N1-C4	2.93	101.45	108.97	7	2
4	A	316	PX4	O7-C23-C24	2.93	117.81	111.50	2	6
4	A	350	PX4	O1-P1-O4	2.93	121.34	107.75	10	3
4	A	353	PX4	O7-C7-C8	2.93	119.00	108.40	3	3
4	A	395	PX4	C5-N1-C4	2.93	116.50	108.97	1	2
4	A	317	PX4	O5-C9-C10	2.92	121.09	111.91	3	5
4	A	365	PX4	O1-P1-O3	2.92	94.16	107.75	6	2
4	A	320	PX4	C11-C10-C9	2.92	102.99	113.62	6	2
4	A	342	PX4	C29-C28-C27	2.92	99.58	114.42	10	2
4	A	366	PX4	C25-C24-C23	2.92	102.99	113.62	8	1
4	A	376	PX4	O4-P1-O2	2.92	120.49	109.07	2	3
4	A	383	PX4	O1-P1-O2	2.92	126.69	112.24	3	9
4	A	383	PX4	C5-N1-C3	2.92	101.46	108.97	7	3
4	A	321	PX4	C5-N1-C3	2.92	101.46	108.97	4	3
4	A	334	PX4	C14-C13-C12	2.92	99.59	114.42	11	3
4	A	357	PX4	O5-C9-C10	2.92	121.08	111.91	12	4
4	A	396	PX4	C7-O7-C23	2.92	124.98	117.79	7	2
4	A	399	PX4	C1-C2-N1	2.92	125.53	115.78	10	5
4	A	317	PX4	C5-N1-C3	2.92	116.48	108.97	13	2
4	A	329	PX4	O7-C7-C8	2.92	118.97	108.40	12	8
4	A	340	PX4	C5-N1-C3	2.92	101.47	108.97	1	3
4	A	404	PX4	O3-C1-C2	2.92	124.52	109.16	13	1
4	A	337	PX4	C12-C11-C10	2.92	102.70	113.19	4	3
4	A	332	PX4	O7-C7-C6	2.92	118.97	108.40	4	4
4	A	306	PX4	C26-C25-C24	2.92	102.71	113.19	12	3
4	A	358	PX4	C3-N1-C2	2.92	97.98	109.92	8	1
4	A	368	PX4	O7-C23-O8	2.92	116.65	123.70	6	4
4	A	428	PX4	C3-N1-C2	2.92	97.98	109.92	14	3
4	A	378	PX4	C1-C2-N1	2.92	125.52	115.78	10	1
4	A	328	PX4	O7-C7-C8	2.92	118.96	108.40	1	7
4	A	335	PX4	C27-C26-C25	2.91	99.63	114.42	7	2
4	A	371	PX4	O3-P1-O2	2.92	97.68	109.07	3	1
4	A	314	PX4	C15-C14-C13	2.91	99.64	114.42	12	1
4	A	363	PX4	O4-P1-O2	2.91	120.44	109.07	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	380	PX4	O1-P1-O4	2.91	121.27	107.75	11	5
4	A	395	PX4	O7-C23-O8	2.91	116.67	123.70	1	3
4	A	402	PX4	P1-O3-C1	2.91	107.27	121.59	8	9
4	A	403	PX4	O7-C23-O8	2.91	130.74	123.70	10	3
4	A	322	PX4	C25-C24-C23	2.91	124.20	113.62	13	1
4	A	329	PX4	O1-P1-O4	2.91	121.25	107.75	4	1
4	A	320	PX4	C8-O5-C9	2.91	106.36	117.12	6	4
4	A	334	PX4	C5-N1-C3	2.91	116.45	108.97	14	3
4	A	334	PX4	O7-C7-C6	2.91	118.93	108.40	6	3
4	A	371	PX4	O1-P1-O2	2.91	126.62	112.24	4	7
4	A	346	PX4	C11-C10-C9	2.91	103.05	113.62	11	2
4	A	395	PX4	O4-P1-O2	2.91	97.71	109.07	5	1
4	A	410	PX4	O7-C7-C6	2.91	118.92	108.40	9	2
4	A	371	PX4	C25-C24-C23	2.90	103.06	113.62	8	3
4	A	349	PX4	O3-P1-O2	2.90	120.41	109.07	3	3
4	A	355	PX4	O1-P1-O2	2.90	126.59	112.24	8	8
4	A	374	PX4	C4-N1-C2	2.90	121.80	109.92	11	1
4	A	399	PX4	C20-C19-C18	2.90	99.69	114.42	13	2
4	A	317	PX4	P1-O4-C6	2.90	104.67	121.68	1	8
4	A	333	PX4	C5-N1-C4	2.90	116.43	108.97	8	5
4	A	350	PX4	C34-C33-C32	2.90	99.70	114.42	3	1
4	A	372	PX4	O5-C9-C10	2.90	121.01	111.91	10	3
4	A	375	PX4	O7-C23-O8	2.90	116.69	123.70	7	4
4	A	328	PX4	O5-C9-C10	2.90	121.01	111.91	13	7
4	A	333	PX4	C31-C30-C29	2.90	99.71	114.42	9	3
4	A	355	PX4	O7-C23-C24	2.90	117.75	111.50	10	6
4	A	368	PX4	C25-C24-C23	2.90	103.08	113.62	13	2
4	A	423	PX4	O5-C9-C10	2.90	121.01	111.91	3	3
4	A	423	PX4	O7-C7-C8	2.90	118.90	108.40	11	2
4	A	309	PX4	C15-C14-C13	2.90	99.72	114.42	10	1
4	A	339	PX4	C1-C2-N1	2.90	125.45	115.78	11	3
4	A	344	PX4	O7-C7-C8	2.90	118.89	108.40	12	4
4	A	375	PX4	O1-P1-O3	2.90	94.28	107.75	4	2
4	A	407	PX4	O5-C9-C10	2.90	121.00	111.91	6	3
4	A	385	PX4	C17-C16-C15	2.90	99.72	114.42	2	2
4	A	421	PX4	C14-C13-C12	2.90	99.72	114.42	14	1
4	A	334	PX4	C15-C14-C13	2.90	99.72	114.42	8	2
4	A	309	PX4	P1-O4-C6	2.89	104.71	121.68	9	2
4	A	316	PX4	O1-P1-O3	2.90	94.30	107.75	14	3
4	A	388	PX4	C17-C16-C15	2.90	99.72	114.42	5	2
4	A	407	PX4	C34-C33-C32	2.90	99.72	114.42	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	C5-N1-C4	2.89	101.53	108.97	4	2
4	A	345	PX4	C8-O5-C9	2.89	106.40	117.12	11	1
4	A	347	PX4	C15-C14-C13	2.89	99.73	114.42	7	2
4	A	378	PX4	C31-C30-C29	2.89	99.73	114.42	9	3
4	A	340	PX4	C30-C29-C28	2.89	99.75	114.42	14	1
4	A	343	PX4	O6-C9-C10	2.89	112.45	123.73	9	2
4	A	418	PX4	O7-C7-C6	2.89	118.88	108.40	8	3
4	A	344	PX4	C28-C27-C26	2.89	99.75	114.42	13	1
4	A	345	PX4	O7-C7-C8	2.89	118.87	108.40	13	3
4	A	371	PX4	O7-C7-C6	2.89	118.87	108.40	9	4
4	A	383	PX4	C17-C16-C15	2.89	99.75	114.42	6	1
4	A	347	PX4	O5-C9-O6	2.89	116.30	123.59	11	4
4	A	307	PX4	C28-C27-C26	2.89	99.76	114.42	4	1
4	A	322	PX4	C32-C31-C30	2.89	99.76	114.42	6	1
4	A	420	PX4	C31-C30-C29	2.89	99.76	114.42	9	1
4	A	320	PX4	C4-N1-C3	2.89	101.55	108.97	10	3
4	A	338	PX4	O5-C9-C10	2.89	120.97	111.91	8	3
4	A	341	PX4	C14-C13-C12	2.89	99.77	114.42	6	1
4	A	367	PX4	O1-P1-O2	2.89	126.51	112.24	8	9
4	A	380	PX4	C4-N1-C3	2.89	116.39	108.97	11	4
4	A	380	PX4	C5-N1-C4	2.89	101.55	108.97	10	3
4	A	404	PX4	C1-C2-N1	2.89	125.42	115.78	7	4
4	A	420	PX4	O7-C7-C6	2.89	118.85	108.40	1	5
4	A	307	PX4	O3-P1-O2	2.88	97.80	109.07	9	1
4	A	318	PX4	C31-C30-C29	2.89	99.78	114.42	6	3
4	A	333	PX4	O1-P1-O2	2.88	126.50	112.24	10	7
4	A	419	PX4	O1-P1-O3	2.88	94.35	107.75	2	2
4	A	311	PX4	O1-P1-O3	2.88	94.36	107.75	5	3
4	A	357	PX4	C12-C11-C10	2.88	102.83	113.19	10	3
4	A	367	PX4	C27-C26-C25	2.88	99.79	114.42	2	2
4	A	393	PX4	C20-C19-C18	2.88	99.80	114.42	7	1
4	A	306	PX4	C1-C2-N1	2.88	125.39	115.78	12	1
4	A	307	PX4	O1-P1-O2	2.88	126.47	112.24	2	6
4	A	376	PX4	C34-C33-C32	2.88	99.81	114.42	2	3
4	A	341	PX4	O5-C9-C10	2.88	120.94	111.91	1	4
4	A	423	PX4	C4-N1-C3	2.88	101.58	108.97	2	3
4	A	427	PX4	C7-O7-C23	2.88	110.71	117.79	10	4
4	A	364	PX4	C18-C17-C16	2.87	99.83	114.42	10	1
4	A	397	PX4	C18-C17-C16	2.87	99.83	114.42	2	1
4	A	394	PX4	O1-P1-O2	2.87	126.44	112.24	11	7
4	A	403	PX4	O3-P1-O2	2.87	97.84	109.07	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	C12-C11-C10	2.87	102.87	113.19	10	3
4	A	331	PX4	C5-N1-C4	2.87	101.59	108.97	14	4
4	A	334	PX4	C1-C2-N1	2.87	125.36	115.78	4	2
4	A	351	PX4	C1-C2-N1	2.87	125.37	115.78	11	3
4	A	354	PX4	C8-O5-C9	2.87	106.49	117.12	1	3
4	A	428	PX4	C8-O5-C9	2.87	106.49	117.12	4	2
4	A	309	PX4	C18-C17-C16	2.87	99.86	114.42	11	3
4	A	388	PX4	O5-C9-C10	2.87	120.91	111.91	14	5
4	A	343	PX4	C13-C12-C11	2.87	99.86	114.42	4	2
4	A	409	PX4	O7-C7-C6	2.87	118.79	108.40	3	6
4	A	314	PX4	O5-C9-O6	2.87	116.36	123.59	3	5
4	A	315	PX4	C8-O5-C9	2.87	106.51	117.12	8	1
4	A	409	PX4	C4-N1-C3	2.87	101.60	108.97	11	3
4	A	326	PX4	O1-P1-O2	2.87	126.41	112.24	9	8
4	A	315	PX4	O5-C9-O6	2.86	116.36	123.59	9	5
4	A	322	PX4	O5-C9-C10	2.86	120.90	111.91	6	3
4	A	356	PX4	C5-N1-C2	2.87	121.64	109.92	2	1
4	A	408	PX4	O5-C9-O6	2.87	116.36	123.59	8	7
4	A	422	PX4	C8-O5-C9	2.87	106.51	117.12	6	3
4	A	357	PX4	C5-N1-C4	2.86	116.34	108.97	2	2
4	A	379	PX4	O7-C7-C6	2.86	118.77	108.40	9	4
4	A	420	PX4	C19-C18-C17	2.86	99.89	114.42	4	2
4	A	385	PX4	O5-C9-C10	2.86	120.89	111.91	13	3
4	A	359	PX4	C15-C14-C13	2.86	99.90	114.42	14	2
4	A	419	PX4	C5-N1-C3	2.86	116.33	108.97	8	2
4	A	430	PX4	O1-P1-O2	2.86	126.38	112.24	8	8
4	A	312	PX4	O7-C7-C6	2.86	118.75	108.40	5	3
4	A	320	PX4	C3-N1-C2	2.86	98.22	109.92	5	1
4	A	341	PX4	O3-P1-O2	2.86	97.90	109.07	11	4
4	A	403	PX4	O5-C9-O6	2.86	116.38	123.59	6	4
4	A	409	PX4	C1-C2-N1	2.86	125.32	115.78	2	2
4	A	334	PX4	O1-P1-O3	2.86	94.48	107.75	4	1
4	A	340	PX4	C5-N1-C4	2.86	101.63	108.97	6	5
4	A	358	PX4	O3-P1-O2	2.86	97.91	109.07	8	2
4	A	365	PX4	C5-N1-C2	2.86	98.23	109.92	13	1
4	A	414	PX4	C15-C14-C13	2.86	99.92	114.42	1	3
4	A	397	PX4	C5-N1-C3	2.86	116.31	108.97	3	1
4	A	310	PX4	C11-C10-C9	2.85	103.25	113.62	14	4
4	A	319	PX4	C20-C19-C18	2.85	99.95	114.42	12	1
4	A	328	PX4	C4-N1-C3	2.85	101.64	108.97	2	4
4	A	328	PX4	O7-C7-C6	2.85	118.72	108.40	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	359	PX4	C11-C10-C9	2.85	103.25	113.62	9	1
4	A	337	PX4	O1-P1-O2	2.85	126.33	112.24	13	3
4	A	388	PX4	C5-N1-C2	2.85	121.58	109.92	7	1
4	A	416	PX4	C4-N1-C2	2.85	121.58	109.92	14	3
4	A	335	PX4	C12-C11-C10	2.85	102.96	113.19	2	3
4	A	340	PX4	C1-C2-N1	2.85	125.29	115.78	11	3
4	A	342	PX4	O3-P1-O2	2.85	97.94	109.07	9	2
4	A	365	PX4	O3-C1-C2	2.85	124.14	109.16	11	2
4	A	372	PX4	O7-C23-O8	2.85	116.82	123.70	4	2
4	A	375	PX4	O5-C9-C10	2.85	120.85	111.91	11	4
4	A	396	PX4	O7-C7-C6	2.85	118.71	108.40	11	4
4	A	330	PX4	C26-C25-C24	2.84	102.97	113.19	6	2
4	A	356	PX4	C4-N1-C2	2.84	98.28	109.92	2	1
4	A	412	PX4	C4-N1-C3	2.85	116.29	108.97	3	2
4	A	308	PX4	C7-O7-C23	2.84	124.79	117.79	13	1
4	A	352	PX4	C4-N1-C3	2.84	101.67	108.97	3	3
4	A	353	PX4	C3-N1-C2	2.84	121.55	109.92	8	2
4	A	406	PX4	O5-C9-C10	2.84	120.83	111.91	12	4
4	A	391	PX4	C18-C17-C16	2.84	100.00	114.42	12	2
4	A	402	PX4	C27-C26-C25	2.84	100.00	114.42	2	2
4	A	370	PX4	C30-C29-C28	2.84	100.01	114.42	3	2
4	A	380	PX4	O8-C23-C24	2.84	112.65	123.73	10	2
4	A	309	PX4	C4-N1-C3	2.84	101.68	108.97	13	2
4	A	349	PX4	C19-C18-C17	2.84	100.02	114.42	4	3
4	A	406	PX4	C12-C11-C10	2.84	102.99	113.19	6	3
4	A	388	PX4	C32-C31-C30	2.84	100.03	114.42	8	2
4	A	389	PX4	O5-C9-C10	2.84	120.81	111.91	4	5
4	A	416	PX4	C5-N1-C3	2.84	116.27	108.97	4	7
4	A	328	PX4	C29-C28-C27	2.84	100.03	114.42	12	2
4	A	336	PX4	C18-C17-C16	2.84	100.03	114.42	11	2
4	A	359	PX4	C5-N1-C3	2.83	101.69	108.97	9	4
4	A	372	PX4	P1-O4-C6	2.83	105.06	121.68	11	9
4	A	399	PX4	C15-C14-C13	2.83	100.03	114.42	4	2
4	A	402	PX4	O4-P1-O2	2.83	120.14	109.07	4	2
4	A	413	PX4	C3-N1-C2	2.83	98.32	109.92	6	1
4	A	321	PX4	C7-O7-C23	2.83	124.76	117.79	4	4
4	A	364	PX4	C14-C13-C12	2.83	100.05	114.42	5	2
4	A	365	PX4	C14-C13-C12	2.83	100.05	114.42	2	3
4	A	372	PX4	O1-P1-O2	2.83	126.24	112.24	10	7
4	A	332	PX4	C4-N1-C3	2.83	101.70	108.97	10	3
4	A	338	PX4	C25-C24-C23	2.83	103.33	113.62	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	C27-C26-C25	2.83	100.06	114.42	5	2
4	A	353	PX4	C33-C32-C31	2.83	100.06	114.42	14	1
4	A	429	PX4	C1-C2-N1	2.83	125.23	115.78	12	5
4	A	350	PX4	C1-C2-N1	2.83	125.22	115.78	2	3
4	A	416	PX4	C25-C24-C23	2.83	123.90	113.62	14	3
4	A	335	PX4	C5-N1-C3	2.82	116.23	108.97	5	4
4	A	428	PX4	C11-C10-C9	2.82	103.35	113.62	9	1
4	A	365	PX4	O5-C8-C7	2.82	116.65	108.43	3	8
4	A	382	PX4	C32-C31-C30	2.82	100.10	114.42	5	1
4	A	395	PX4	O3-P1-O2	2.82	98.04	109.07	9	2
4	A	400	PX4	O7-C23-O8	2.82	116.88	123.70	14	5
4	A	307	PX4	C31-C30-C29	2.82	100.10	114.42	5	4
4	A	430	PX4	C11-C10-C9	2.82	103.36	113.62	12	2
4	A	351	PX4	C5-N1-C4	2.82	101.72	108.97	8	2
4	A	340	PX4	C5-N1-C2	2.82	98.38	109.92	2	2
4	A	348	PX4	C5-N1-C4	2.82	101.72	108.97	10	2
4	A	357	PX4	O8-C23-C24	2.82	112.73	123.73	5	2
4	A	365	PX4	C4-N1-C3	2.82	116.22	108.97	8	1
4	A	383	PX4	O1-P1-O3	2.82	94.65	107.75	3	4
4	A	353	PX4	C8-O5-C9	2.82	106.69	117.12	9	4
4	A	360	PX4	O3-P1-O2	2.82	98.05	109.07	6	1
4	A	365	PX4	O4-P1-O2	2.82	120.08	109.07	10	2
4	A	389	PX4	C26-C25-C24	2.82	103.06	113.19	4	2
4	A	401	PX4	O5-C9-O6	2.82	116.48	123.59	13	5
4	A	422	PX4	C31-C30-C29	2.82	100.12	114.42	2	2
4	A	372	PX4	C1-C2-N1	2.82	125.18	115.78	5	1
4	A	410	PX4	C19-C18-C17	2.82	100.12	114.42	10	2
4	A	327	PX4	C12-C11-C10	2.82	103.07	113.19	5	2
4	A	407	PX4	C33-C32-C31	2.82	100.13	114.42	7	1
4	A	357	PX4	C26-C25-C24	2.81	103.08	113.19	6	2
4	A	318	PX4	C5-N1-C3	2.81	116.20	108.97	10	4
4	A	317	PX4	C11-C10-C9	2.81	103.40	113.62	13	1
4	A	322	PX4	C12-C11-C10	2.81	123.30	113.19	7	4
4	A	391	PX4	C17-C16-C15	2.81	100.15	114.42	13	1
4	A	378	PX4	O1-P1-O4	2.81	94.69	107.75	14	2
4	A	392	PX4	O1-P1-O2	2.81	126.14	112.24	13	12
4	A	404	PX4	C4-N1-C2	2.81	121.42	109.92	9	2
4	A	417	PX4	C20-C19-C18	2.81	100.15	114.42	5	2
4	A	402	PX4	O1-P1-O3	2.81	94.69	107.75	6	2
4	A	417	PX4	O1-P1-O2	2.81	126.14	112.24	12	5
4	A	428	PX4	O7-C7-C8	2.81	118.58	108.40	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	371	PX4	C31-C30-C29	2.81	100.17	114.42	5	1
4	A	398	PX4	C18-C17-C16	2.81	100.16	114.42	2	3
4	A	339	PX4	C31-C30-C29	2.81	100.17	114.42	10	3
4	A	331	PX4	O5-C9-C10	2.81	120.72	111.91	7	4
4	A	404	PX4	C30-C29-C28	2.81	100.17	114.42	1	2
4	A	427	PX4	O3-C1-C2	2.81	123.93	109.16	6	1
4	A	354	PX4	O5-C9-C10	2.81	120.71	111.91	11	4
4	A	370	PX4	O1-P1-O4	2.81	120.78	107.75	1	2
4	A	373	PX4	C11-C10-C9	2.81	103.42	113.62	3	2
4	A	317	PX4	O7-C23-O8	2.80	130.48	123.70	2	3
4	A	334	PX4	O3-P1-O2	2.80	98.11	109.07	11	2
4	A	342	PX4	C12-C11-C10	2.80	103.11	113.19	1	3
4	A	368	PX4	C17-C16-C15	2.80	100.20	114.42	7	1
4	A	369	PX4	C11-C10-C9	2.80	123.82	113.62	4	2
4	A	369	PX4	O1-P1-O4	2.80	120.77	107.75	13	3
4	A	404	PX4	C25-C24-C23	2.80	123.82	113.62	14	3
4	A	410	PX4	C33-C32-C31	2.80	100.19	114.42	7	1
4	A	348	PX4	C14-C13-C12	2.80	100.21	114.42	5	2
4	A	353	PX4	C14-C13-C12	2.80	100.21	114.42	7	1
4	A	387	PX4	C25-C24-C23	2.80	103.43	113.62	10	2
4	A	381	PX4	C26-C25-C24	2.80	103.13	113.19	1	2
4	A	390	PX4	C5-N1-C3	2.80	101.77	108.97	2	3
4	A	415	PX4	O5-C9-C10	2.80	120.70	111.91	13	2
4	A	392	PX4	C12-C11-C10	2.80	103.13	113.19	7	1
4	A	427	PX4	C5-N1-C3	2.80	101.78	108.97	11	4
4	A	344	PX4	C27-C26-C25	2.80	100.22	114.42	10	2
4	A	366	PX4	C32-C31-C30	2.80	100.23	114.42	1	1
4	A	386	PX4	C15-C14-C13	2.80	100.23	114.42	5	2
4	A	403	PX4	C16-C15-C14	2.80	100.23	114.42	5	2
4	A	330	PX4	C25-C24-C23	2.79	103.46	113.62	6	1
4	A	340	PX4	C31-C30-C29	2.79	100.24	114.42	14	2
4	A	337	PX4	O5-C9-C10	2.79	120.67	111.91	5	1
4	A	356	PX4	C4-N1-C3	2.79	101.80	108.97	9	4
4	A	381	PX4	C14-C13-C12	2.79	100.26	114.42	7	1
4	A	399	PX4	C27-C26-C25	2.79	100.25	114.42	3	2
4	A	411	PX4	O5-C9-C10	2.79	120.67	111.91	13	4
4	A	315	PX4	C12-C11-C10	2.79	103.16	113.19	2	4
4	A	320	PX4	O1-P1-O3	2.79	94.79	107.75	8	2
4	A	404	PX4	O5-C9-C10	2.79	120.66	111.91	2	4
4	A	322	PX4	O5-C8-C7	2.79	116.55	108.43	6	4
4	A	422	PX4	O1-P1-O2	2.79	126.03	112.24	7	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	C26-C25-C24	2.79	103.17	113.19	13	2
4	A	326	PX4	C31-C30-C29	2.79	100.28	114.42	4	1
4	A	347	PX4	O1-P1-O3	2.78	94.81	107.75	5	1
4	A	358	PX4	C19-C18-C17	2.79	100.28	114.42	7	1
4	A	363	PX4	O1-P1-O3	2.79	94.80	107.75	6	3
4	A	370	PX4	C13-C12-C11	2.79	100.28	114.42	1	4
4	A	384	PX4	C13-C12-C11	2.79	100.27	114.42	4	1
4	A	365	PX4	O7-C7-C8	2.79	118.49	108.40	13	2
4	A	406	PX4	O1-P1-O3	2.79	94.81	107.75	5	2
4	A	306	PX4	O4-P1-O2	2.78	119.94	109.07	7	1
4	A	308	PX4	O5-C9-C10	2.78	120.64	111.91	6	4
4	A	327	PX4	O7-C7-C6	2.78	118.48	108.40	2	5
4	A	338	PX4	C7-O7-C23	2.78	124.64	117.79	2	8
4	A	405	PX4	O5-C9-C10	2.78	120.64	111.91	4	6
4	A	319	PX4	O7-C7-C8	2.78	118.47	108.40	6	6
4	A	323	PX4	C7-O7-C23	2.78	124.64	117.79	8	2
4	A	345	PX4	C3-N1-C2	2.78	98.54	109.92	2	2
4	A	388	PX4	C16-C15-C14	2.78	100.31	114.42	4	3
4	A	402	PX4	C15-C14-C13	2.78	100.30	114.42	14	2
4	A	419	PX4	C17-C16-C15	2.78	100.31	114.42	4	1
4	A	340	PX4	C11-C10-C9	2.78	103.52	113.62	14	2
4	A	377	PX4	O7-C7-C6	2.78	118.46	108.40	2	2
4	A	337	PX4	C5-N1-C4	2.78	101.84	108.97	7	2
4	A	343	PX4	C4-N1-C2	2.78	98.56	109.92	5	1
4	A	348	PX4	O1-P1-O2	2.78	125.97	112.24	1	5
4	A	380	PX4	O5-C9-O6	2.78	116.58	123.59	12	5
4	A	383	PX4	C4-N1-C3	2.78	101.84	108.97	4	1
4	A	414	PX4	O7-C7-C8	2.78	118.45	108.40	2	2
4	A	317	PX4	C3-N1-C2	2.77	98.56	109.92	14	1
4	A	327	PX4	C18-C17-C16	2.77	100.34	114.42	14	1
4	A	367	PX4	C34-C33-C32	2.77	100.34	114.42	11	2
4	A	368	PX4	O4-P1-O2	2.77	119.91	109.07	9	1
4	A	344	PX4	C4-N1-C3	2.77	101.85	108.97	6	3
4	A	369	PX4	C12-C11-C10	2.77	103.22	113.19	5	4
4	A	377	PX4	O7-C7-C8	2.77	118.44	108.40	5	6
4	A	342	PX4	O1-P1-O3	2.77	94.88	107.75	8	1
4	A	360	PX4	O5-C9-C10	2.77	120.60	111.91	11	1
4	A	392	PX4	C3-N1-C2	2.77	121.26	109.92	1	2
4	A	342	PX4	C4-N1-C3	2.77	101.85	108.97	12	2
4	A	350	PX4	O1-P1-O2	2.77	125.93	112.24	5	7
4	A	361	PX4	C8-O5-C9	2.77	106.86	117.12	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	374	PX4	C7-O7-C23	2.77	124.61	117.79	12	4
4	A	321	PX4	C3-N1-C2	2.77	121.24	109.92	13	2
4	A	374	PX4	O1-P1-O4	2.77	120.60	107.75	8	2
4	A	356	PX4	O5-C9-C10	2.77	120.59	111.91	10	3
4	A	377	PX4	O5-C9-O6	2.77	116.61	123.59	6	2
4	A	415	PX4	C11-C10-C9	2.77	103.56	113.62	14	1
4	A	430	PX4	C5-N1-C4	2.77	101.86	108.97	5	3
4	A	316	PX4	O4-P1-O2	2.76	119.87	109.07	14	3
4	A	337	PX4	C26-C25-C24	2.76	103.25	113.19	6	1
4	A	352	PX4	O5-C9-C10	2.76	120.58	111.91	6	6
4	A	425	PX4	O7-C7-C6	2.76	118.41	108.40	1	4
4	A	307	PX4	C11-C10-C9	2.76	103.57	113.62	14	3
4	A	379	PX4	C26-C25-C24	2.76	103.26	113.19	1	3
4	A	379	PX4	C8-O5-C9	2.76	106.89	117.12	9	1
4	A	381	PX4	O5-C9-O6	2.76	116.62	123.59	7	2
4	A	415	PX4	O1-P1-O3	2.76	94.91	107.75	14	5
4	A	312	PX4	C25-C24-C23	2.76	103.58	113.62	5	3
4	A	333	PX4	O1-P1-O4	2.76	120.57	107.75	3	4
4	A	352	PX4	O6-C9-C10	2.76	112.96	123.73	3	2
4	A	362	PX4	C8-O5-C9	2.76	106.90	117.12	3	2
4	A	376	PX4	O7-C7-C6	2.76	118.40	108.40	3	3
4	A	321	PX4	C12-C11-C10	2.76	103.27	113.19	4	2
4	A	323	PX4	O1-P1-O2	2.76	125.88	112.24	9	6
4	A	325	PX4	O4-P1-O2	2.76	119.84	109.07	11	3
4	A	340	PX4	C3-N1-C2	2.76	121.20	109.92	1	2
4	A	366	PX4	O5-C9-C10	2.76	120.57	111.91	10	2
4	A	396	PX4	O3-P1-O2	2.76	98.28	109.07	11	4
4	A	406	PX4	C8-O5-C9	2.76	106.91	117.12	6	1
4	A	414	PX4	C30-C29-C28	2.76	100.42	114.42	8	2
4	A	329	PX4	C3-N1-C2	2.76	121.19	109.92	5	2
4	A	346	PX4	O1-P1-O4	2.76	94.95	107.75	6	1
4	A	370	PX4	O7-C7-C6	2.76	118.38	108.40	11	4
4	A	380	PX4	C8-O5-C9	2.76	106.92	117.12	6	3
4	A	420	PX4	C16-C15-C14	2.76	100.44	114.42	11	1
4	A	423	PX4	C19-C18-C17	2.76	100.44	114.42	11	3
4	A	349	PX4	C26-C25-C24	2.75	103.29	113.19	9	2
4	A	360	PX4	C11-C10-C9	2.75	103.61	113.62	2	1
4	A	426	PX4	O7-C23-O8	2.75	117.05	123.70	7	4
4	A	306	PX4	O1-P1-O4	2.75	120.53	107.75	8	1
4	A	318	PX4	O3-C1-C2	2.75	123.62	109.16	10	1
4	A	326	PX4	C5-N1-C4	2.75	101.91	108.97	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	366	PX4	O8-C23-C24	2.75	113.00	123.73	13	2
4	A	372	PX4	C4-N1-C2	2.75	121.17	109.92	11	1
4	A	397	PX4	C25-C24-C23	2.75	103.62	113.62	9	2
4	A	368	PX4	O3-C1-C2	2.75	123.61	109.16	9	1
4	A	422	PX4	C3-N1-C2	2.75	121.16	109.92	5	1
4	A	353	PX4	C5-N1-C4	2.75	101.91	108.97	10	2
4	A	380	PX4	C5-N1-C3	2.75	101.92	108.97	12	3
4	A	387	PX4	O7-C7-C6	2.75	118.34	108.40	5	4
4	A	316	PX4	O7-C23-O8	2.75	117.07	123.70	7	3
4	A	330	PX4	O1-P1-O2	2.75	125.81	112.24	12	5
4	A	340	PX4	O7-C23-O8	2.75	117.07	123.70	11	7
4	A	377	PX4	C11-C10-C9	2.74	103.64	113.62	8	3
4	A	399	PX4	C14-C13-C12	2.74	100.49	114.42	7	3
4	A	413	PX4	O5-C9-O6	2.74	116.67	123.59	7	4
4	A	316	PX4	C11-C10-C9	2.74	123.60	113.62	5	1
4	A	350	PX4	O8-C23-C24	2.74	113.03	123.73	7	2
4	A	417	PX4	O7-C7-C8	2.74	118.33	108.40	11	5
4	A	420	PX4	C4-N1-C3	2.74	116.02	108.97	7	3
4	A	318	PX4	C7-O7-C23	2.74	124.53	117.79	11	6
4	A	335	PX4	C28-C27-C26	2.74	100.52	114.42	4	2
4	A	352	PX4	O1-P1-O3	2.74	95.02	107.75	4	1
4	A	361	PX4	C19-C18-C17	2.74	100.52	114.42	9	1
4	A	373	PX4	C4-N1-C3	2.74	116.02	108.97	10	1
4	A	389	PX4	O7-C7-C8	2.74	118.32	108.40	13	3
4	A	321	PX4	C4-N1-C3	2.74	101.94	108.97	2	2
4	A	339	PX4	C11-C10-C9	2.74	103.66	113.62	14	2
4	A	351	PX4	O1-P1-O2	2.74	125.78	112.24	4	3
4	A	361	PX4	O5-C9-C10	2.74	120.50	111.91	6	4
4	A	428	PX4	O4-P1-O2	2.74	119.77	109.07	5	2
4	A	379	PX4	C5-N1-C3	2.74	116.01	108.97	14	3
4	A	309	PX4	C28-C27-C26	2.74	100.54	114.42	13	3
4	A	325	PX4	C1-C2-N1	2.74	124.91	115.78	12	1
4	A	369	PX4	C8-O5-C9	2.74	106.99	117.12	7	2
4	A	315	PX4	O3-C1-C2	2.73	123.54	109.16	13	2
4	A	353	PX4	O4-P1-O2	2.73	119.75	109.07	2	3
4	A	370	PX4	C5-N1-C3	2.73	101.94	108.97	6	3
4	A	313	PX4	C1-C2-N1	2.73	124.90	115.78	8	4
4	A	323	PX4	C4-N1-C3	2.73	101.95	108.97	11	4
4	A	331	PX4	O3-P1-O2	2.73	98.39	109.07	7	4
4	A	371	PX4	C32-C31-C30	2.73	100.55	114.42	2	2
4	A	314	PX4	C26-C25-C24	2.73	103.37	113.19	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	337	PX4	C29-C28-C27	2.73	100.56	114.42	5	1
4	A	334	PX4	C27-C26-C25	2.73	100.57	114.42	14	2
4	A	361	PX4	O1-P1-O4	2.73	120.43	107.75	10	3
4	A	365	PX4	C8-C7-C6	2.73	105.33	111.79	8	9
4	A	406	PX4	C28-C27-C26	2.73	100.56	114.42	6	3
4	A	362	PX4	C14-C13-C12	2.73	100.57	114.42	13	2
4	A	397	PX4	C5-N1-C2	2.73	121.08	109.92	8	3
4	A	421	PX4	C4-N1-C3	2.73	101.96	108.97	2	1
4	A	346	PX4	O4-P1-O2	2.73	98.41	109.07	7	2
4	A	421	PX4	C5-N1-C3	2.73	101.96	108.97	7	2
4	A	371	PX4	C1-C2-N1	2.73	124.88	115.78	2	2
4	A	406	PX4	C19-C18-C17	2.73	100.58	114.42	12	1
4	A	312	PX4	C30-C29-C28	2.72	100.59	114.42	4	1
4	A	385	PX4	O5-C9-O6	2.73	116.71	123.59	4	3
4	A	314	PX4	C12-C11-C10	2.72	103.40	113.19	11	2
4	A	324	PX4	C34-C33-C32	2.72	100.61	114.42	11	1
4	A	371	PX4	C33-C32-C31	2.72	100.61	114.42	7	2
4	A	375	PX4	C14-C13-C12	2.72	100.61	114.42	8	1
4	A	405	PX4	O3-C1-C2	2.72	123.48	109.16	14	1
4	A	372	PX4	C5-N1-C2	2.72	121.04	109.92	4	2
4	A	376	PX4	O6-C9-C10	2.72	113.12	123.73	11	4
4	A	385	PX4	C1-C2-N1	2.72	124.86	115.78	7	3
4	A	399	PX4	O1-P1-O4	2.72	120.37	107.75	10	1
4	A	307	PX4	C20-C19-C18	2.72	100.63	114.42	2	2
4	A	398	PX4	C4-N1-C2	2.72	121.03	109.92	1	2
4	A	394	PX4	C11-C10-C9	2.72	123.50	113.62	14	2
4	A	389	PX4	C1-C2-N1	2.71	124.84	115.78	12	2
4	A	401	PX4	O1-P1-O2	2.72	125.66	112.24	10	4
4	A	315	PX4	C25-C24-C23	2.71	103.75	113.62	9	2
4	A	392	PX4	C11-C10-C9	2.71	103.75	113.62	4	2
4	A	399	PX4	C19-C18-C17	2.71	100.65	114.42	3	2
4	A	403	PX4	C14-C13-C12	2.71	100.65	114.42	11	3
4	A	307	PX4	C15-C14-C13	2.71	100.66	114.42	1	1
4	A	349	PX4	C27-C26-C25	2.71	100.66	114.42	14	2
4	A	352	PX4	O1-P1-O4	2.71	120.34	107.75	5	1
4	A	401	PX4	C8-O5-C9	2.71	107.08	117.12	8	5
4	A	324	PX4	O3-C1-C2	2.71	123.41	109.16	11	3
4	A	325	PX4	C4-N1-C3	2.71	102.01	108.97	9	2
4	A	391	PX4	C27-C26-C25	2.71	100.67	114.42	2	1
4	A	412	PX4	O1-P1-O3	2.71	95.16	107.75	8	3
4	A	426	PX4	O3-P1-O2	2.71	98.48	109.07	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	399	PX4	C4-N1-C3	2.71	115.94	108.97	1	3
4	A	342	PX4	O1-P1-O4	2.71	120.32	107.75	8	2
4	A	358	PX4	C29-C28-C27	2.71	100.68	114.42	8	3
4	A	376	PX4	C19-C18-C17	2.71	100.68	114.42	4	1
4	A	393	PX4	C17-C16-C15	2.71	100.68	114.42	13	1
4	A	423	PX4	C12-C11-C10	2.71	122.93	113.19	2	3
4	A	413	PX4	C31-C30-C29	2.71	100.68	114.42	9	1
4	A	329	PX4	C5-N1-C4	2.71	102.02	108.97	4	3
4	A	330	PX4	P1-O4-C6	2.71	105.81	121.68	7	6
4	A	349	PX4	C34-C33-C32	2.71	100.69	114.42	5	2
4	A	371	PX4	O5-C9-O6	2.71	116.76	123.59	10	2
4	A	392	PX4	C4-N1-C2	2.71	120.99	109.92	9	3
4	A	414	PX4	C1-C2-N1	2.71	124.81	115.78	14	3
4	A	425	PX4	C14-C13-C12	2.71	100.69	114.42	8	1
4	A	409	PX4	C25-C24-C23	2.70	103.79	113.62	6	2
4	A	416	PX4	P1-O4-C6	2.70	105.82	121.68	9	4
4	A	420	PX4	C20-C19-C18	2.70	100.69	114.42	6	2
4	A	334	PX4	C29-C28-C27	2.70	100.70	114.42	12	3
4	A	344	PX4	C33-C32-C31	2.70	100.70	114.42	8	1
4	A	343	PX4	O1-P1-O2	2.70	125.60	112.24	4	6
4	A	358	PX4	C7-O7-C23	2.70	124.44	117.79	1	3
4	A	365	PX4	O7-C7-C6	2.70	118.19	108.40	12	2
4	A	368	PX4	O5-C9-C10	2.70	120.39	111.91	9	1
4	A	357	PX4	O7-C7-C6	2.70	118.18	108.40	11	3
4	A	348	PX4	O7-C7-C8	2.70	118.18	108.40	3	2
4	A	373	PX4	C5-N1-C3	2.70	115.92	108.97	11	1
4	A	396	PX4	C18-C17-C16	2.70	100.72	114.42	8	2
4	A	403	PX4	C11-C10-C9	2.70	103.80	113.62	3	1
4	A	342	PX4	C25-C24-C23	2.70	103.81	113.62	11	3
4	A	356	PX4	C29-C28-C27	2.70	100.73	114.42	4	1
4	A	360	PX4	C27-C26-C25	2.70	100.73	114.42	6	2
4	A	381	PX4	O7-C23-O8	2.70	117.18	123.70	5	3
4	A	413	PX4	C12-C11-C10	2.70	103.49	113.19	4	3
4	A	326	PX4	C19-C18-C17	2.70	100.74	114.42	4	2
4	A	327	PX4	C3-N1-C2	2.70	120.95	109.92	3	1
4	A	344	PX4	C25-C24-C23	2.70	123.42	113.62	4	1
4	A	362	PX4	P1-O4-C6	2.70	105.87	121.68	4	5
4	A	364	PX4	C20-C19-C18	2.70	100.74	114.42	11	1
4	A	401	PX4	C16-C15-C14	2.70	100.74	114.42	13	1
4	A	385	PX4	O7-C23-O8	2.69	117.19	123.70	1	2
4	A	371	PX4	O6-C9-C10	2.69	134.24	123.73	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	387	PX4	C26-C25-C24	2.69	103.50	113.19	9	4
4	A	324	PX4	C5-N1-C4	2.69	102.05	108.97	10	2
4	A	324	PX4	C32-C31-C30	2.69	100.76	114.42	11	1
4	A	330	PX4	C1-C2-N1	2.69	124.77	115.78	8	3
4	A	356	PX4	O8-C23-C24	2.69	113.22	123.73	7	1
4	A	375	PX4	O6-C9-C10	2.69	113.23	123.73	12	1
4	A	393	PX4	C18-C17-C16	2.69	100.75	114.42	6	1
4	A	397	PX4	C13-C12-C11	2.69	100.75	114.42	14	2
4	A	425	PX4	C1-C2-N1	2.69	124.77	115.78	8	2
4	A	374	PX4	O1-P1-O3	2.69	95.24	107.75	3	3
4	A	380	PX4	C13-C12-C11	2.69	100.76	114.42	6	1
4	A	348	PX4	C25-C24-C23	2.69	103.84	113.62	5	1
4	A	355	PX4	O5-C9-C10	2.69	120.35	111.91	5	2
4	A	322	PX4	C1-C2-N1	2.69	124.76	115.78	6	1
4	A	348	PX4	O5-C9-C10	2.69	120.34	111.91	7	6
4	A	394	PX4	C3-N1-C2	2.69	120.92	109.92	8	1
4	A	406	PX4	C5-N1-C3	2.69	102.06	108.97	13	1
4	A	384	PX4	C25-C24-C23	2.69	103.85	113.62	9	1
4	A	318	PX4	C1-C2-N1	2.69	124.75	115.78	1	2
4	A	398	PX4	O6-C9-C10	2.69	113.25	123.73	2	1
4	A	419	PX4	O3-C1-C2	2.69	123.29	109.16	10	1
4	A	321	PX4	O1-P1-O4	2.68	120.22	107.75	1	5
4	A	356	PX4	O4-P1-O2	2.69	119.56	109.07	14	3
4	A	308	PX4	C20-C19-C18	2.68	100.80	114.42	9	1
4	A	374	PX4	C30-C29-C28	2.68	100.80	114.42	3	1
4	A	381	PX4	C8-O5-C9	2.68	127.06	117.12	2	1
4	A	392	PX4	C20-C19-C18	2.68	100.80	114.42	14	2
4	A	411	PX4	O4-P1-O2	2.68	119.55	109.07	14	5
4	A	414	PX4	C25-C24-C23	2.68	123.38	113.62	7	1
4	A	317	PX4	O4-P1-O2	2.68	119.55	109.07	3	1
4	A	362	PX4	O7-C23-O8	2.68	117.22	123.70	4	1
4	A	320	PX4	C12-C11-C10	2.68	103.55	113.19	13	2
4	A	377	PX4	O1-P1-O4	2.68	120.20	107.75	9	1
4	A	385	PX4	C19-C18-C17	2.68	100.81	114.42	12	1
4	A	404	PX4	C34-C33-C32	2.68	100.81	114.42	11	1
4	A	418	PX4	C17-C16-C15	2.68	100.82	114.42	12	1
4	A	326	PX4	O6-C9-C10	2.68	113.28	123.73	7	2
4	A	399	PX4	C7-O7-C23	2.68	111.20	117.79	8	3
4	A	386	PX4	C26-C25-C24	2.68	103.57	113.19	5	2
4	A	389	PX4	O4-P1-O2	2.68	119.53	109.07	3	1
4	A	420	PX4	C5-N1-C4	2.68	102.09	108.97	1	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	322	PX4	C29-C28-C27	2.68	100.84	114.42	6	2
4	A	344	PX4	C26-C25-C24	2.68	103.57	113.19	14	2
4	A	356	PX4	C13-C12-C11	2.68	100.84	114.42	5	2
4	A	373	PX4	C20-C19-C18	2.68	100.84	114.42	14	3
4	A	388	PX4	C25-C24-C23	2.68	103.89	113.62	5	1
4	A	419	PX4	C8-O5-C9	2.68	107.21	117.12	5	2
4	A	401	PX4	O7-C23-O8	2.67	117.24	123.70	8	1
4	A	412	PX4	O4-P1-O2	2.67	98.62	109.07	4	6
4	A	324	PX4	C29-C28-C27	2.67	100.86	114.42	14	3
4	A	351	PX4	C31-C30-C29	2.67	100.85	114.42	4	2
4	A	404	PX4	C5-N1-C2	2.67	120.85	109.92	10	1
4	A	405	PX4	C12-C11-C10	2.67	103.58	113.19	6	3
4	A	417	PX4	C27-C26-C25	2.67	100.85	114.42	14	2
4	A	407	PX4	C29-C28-C27	2.67	100.86	114.42	11	2
4	A	409	PX4	O8-C23-C24	2.67	113.31	123.73	4	1
4	A	419	PX4	O4-P1-O2	2.67	98.62	109.07	12	2
4	A	385	PX4	O7-C7-C6	2.67	118.08	108.40	3	3
4	A	323	PX4	C28-C27-C26	2.67	100.87	114.42	3	2
4	A	326	PX4	O1-P1-O4	2.67	120.15	107.75	11	2
4	A	339	PX4	C4-N1-C2	2.67	98.99	109.92	10	3
4	A	346	PX4	O5-C9-C10	2.67	120.29	111.91	3	2
4	A	312	PX4	O5-C9-O6	2.67	116.86	123.59	2	2
4	A	337	PX4	C34-C33-C32	2.67	100.87	114.42	5	3
4	A	373	PX4	C17-C16-C15	2.67	100.87	114.42	3	1
4	A	391	PX4	C33-C32-C31	2.67	100.87	114.42	7	2
4	A	338	PX4	O1-P1-O2	2.67	125.44	112.24	1	7
4	A	314	PX4	O3-C1-C2	2.67	123.19	109.16	5	1
4	A	328	PX4	C16-C15-C14	2.67	100.88	114.42	5	2
4	A	353	PX4	C12-C11-C10	2.67	103.60	113.19	10	3
4	A	367	PX4	C5-N1-C4	2.67	115.83	108.97	5	2
4	A	398	PX4	C17-C16-C15	2.67	100.88	114.42	2	2
4	A	404	PX4	O1-P1-O2	2.67	125.43	112.24	3	4
4	A	375	PX4	C11-C10-C9	2.67	103.92	113.62	1	3
4	A	391	PX4	O7-C23-O8	2.67	117.26	123.70	7	2
4	A	400	PX4	C7-O7-C23	2.67	124.36	117.79	4	4
4	A	414	PX4	C4-N1-C3	2.67	102.12	108.97	13	3
4	A	367	PX4	C7-O7-C23	2.67	124.35	117.79	3	4
4	A	319	PX4	O7-C23-O8	2.66	117.26	123.70	13	4
4	A	320	PX4	C15-C14-C13	2.66	100.90	114.42	2	2
4	A	406	PX4	C33-C32-C31	2.66	100.90	114.42	11	2
4	A	407	PX4	O1-P1-O3	2.67	95.37	107.75	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	340	PX4	O1-P1-O2	2.66	125.41	112.24	1	5
4	A	318	PX4	C4-N1-C3	2.66	102.13	108.97	10	2
4	A	319	PX4	C4-N1-C3	2.66	102.13	108.97	5	4
4	A	354	PX4	C4-N1-C3	2.66	102.13	108.97	13	4
4	A	308	PX4	C33-C32-C31	2.66	100.92	114.42	8	1
4	A	324	PX4	C11-C10-C9	2.66	103.94	113.62	2	1
4	A	375	PX4	C5-N1-C4	2.66	102.13	108.97	14	1
4	A	340	PX4	C15-C14-C13	2.66	100.93	114.42	13	1
4	A	346	PX4	C4-N1-C2	2.66	99.04	109.92	12	3
4	A	378	PX4	C4-N1-C2	2.66	120.80	109.92	8	1
4	A	345	PX4	O7-C23-C24	2.66	117.23	111.50	7	3
4	A	374	PX4	C33-C32-C31	2.66	100.93	114.42	6	3
4	A	318	PX4	C14-C13-C12	2.66	100.94	114.42	8	1
4	A	334	PX4	C8-O5-C9	2.66	107.28	117.12	12	2
4	A	380	PX4	O6-C9-C10	2.66	113.37	123.73	10	2
4	A	414	PX4	C5-N1-C3	2.66	102.14	108.97	6	2
4	A	309	PX4	O4-P1-O2	2.65	119.44	109.07	14	7
4	A	327	PX4	C8-O5-C9	2.65	107.29	117.12	12	1
4	A	329	PX4	O5-C9-C10	2.66	120.24	111.91	9	7
4	A	330	PX4	O7-C7-C8	2.66	118.02	108.40	1	6
4	A	382	PX4	C15-C14-C13	2.66	100.94	114.42	2	2
4	A	308	PX4	C13-C12-C11	2.65	100.96	114.42	8	2
4	A	311	PX4	O1-P1-O2	2.65	125.36	112.24	8	3
4	A	316	PX4	O3-C1-C2	2.65	123.12	109.16	3	1
4	A	374	PX4	C4-N1-C3	2.65	102.15	108.97	5	3
4	A	376	PX4	C12-C11-C10	2.65	103.65	113.19	10	2
4	A	359	PX4	C1-C2-N1	2.65	124.63	115.78	4	4
4	A	367	PX4	C12-C11-C10	2.65	103.66	113.19	9	1
4	A	390	PX4	C8-O5-C9	2.65	107.30	117.12	5	2
4	A	391	PX4	C19-C18-C17	2.65	100.96	114.42	12	2
4	A	390	PX4	C30-C29-C28	2.65	100.97	114.42	12	1
4	A	410	PX4	C3-N1-C2	2.65	120.77	109.92	13	2
4	A	420	PX4	O6-C9-C10	2.65	113.39	123.73	13	2
4	A	307	PX4	C13-C12-C11	2.65	100.97	114.42	10	2
4	A	419	PX4	C30-C29-C28	2.65	100.97	114.42	12	1
4	A	422	PX4	O1-P1-O3	2.65	95.44	107.75	4	3
4	A	325	PX4	C20-C19-C18	2.65	100.98	114.42	5	2
4	A	348	PX4	C12-C11-C10	2.65	103.67	113.19	2	3
4	A	350	PX4	O4-P1-O2	2.65	119.42	109.07	7	6
4	A	426	PX4	C19-C18-C17	2.65	100.98	114.42	10	1
4	A	430	PX4	C13-C12-C11	2.65	100.97	114.42	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	385	PX4	O1-P1-O4	2.65	120.04	107.75	4	1
4	A	323	PX4	C11-C10-C9	2.65	103.99	113.62	9	2
4	A	345	PX4	O8-C23-C24	2.65	113.41	123.73	2	1
4	A	360	PX4	C12-C11-C10	2.65	103.68	113.19	5	1
4	A	315	PX4	O5-C9-C10	2.64	120.21	111.91	11	2
4	A	337	PX4	C5-N1-C2	2.65	120.74	109.92	2	2
4	A	384	PX4	C4-N1-C3	2.65	102.17	108.97	12	2
4	A	400	PX4	C1-C2-N1	2.65	124.61	115.78	5	3
4	A	348	PX4	C31-C30-C29	2.64	101.00	114.42	1	2
4	A	364	PX4	C31-C30-C29	2.64	101.00	114.42	6	1
4	A	320	PX4	C16-C15-C14	2.64	101.01	114.42	12	4
4	A	322	PX4	C8-O5-C9	2.64	107.33	117.12	14	2
4	A	382	PX4	O1-P1-O4	2.64	120.02	107.75	6	3
4	A	414	PX4	C7-O7-C23	2.64	124.30	117.79	11	2
4	A	341	PX4	O4-P1-O2	2.64	98.75	109.07	7	1
4	A	372	PX4	O1-P1-O3	2.64	95.48	107.75	3	2
4	A	358	PX4	C27-C26-C25	2.64	101.02	114.42	2	1
4	A	320	PX4	C18-C17-C16	2.64	101.03	114.42	10	3
4	A	333	PX4	C14-C13-C12	2.64	101.04	114.42	9	2
4	A	354	PX4	C12-C11-C10	2.64	103.71	113.19	2	2
4	A	365	PX4	O8-C23-C24	2.64	113.44	123.73	13	1
4	A	391	PX4	C26-C25-C24	2.64	103.71	113.19	12	1
4	A	366	PX4	C1-C2-N1	2.64	124.58	115.78	2	3
4	A	383	PX4	C1-C2-N1	2.64	124.58	115.78	9	2
4	A	388	PX4	C15-C14-C13	2.64	101.04	114.42	14	2
4	A	316	PX4	C5-N1-C3	2.63	115.75	108.97	5	1
4	A	335	PX4	C15-C14-C13	2.63	101.05	114.42	1	3
4	A	375	PX4	O3-C1-C2	2.63	123.02	109.16	13	1
4	A	423	PX4	C3-N1-C2	2.64	120.70	109.92	9	2
4	A	356	PX4	C34-C33-C32	2.63	101.06	114.42	12	2
4	A	377	PX4	C1-C2-N1	2.63	124.57	115.78	3	2
4	A	417	PX4	O1-P1-O4	2.63	119.97	107.75	14	2
4	A	312	PX4	C28-C27-C26	2.63	101.06	114.42	1	3
4	A	335	PX4	C31-C30-C29	2.63	101.07	114.42	6	1
4	A	338	PX4	C31-C30-C29	2.63	101.07	114.42	8	1
4	A	365	PX4	C20-C19-C18	2.63	101.07	114.42	13	1
4	A	379	PX4	C20-C19-C18	2.63	101.08	114.42	2	1
4	A	392	PX4	C33-C32-C31	2.63	101.07	114.42	9	1
4	A	408	PX4	C27-C26-C25	2.63	101.07	114.42	5	5
4	A	329	PX4	O6-C9-C10	2.63	113.47	123.73	5	1
4	A	410	PX4	C8-O5-C9	2.63	126.86	117.12	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	421	PX4	C1-C2-N1	2.63	124.56	115.78	9	2
4	A	428	PX4	C5-N1-C4	2.63	115.74	108.97	1	3
4	A	307	PX4	O5-C9-O6	2.63	116.96	123.59	4	1
4	A	308	PX4	C32-C31-C30	2.63	101.08	114.42	13	2
4	A	316	PX4	C1-C2-N1	2.63	124.56	115.78	4	4
4	A	336	PX4	C33-C32-C31	2.63	101.08	114.42	4	1
4	A	351	PX4	C5-N1-C2	2.63	99.16	109.92	1	4
4	A	406	PX4	C5-N1-C4	2.63	102.22	108.97	12	2
4	A	320	PX4	C13-C12-C11	2.63	101.10	114.42	1	2
4	A	352	PX4	C34-C33-C32	2.63	101.09	114.42	8	2
4	A	373	PX4	O3-C1-C2	2.63	122.97	109.16	4	1
4	A	382	PX4	C5-N1-C4	2.63	102.22	108.97	4	2
4	A	393	PX4	C4-N1-C2	2.63	120.66	109.92	12	1
4	A	351	PX4	C32-C31-C30	2.63	101.10	114.42	13	1
4	A	320	PX4	O4-P1-O2	2.62	119.32	109.07	2	3
4	A	330	PX4	O4-P1-O2	2.62	98.81	109.07	8	3
4	A	343	PX4	C32-C31-C30	2.62	101.11	114.42	2	3
4	A	358	PX4	O7-C7-C6	2.62	117.90	108.40	10	6
4	A	416	PX4	C1-C2-N1	2.62	124.54	115.78	14	3
4	A	310	PX4	O1-P1-O4	2.62	119.92	107.75	11	4
4	A	386	PX4	C5-N1-C4	2.62	102.23	108.97	7	3
4	A	355	PX4	C8-O5-C9	2.62	126.83	117.12	10	1
4	A	398	PX4	C25-C24-C23	2.62	104.08	113.62	2	2
4	A	410	PX4	C1-C2-N1	2.62	124.53	115.78	7	5
4	A	312	PX4	C12-C11-C10	2.62	103.77	113.19	4	2
4	A	316	PX4	C29-C28-C27	2.62	101.13	114.42	9	1
4	A	334	PX4	C17-C16-C15	2.62	101.12	114.42	14	1
4	A	397	PX4	O7-C7-C6	2.62	117.88	108.40	8	2
4	A	403	PX4	O4-P1-O2	2.62	119.30	109.07	8	1
4	A	405	PX4	C30-C29-C28	2.62	101.13	114.42	13	1
4	A	339	PX4	C7-O7-C23	2.62	111.35	117.79	2	2
4	A	354	PX4	O1-P1-O3	2.62	95.59	107.75	4	3
4	A	356	PX4	O7-C23-O8	2.62	117.38	123.70	10	1
4	A	376	PX4	C26-C25-C24	2.62	103.78	113.19	2	3
4	A	399	PX4	C3-N1-C2	2.62	99.21	109.92	12	3
4	A	347	PX4	O1-P1-O4	2.62	119.89	107.75	5	2
4	A	360	PX4	C8-O5-C9	2.62	107.43	117.12	13	1
4	A	403	PX4	C34-C33-C32	2.62	101.14	114.42	1	1
4	A	412	PX4	C25-C24-C23	2.62	104.10	113.62	7	3
4	A	418	PX4	C30-C29-C28	2.62	101.14	114.42	5	1
4	A	363	PX4	C32-C31-C30	2.62	101.15	114.42	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	C7-O7-C23	2.62	124.23	117.79	8	5
4	A	381	PX4	O4-P1-O2	2.61	119.28	109.07	6	2
4	A	351	PX4	C34-C33-C32	2.61	101.16	114.42	14	1
4	A	408	PX4	C19-C18-C17	2.61	101.16	114.42	7	2
4	A	347	PX4	C27-C26-C25	2.61	127.68	114.42	5	1
4	A	354	PX4	C5-N1-C2	2.61	120.60	109.92	9	3
4	A	371	PX4	C5-N1-C4	2.61	102.26	108.97	7	2
4	A	388	PX4	C1-C2-N1	2.61	124.50	115.78	6	3
4	A	407	PX4	C16-C15-C14	2.61	101.17	114.42	12	1
4	A	428	PX4	O1-P1-O2	2.61	125.15	112.24	5	7
4	A	318	PX4	C27-C26-C25	2.61	101.18	114.42	14	1
4	A	351	PX4	O3-C1-C2	2.61	122.88	109.16	6	2
4	A	366	PX4	C8-O5-C9	2.61	107.46	117.12	13	1
4	A	366	PX4	C5-N1-C4	2.61	102.27	108.97	7	3
4	A	374	PX4	C5-N1-C4	2.61	102.27	108.97	13	3
4	A	326	PX4	O4-P1-O2	2.61	119.25	109.07	11	3
4	A	347	PX4	C4-N1-C3	2.61	102.27	108.97	10	1
4	A	323	PX4	C8-O5-C9	2.61	107.47	117.12	1	2
4	A	323	PX4	C30-C29-C28	2.61	101.20	114.42	5	1
4	A	363	PX4	C13-C12-C11	2.61	101.20	114.42	2	2
4	A	421	PX4	O6-C9-C10	2.61	113.57	123.73	9	1
4	A	374	PX4	C11-C10-C9	2.60	104.15	113.62	1	2
4	A	393	PX4	C12-C11-C10	2.60	103.83	113.19	9	5
4	A	428	PX4	O3-C1-C2	2.60	122.86	109.16	9	1
4	A	317	PX4	C25-C24-C23	2.60	123.09	113.62	7	2
4	A	340	PX4	C29-C28-C27	2.60	101.21	114.42	6	2
4	A	359	PX4	O5-C9-C10	2.60	120.07	111.91	6	4
4	A	376	PX4	C32-C31-C30	2.60	101.21	114.42	11	2
4	A	382	PX4	C12-C11-C10	2.60	103.83	113.19	5	1
4	A	338	PX4	C4-N1-C2	2.60	120.56	109.92	13	2
4	A	351	PX4	C25-C24-C23	2.60	104.16	113.62	14	1
4	A	359	PX4	C4-N1-C3	2.60	102.29	108.97	3	3
4	A	393	PX4	O5-C9-O6	2.60	117.03	123.59	4	4
4	A	371	PX4	C8-O5-C9	2.60	107.50	117.12	5	2
4	A	410	PX4	C28-C27-C26	2.60	101.23	114.42	3	2
4	A	323	PX4	C14-C13-C12	2.60	101.24	114.42	9	3
4	A	327	PX4	C33-C32-C31	2.60	101.24	114.42	13	1
4	A	337	PX4	C33-C32-C31	2.60	101.24	114.42	8	2
4	A	345	PX4	C11-C10-C9	2.60	104.17	113.62	10	2
4	A	350	PX4	O1-P1-O3	2.60	95.68	107.75	13	2
4	A	426	PX4	C28-C27-C26	2.60	101.24	114.42	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	340	PX4	O8-C23-C24	2.60	113.61	123.73	12	2
4	A	370	PX4	O7-C7-C8	2.60	117.80	108.40	8	2
4	A	370	PX4	C31-C30-C29	2.60	101.24	114.42	7	1
4	A	426	PX4	C17-C16-C15	2.60	101.25	114.42	2	1
4	A	430	PX4	C29-C28-C27	2.60	101.24	114.42	1	1
4	A	344	PX4	O3-C1-C2	2.59	122.81	109.16	11	2
4	A	360	PX4	C5-N1-C2	2.59	120.53	109.92	12	3
4	A	311	PX4	C20-C19-C18	2.59	101.26	114.42	8	2
4	A	327	PX4	C20-C19-C18	2.59	101.26	114.42	5	3
4	A	373	PX4	C5-N1-C4	2.59	102.31	108.97	5	1
4	A	412	PX4	O5-C9-C10	2.59	120.05	111.91	7	2
4	A	329	PX4	C32-C31-C30	2.59	127.58	114.42	11	1
4	A	330	PX4	O1-P1-O4	2.59	119.78	107.75	3	2
4	A	308	PX4	O7-C7-C6	2.59	117.78	108.40	5	2
4	A	313	PX4	C17-C16-C15	2.59	101.28	114.42	7	1
4	A	393	PX4	C5-N1-C3	2.59	102.32	108.97	7	3
4	A	319	PX4	C28-C27-C26	2.59	101.29	114.42	9	2
4	A	378	PX4	C33-C32-C31	2.59	101.29	114.42	1	2
4	A	387	PX4	O6-C9-C10	2.59	113.64	123.73	9	1
4	A	427	PX4	C16-C15-C14	2.59	101.28	114.42	1	3
4	A	308	PX4	C18-C17-C16	2.59	101.30	114.42	9	1
4	A	332	PX4	C27-C26-C25	2.59	101.29	114.42	12	1
4	A	346	PX4	C1-C2-N1	2.59	124.42	115.78	9	3
4	A	328	PX4	C18-C17-C16	2.59	101.30	114.42	5	2
4	A	350	PX4	O5-C9-C10	2.59	120.02	111.91	11	3
4	A	405	PX4	O5-C9-O6	2.59	117.06	123.59	1	2
4	A	407	PX4	C15-C14-C13	2.59	101.29	114.42	13	1
4	A	307	PX4	C8-O5-C9	2.58	107.55	117.12	5	2
4	A	369	PX4	C30-C29-C28	2.58	101.30	114.42	12	2
4	A	306	PX4	C16-C15-C14	2.58	101.31	114.42	7	1
4	A	327	PX4	C14-C13-C12	2.58	101.31	114.42	12	1
4	A	359	PX4	O1-P1-O4	2.58	119.75	107.75	11	2
4	A	382	PX4	C14-C13-C12	2.58	101.31	114.42	3	1
4	A	407	PX4	C26-C25-C24	2.58	122.48	113.19	6	2
4	A	342	PX4	C5-N1-C4	2.58	115.61	108.97	6	3
4	A	416	PX4	O4-P1-O2	2.58	119.16	109.07	10	4
4	A	376	PX4	C16-C15-C14	2.58	101.31	114.42	5	1
4	A	419	PX4	O5-C9-C10	2.58	120.01	111.91	3	3
4	A	421	PX4	C25-C24-C23	2.58	104.23	113.62	4	2
4	A	328	PX4	C20-C19-C18	2.58	101.32	114.42	13	1
4	A	348	PX4	C30-C29-C28	2.58	101.33	114.42	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	429	PX4	C5-N1-C2	2.58	99.36	109.92	13	1
4	A	317	PX4	C26-C25-C24	2.58	103.92	113.19	5	1
4	A	330	PX4	C12-C11-C10	2.58	103.92	113.19	10	1
4	A	363	PX4	C26-C25-C24	2.58	103.92	113.19	7	3
4	A	309	PX4	C25-C24-C23	2.58	104.25	113.62	5	1
4	A	343	PX4	O4-P1-O2	2.58	119.13	109.07	2	2
4	A	351	PX4	C18-C17-C16	2.58	101.34	114.42	11	1
4	A	390	PX4	O7-C7-C6	2.58	117.73	108.40	10	2
4	A	371	PX4	C14-C13-C12	2.58	101.35	114.42	12	1
4	A	397	PX4	C17-C16-C15	2.58	101.35	114.42	6	1
4	A	402	PX4	C19-C18-C17	2.58	101.35	114.42	13	1
4	A	310	PX4	C1-C2-N1	2.57	124.36	115.78	8	3
4	A	364	PX4	O4-P1-O2	2.57	119.11	109.07	13	3
4	A	316	PX4	C34-C33-C32	2.57	101.38	114.42	14	1
4	A	323	PX4	O3-P1-O2	2.57	99.02	109.07	12	2
4	A	325	PX4	C13-C12-C11	2.57	101.37	114.42	12	2
4	A	326	PX4	O1-P1-O3	2.57	95.80	107.75	6	1
4	A	378	PX4	C8-O5-C9	2.57	107.60	117.12	3	2
4	A	400	PX4	O5-C9-O6	2.57	117.10	123.59	11	3
4	A	329	PX4	C14-C13-C12	2.57	101.37	114.42	2	2
4	A	374	PX4	C20-C19-C18	2.57	101.37	114.42	6	1
4	A	400	PX4	O5-C9-C10	2.57	119.98	111.91	11	2
4	A	416	PX4	O1-P1-O4	2.57	119.69	107.75	13	2
4	A	358	PX4	C15-C14-C13	2.57	101.38	114.42	10	1
4	A	419	PX4	C12-C11-C10	2.57	103.95	113.19	13	3
4	A	402	PX4	C32-C31-C30	2.57	101.38	114.42	9	1
4	A	423	PX4	O4-P1-O2	2.57	119.11	109.07	1	2
4	A	357	PX4	C5-N1-C2	2.57	99.41	109.92	5	2
4	A	414	PX4	C33-C32-C31	2.57	101.38	114.42	1	1
4	A	417	PX4	O5-C9-C10	2.57	119.97	111.91	7	3
4	A	362	PX4	C30-C29-C28	2.57	101.39	114.42	6	1
4	A	340	PX4	O5-C9-C10	2.57	119.96	111.91	12	3
4	A	361	PX4	C11-C10-C9	2.57	104.29	113.62	14	2
4	A	372	PX4	O7-C7-C6	2.57	117.69	108.40	1	5
4	A	384	PX4	O7-C7-C6	2.57	117.69	108.40	1	2
4	A	388	PX4	O4-P1-O2	2.57	119.10	109.07	10	1
4	A	393	PX4	C25-C24-C23	2.57	104.29	113.62	14	1
4	A	409	PX4	C13-C12-C11	2.57	101.40	114.42	10	1
4	A	310	PX4	C3-N1-C2	2.56	120.41	109.92	1	1
4	A	366	PX4	C34-C33-C32	2.56	101.41	114.42	6	2
4	A	423	PX4	C28-C27-C26	2.56	101.42	114.42	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	372	PX4	C27-C26-C25	2.56	101.42	114.42	13	1
4	A	378	PX4	C14-C13-C12	2.56	101.42	114.42	1	1
4	A	381	PX4	C29-C28-C27	2.56	101.43	114.42	8	2
4	A	392	PX4	C28-C27-C26	2.56	101.43	114.42	14	2
4	A	394	PX4	C31-C30-C29	2.56	101.42	114.42	9	1
4	A	309	PX4	O1-P1-O3	2.56	95.86	107.75	11	4
4	A	318	PX4	C5-N1-C4	2.56	102.39	108.97	2	2
4	A	347	PX4	C5-N1-C3	2.56	102.39	108.97	4	3
4	A	369	PX4	C3-N1-C2	2.56	120.39	109.92	12	2
4	A	404	PX4	C31-C30-C29	2.56	101.43	114.42	5	1
4	A	420	PX4	O4-P1-O2	2.56	99.06	109.07	13	1
4	A	422	PX4	C5-N1-C4	2.56	102.39	108.97	9	3
4	A	364	PX4	C4-N1-C2	2.56	120.38	109.92	13	2
4	A	306	PX4	C20-C19-C18	2.56	101.45	114.42	1	1
4	A	336	PX4	O7-C23-O8	2.56	117.53	123.70	2	1
4	A	338	PX4	C18-C17-C16	2.56	101.44	114.42	14	4
4	A	390	PX4	C16-C15-C14	2.56	101.44	114.42	3	2
4	A	392	PX4	C25-C24-C23	2.56	122.92	113.62	2	2
4	A	410	PX4	O7-C7-C8	2.56	117.66	108.40	9	2
4	A	395	PX4	C31-C30-C29	2.56	101.45	114.42	7	3
4	A	416	PX4	C14-C13-C12	2.56	101.45	114.42	5	3
4	A	315	PX4	O1-P1-O4	2.55	119.60	107.75	9	1
4	A	318	PX4	C12-C11-C10	2.55	104.01	113.19	5	2
4	A	328	PX4	C30-C29-C28	2.55	101.46	114.42	3	2
4	A	375	PX4	C28-C27-C26	2.55	101.46	114.42	8	2
4	A	410	PX4	C5-N1-C4	2.55	102.41	108.97	6	3
4	A	425	PX4	O3-C1-C2	2.55	122.60	109.16	1	2
4	A	340	PX4	O3-P1-O2	2.55	99.09	109.07	4	1
4	A	367	PX4	C25-C24-C23	2.55	104.33	113.62	9	2
4	A	335	PX4	C11-C10-C9	2.55	104.34	113.62	6	2
4	A	335	PX4	O5-C9-O6	2.55	117.15	123.59	13	3
4	A	392	PX4	C7-O7-C23	2.55	111.51	117.79	14	2
4	A	398	PX4	C4-N1-C3	2.55	102.41	108.97	7	3
4	A	416	PX4	C20-C19-C18	2.55	101.47	114.42	10	4
4	A	427	PX4	O6-C9-C10	2.55	113.78	123.73	12	1
4	A	336	PX4	C5-N1-C3	2.55	102.42	108.97	9	3
4	A	323	PX4	C27-C26-C25	2.55	101.49	114.42	8	3
4	A	334	PX4	C33-C32-C31	2.55	101.48	114.42	5	1
4	A	375	PX4	O7-C7-C8	2.55	117.63	108.40	7	5
4	A	420	PX4	C8-O5-C9	2.55	107.68	117.12	13	2
4	A	426	PX4	C26-C25-C24	2.55	104.03	113.19	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	C30-C29-C28	2.55	101.48	114.42	3	1
4	A	411	PX4	C28-C27-C26	2.55	101.49	114.42	6	2
4	A	331	PX4	C18-C17-C16	2.55	101.50	114.42	9	1
4	A	336	PX4	C27-C26-C25	2.55	101.50	114.42	8	3
4	A	349	PX4	O7-C23-O8	2.55	117.55	123.70	9	4
4	A	384	PX4	C18-C17-C16	2.55	101.50	114.42	14	2
4	A	418	PX4	C4-N1-C2	2.55	120.34	109.92	9	1
4	A	420	PX4	O7-C7-C8	2.55	117.62	108.40	1	1
4	A	430	PX4	C5-N1-C3	2.55	102.43	108.97	2	2
4	A	335	PX4	C5-N1-C2	2.54	120.33	109.92	3	1
4	A	368	PX4	C8-O5-C9	2.54	107.70	117.12	6	4
4	A	389	PX4	C12-C11-C10	2.54	104.04	113.19	7	2
4	A	400	PX4	C15-C14-C13	2.54	101.51	114.42	6	1
4	A	307	PX4	O5-C9-C10	2.54	119.89	111.91	7	4
4	A	327	PX4	O4-P1-O2	2.54	119.00	109.07	5	1
4	A	334	PX4	O4-P1-O2	2.54	119.00	109.07	10	5
4	A	353	PX4	O5-C9-C10	2.54	119.89	111.91	6	5
4	A	426	PX4	C25-C24-C23	2.54	104.37	113.62	12	1
4	A	391	PX4	C32-C31-C30	2.54	101.52	114.42	2	2
4	A	403	PX4	C3-N1-C2	2.54	99.52	109.92	12	1
4	A	410	PX4	C26-C25-C24	2.54	104.06	113.19	8	2
4	A	420	PX4	C12-C11-C10	2.54	104.05	113.19	12	2
4	A	326	PX4	C11-C10-C9	2.54	122.85	113.62	13	3
4	A	377	PX4	O1-P1-O2	2.54	124.79	112.24	7	4
4	A	365	PX4	O5-C9-C10	2.54	119.87	111.91	3	1
4	A	316	PX4	C7-O7-C23	2.54	124.04	117.79	11	2
4	A	332	PX4	C19-C18-C17	2.54	101.54	114.42	2	1
4	A	396	PX4	C34-C33-C32	2.54	101.54	114.42	1	2
4	A	342	PX4	C16-C15-C14	2.54	101.55	114.42	3	2
4	A	376	PX4	C4-N1-C3	2.54	115.50	108.97	3	1
4	A	409	PX4	C20-C19-C18	2.54	101.55	114.42	2	1
4	A	355	PX4	C4-N1-C2	2.54	99.54	109.92	10	3
4	A	395	PX4	C26-C25-C24	2.53	104.08	113.19	4	1
4	A	411	PX4	C14-C13-C12	2.53	101.56	114.42	8	2
4	A	413	PX4	O5-C9-C10	2.54	119.86	111.91	2	4
4	A	343	PX4	C17-C16-C15	2.53	101.56	114.42	14	1
4	A	407	PX4	C18-C17-C16	2.53	101.56	114.42	9	2
4	A	336	PX4	C3-N1-C2	2.53	120.28	109.92	10	1
4	A	358	PX4	C34-C33-C32	2.53	101.57	114.42	7	1
4	A	386	PX4	C7-O7-C23	2.53	111.56	117.79	12	1
4	A	399	PX4	C18-C17-C16	2.53	101.57	114.42	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	407	PX4	C32-C31-C30	2.53	101.56	114.42	4	3
4	A	410	PX4	C18-C17-C16	2.53	101.57	114.42	4	1
4	A	307	PX4	C34-C33-C32	2.53	101.58	114.42	1	2
4	A	337	PX4	O3-C1-C2	2.53	122.47	109.16	8	1
4	A	361	PX4	C18-C17-C16	2.53	101.58	114.42	1	2
4	A	412	PX4	C18-C17-C16	2.53	101.58	114.42	14	1
4	A	417	PX4	C18-C17-C16	2.53	101.58	114.42	14	2
4	A	356	PX4	C33-C32-C31	2.53	101.59	114.42	6	1
4	A	360	PX4	O6-C9-C10	2.53	113.87	123.73	13	1
4	A	419	PX4	O3-P1-O2	2.53	99.18	109.07	3	1
4	A	370	PX4	O4-P1-O2	2.53	118.94	109.07	3	1
4	A	310	PX4	O3-P1-O2	2.53	99.20	109.07	14	2
4	A	371	PX4	O4-P1-O2	2.53	99.20	109.07	2	3
4	A	383	PX4	C20-C19-C18	2.53	101.60	114.42	8	3
4	A	406	PX4	C16-C15-C14	2.53	101.61	114.42	7	2
4	A	346	PX4	C33-C32-C31	2.52	101.61	114.42	5	2
4	A	357	PX4	C30-C29-C28	2.52	101.62	114.42	1	1
4	A	314	PX4	C1-C2-N1	2.52	124.20	115.78	1	2
4	A	344	PX4	O4-P1-O2	2.52	118.92	109.07	4	1
4	A	345	PX4	C5-N1-C4	2.52	102.49	108.97	14	3
4	A	362	PX4	C27-C26-C25	2.52	101.62	114.42	5	1
4	A	363	PX4	C27-C26-C25	2.52	101.62	114.42	8	1
4	A	409	PX4	C30-C29-C28	2.52	101.62	114.42	7	1
4	A	421	PX4	C16-C15-C14	2.52	101.62	114.42	11	2
4	A	428	PX4	C27-C26-C25	2.52	101.62	114.42	1	1
4	A	367	PX4	C3-N1-C2	2.52	99.60	109.92	13	1
4	A	375	PX4	C27-C26-C25	2.52	101.62	114.42	3	1
4	A	415	PX4	C17-C16-C15	2.52	101.63	114.42	8	1
4	A	346	PX4	C5-N1-C4	2.52	102.50	108.97	11	2
4	A	403	PX4	C20-C19-C18	2.52	101.64	114.42	2	1
4	A	409	PX4	O3-C1-C2	2.52	122.41	109.16	11	3
4	A	411	PX4	O1-P1-O4	2.52	119.44	107.75	1	4
4	A	413	PX4	C33-C32-C31	2.52	101.64	114.42	7	2
4	A	349	PX4	O6-C9-C10	2.52	113.91	123.73	14	1
4	A	380	PX4	C7-O7-C23	2.52	111.59	117.79	5	3
4	A	385	PX4	C16-C15-C14	2.52	101.65	114.42	8	1
4	A	324	PX4	O3-P1-O2	2.52	99.24	109.07	4	4
4	A	344	PX4	C3-N1-C2	2.51	99.63	109.92	1	2
4	A	357	PX4	C11-C10-C9	2.52	104.47	113.62	8	1
4	A	392	PX4	C32-C31-C30	2.51	101.66	114.42	6	1
4	A	320	PX4	C33-C32-C31	2.51	101.67	114.42	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	380	PX4	C27-C26-C25	2.51	101.67	114.42	10	4
4	A	401	PX4	O7-C7-C8	2.51	117.50	108.40	8	3
4	A	404	PX4	C5-N1-C3	2.51	115.43	108.97	2	3
4	A	422	PX4	C5-N1-C3	2.51	115.43	108.97	7	2
4	A	347	PX4	C8-O5-C9	2.51	107.83	117.12	13	2
4	A	398	PX4	C3-N1-C2	2.51	120.18	109.92	6	1
4	A	319	PX4	O7-C7-C6	2.51	117.48	108.40	3	2
4	A	395	PX4	C5-N1-C3	2.51	102.53	108.97	8	1
4	A	396	PX4	C8-O5-C9	2.51	107.84	117.12	2	1
4	A	318	PX4	C25-C24-C23	2.51	122.73	113.62	7	3
4	A	320	PX4	O7-C23-O8	2.51	117.64	123.70	6	2
4	A	328	PX4	C25-C24-C23	2.51	104.51	113.62	9	1
4	A	343	PX4	C1-C2-N1	2.51	124.14	115.78	2	1
4	A	339	PX4	C17-C16-C15	2.50	127.14	114.42	12	2
4	A	346	PX4	O8-C23-C24	2.50	113.96	123.73	2	2
4	A	384	PX4	C30-C29-C28	2.50	101.71	114.42	1	2
4	A	396	PX4	C25-C24-C23	2.50	104.51	113.62	1	2
4	A	312	PX4	C31-C30-C29	2.50	101.72	114.42	14	3
4	A	312	PX4	C20-C19-C18	2.50	101.72	114.42	12	1
4	A	341	PX4	C8-O5-C9	2.50	107.86	117.12	12	1
4	A	349	PX4	O4-P1-O2	2.50	118.84	109.07	10	2
4	A	351	PX4	C14-C13-C12	2.50	101.72	114.42	8	2
4	A	366	PX4	O1-P1-O3	2.50	96.12	107.75	12	2
4	A	328	PX4	C4-N1-C2	2.50	120.15	109.92	12	2
4	A	410	PX4	C25-C24-C23	2.50	122.72	113.62	3	3
4	A	415	PX4	O3-C1-C2	2.50	122.31	109.16	5	2
4	A	339	PX4	C33-C32-C31	2.50	101.73	114.42	6	1
4	A	352	PX4	C16-C15-C14	2.50	101.73	114.42	13	1
4	A	428	PX4	C1-C2-N1	2.50	124.13	115.78	5	3
4	A	428	PX4	C17-C16-C15	2.50	101.73	114.42	5	2
4	A	363	PX4	C5-N1-C2	2.50	99.70	109.92	3	1
4	A	379	PX4	C27-C26-C25	2.50	101.74	114.42	10	1
4	A	400	PX4	C19-C18-C17	2.50	101.75	114.42	11	3
4	A	400	PX4	O4-P1-O2	2.50	99.31	109.07	12	1
4	A	418	PX4	O5-C9-C10	2.50	119.75	111.91	7	1
4	A	429	PX4	C14-C13-C12	2.50	101.75	114.42	12	1
4	A	347	PX4	C19-C18-C17	2.50	101.75	114.42	13	1
4	A	406	PX4	O3-C1-C2	2.50	122.29	109.16	3	1
4	A	312	PX4	O5-C9-C10	2.49	119.74	111.91	13	2
4	A	323	PX4	C12-C11-C10	2.49	104.22	113.19	6	1
4	A	329	PX4	O4-P1-O2	2.49	118.81	109.07	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	361	PX4	C14-C13-C12	2.49	101.76	114.42	1	2
4	A	368	PX4	C5-N1-C4	2.49	102.56	108.97	12	3
4	A	387	PX4	C15-C14-C13	2.50	101.76	114.42	1	2
4	A	389	PX4	C7-O7-C23	2.49	123.93	117.79	10	3
4	A	427	PX4	C13-C12-C11	2.49	101.76	114.42	13	1
4	A	318	PX4	O1-P1-O4	2.49	119.32	107.75	4	1
4	A	365	PX4	C13-C12-C11	2.49	101.77	114.42	2	2
4	A	364	PX4	O3-C1-C2	2.49	122.26	109.16	11	1
4	A	307	PX4	C25-C24-C23	2.49	104.56	113.62	13	2
4	A	312	PX4	C4-N1-C3	2.49	102.57	108.97	2	1
4	A	365	PX4	C25-C24-C23	2.49	104.56	113.62	10	2
4	A	380	PX4	O3-C1-C2	2.49	122.26	109.16	1	1
4	A	391	PX4	C1-C2-N1	2.49	124.10	115.78	13	3
4	A	331	PX4	O7-C7-C6	2.49	117.41	108.40	5	3
4	A	369	PX4	C29-C28-C27	2.49	101.78	114.42	6	2
4	A	416	PX4	C31-C30-C29	2.49	101.78	114.42	8	2
4	A	420	PX4	C25-C24-C23	2.49	104.56	113.62	3	3
4	A	353	PX4	O8-C23-C24	2.49	114.02	123.73	7	2
4	A	428	PX4	C28-C27-C26	2.49	101.78	114.42	10	1
4	A	352	PX4	C11-C10-C9	2.49	122.67	113.62	9	1
4	A	331	PX4	C14-C13-C12	2.49	101.80	114.42	6	1
4	A	354	PX4	C14-C13-C12	2.49	101.80	114.42	3	3
4	A	362	PX4	C1-C2-N1	2.49	124.08	115.78	12	1
4	A	402	PX4	O8-C23-C24	2.49	114.03	123.73	8	1
4	A	384	PX4	C5-N1-C4	2.48	102.59	108.97	1	3
4	A	405	PX4	O7-C23-O8	2.48	117.70	123.70	9	4
4	A	336	PX4	C8-O5-C9	2.48	107.93	117.12	3	1
4	A	343	PX4	O3-C1-C2	2.48	122.21	109.16	10	1
4	A	354	PX4	C30-C29-C28	2.48	101.82	114.42	7	2
4	A	357	PX4	C29-C28-C27	2.48	101.82	114.42	2	3
4	A	360	PX4	C26-C25-C24	2.48	104.26	113.19	13	1
4	A	391	PX4	C34-C33-C32	2.48	101.82	114.42	11	3
4	A	405	PX4	C31-C30-C29	2.48	101.82	114.42	9	1
4	A	413	PX4	C28-C27-C26	2.48	101.82	114.42	6	1
4	A	338	PX4	O8-C23-C24	2.48	114.06	123.73	9	1
4	A	361	PX4	C4-N1-C2	2.48	120.07	109.92	6	2
4	A	383	PX4	O1-P1-O4	2.48	96.23	107.75	10	4
4	A	387	PX4	C4-N1-C2	2.48	120.06	109.92	9	1
4	A	397	PX4	O1-P1-O4	2.48	119.27	107.75	14	1
4	A	360	PX4	C14-C13-C12	2.48	101.84	114.42	4	2
4	A	412	PX4	C30-C29-C28	2.48	101.83	114.42	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	320	PX4	C14-C13-C12	2.48	101.84	114.42	8	1
4	A	324	PX4	C3-N1-C2	2.48	120.06	109.92	2	1
4	A	336	PX4	O5-C9-C10	2.48	119.69	111.91	9	6
4	A	337	PX4	O5-C9-O6	2.48	117.34	123.59	7	5
4	A	347	PX4	C32-C31-C30	2.48	101.85	114.42	14	2
4	A	348	PX4	C4-N1-C2	2.48	120.06	109.92	10	1
4	A	360	PX4	O4-P1-O2	2.48	118.75	109.07	11	4
4	A	341	PX4	O7-C23-O8	2.48	117.72	123.70	5	1
4	A	345	PX4	C34-C33-C32	2.48	101.85	114.42	7	2
4	A	311	PX4	C30-C29-C28	2.47	101.86	114.42	10	1
4	A	346	PX4	O3-C1-C2	2.48	122.18	109.16	9	1
4	A	356	PX4	C31-C30-C29	2.48	101.85	114.42	2	2
4	A	377	PX4	C25-C24-C23	2.48	104.61	113.62	10	4
4	A	391	PX4	O7-C7-C6	2.48	117.37	108.40	2	2
4	A	426	PX4	C4-N1-C3	2.48	102.60	108.97	10	2
4	A	391	PX4	C14-C13-C12	2.48	101.86	114.42	7	2
4	A	394	PX4	O7-C7-C8	2.47	117.36	108.40	13	2
4	A	324	PX4	C8-O5-C9	2.47	107.97	117.12	1	1
4	A	326	PX4	C14-C13-C12	2.47	101.88	114.42	11	2
4	A	329	PX4	C5-N1-C3	2.47	102.62	108.97	2	1
4	A	338	PX4	O1-P1-O3	2.47	96.27	107.75	9	1
4	A	351	PX4	O4-P1-O2	2.47	118.72	109.07	10	1
4	A	354	PX4	O3-C1-C2	2.47	122.16	109.16	2	1
4	A	379	PX4	C29-C28-C27	2.47	101.89	114.42	11	2
4	A	410	PX4	C14-C13-C12	2.47	101.88	114.42	9	2
4	A	334	PX4	O1-P1-O4	2.47	96.28	107.75	3	1
4	A	366	PX4	C3-N1-C2	2.47	120.02	109.92	14	1
4	A	337	PX4	C27-C26-C25	2.47	101.90	114.42	11	3
4	A	337	PX4	O1-P1-O3	2.47	119.20	107.75	8	2
4	A	389	PX4	C5-N1-C2	2.47	99.82	109.92	2	1
4	A	339	PX4	O7-C7-C8	2.47	117.33	108.40	3	2
4	A	340	PX4	C7-O7-C23	2.47	123.86	117.79	9	1
4	A	394	PX4	O5-C9-C10	2.47	119.65	111.91	4	2
4	A	365	PX4	O1-P1-O4	2.47	119.20	107.75	13	3
4	A	372	PX4	C13-C12-C11	2.47	101.91	114.42	6	3
4	A	430	PX4	C26-C25-C24	2.47	104.32	113.19	6	1
4	A	309	PX4	C26-C25-C24	2.46	104.33	113.19	5	4
4	A	321	PX4	C1-C2-N1	2.47	124.01	115.78	11	3
4	A	339	PX4	O7-C7-C6	2.47	117.33	108.40	13	3
4	A	343	PX4	C11-C10-C9	2.46	104.66	113.62	5	2
4	A	346	PX4	C16-C15-C14	2.47	101.91	114.42	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	352	PX4	C28-C27-C26	2.47	101.91	114.42	13	2
4	A	352	PX4	O4-P1-O2	2.46	118.70	109.07	4	2
4	A	310	PX4	C25-C24-C23	2.46	104.66	113.62	9	1
4	A	325	PX4	C14-C13-C12	2.46	101.92	114.42	8	1
4	A	352	PX4	C5-N1-C2	2.46	99.83	109.92	6	1
4	A	365	PX4	C34-C33-C32	2.46	101.92	114.42	10	1
4	A	393	PX4	O3-C1-C2	2.46	122.11	109.16	12	1
4	A	415	PX4	C5-N1-C2	2.46	99.84	109.92	11	1
4	A	424	PX4	C25-C24-C23	2.46	104.66	113.62	5	2
4	A	350	PX4	C26-C25-C24	2.46	104.34	113.19	4	2
4	A	352	PX4	C4-N1-C2	2.46	99.84	109.92	14	1
4	A	366	PX4	O7-C7-C6	2.46	117.31	108.40	9	2
4	A	379	PX4	O3-C1-C2	2.46	122.10	109.16	5	3
4	A	412	PX4	O3-P1-O2	2.46	99.45	109.07	12	1
4	A	306	PX4	C5-N1-C4	2.46	102.65	108.97	7	2
4	A	378	PX4	O7-C7-C8	2.46	117.31	108.40	11	4
4	A	420	PX4	C1-C2-N1	2.46	124.00	115.78	11	3
4	A	429	PX4	C13-C12-C11	2.46	101.94	114.42	3	1
4	A	320	PX4	O1-P1-O4	2.46	119.16	107.75	8	1
4	A	326	PX4	C4-N1-C2	2.46	119.97	109.92	3	1
4	A	312	PX4	C14-C13-C12	2.46	101.96	114.42	11	1
4	A	328	PX4	O4-P1-O2	2.46	99.47	109.07	10	3
4	A	342	PX4	C32-C31-C30	2.46	101.95	114.42	9	1
4	A	363	PX4	C33-C32-C31	2.46	101.95	114.42	3	1
4	A	382	PX4	C25-C24-C23	2.46	104.69	113.62	11	2
4	A	389	PX4	O5-C9-O6	2.46	117.39	123.59	14	3
4	A	394	PX4	O3-C1-C2	2.46	122.08	109.16	4	1
4	A	418	PX4	O5-C9-O6	2.46	117.39	123.59	2	5
4	A	345	PX4	C13-C12-C11	2.46	101.96	114.42	6	4
4	A	420	PX4	C28-C27-C26	2.46	101.95	114.42	10	2
4	A	324	PX4	C28-C27-C26	2.45	101.97	114.42	1	3
4	A	330	PX4	C34-C33-C32	2.45	101.97	114.42	10	1
4	A	352	PX4	C15-C14-C13	2.45	101.96	114.42	7	1
4	A	389	PX4	C18-C17-C16	2.45	101.97	114.42	6	1
4	A	394	PX4	C34-C33-C32	2.45	101.96	114.42	13	1
4	A	401	PX4	C11-C10-C9	2.45	104.70	113.62	7	5
4	A	407	PX4	C25-C24-C23	2.45	104.70	113.62	1	1
4	A	407	PX4	C8-O5-C9	2.45	126.21	117.12	6	2
4	A	410	PX4	C11-C10-C9	2.45	104.70	113.62	1	2
4	A	427	PX4	O1-P1-O4	2.45	119.14	107.75	7	1
4	A	331	PX4	O1-P1-O4	2.45	119.13	107.75	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	367	PX4	C5-N1-C2	2.45	99.88	109.92	2	1
4	A	372	PX4	O8-C23-C24	2.45	114.16	123.73	1	2
4	A	415	PX4	C25-C24-C23	2.45	104.70	113.62	11	1
4	A	309	PX4	C31-C30-C29	2.45	101.99	114.42	9	2
4	A	317	PX4	C29-C28-C27	2.45	101.98	114.42	2	4
4	A	339	PX4	C25-C24-C23	2.45	104.71	113.62	2	5
4	A	322	PX4	C17-C16-C15	2.45	101.99	114.42	2	5
4	A	354	PX4	C31-C30-C29	2.45	101.98	114.42	14	3
4	A	358	PX4	C4-N1-C2	2.45	119.94	109.92	3	1
4	A	326	PX4	C26-C25-C24	2.45	104.39	113.19	13	2
4	A	335	PX4	C29-C28-C27	2.45	101.99	114.42	5	1
4	A	367	PX4	C8-O5-C9	2.45	108.05	117.12	11	1
4	A	370	PX4	C26-C25-C24	2.45	104.38	113.19	2	2
4	A	385	PX4	C25-C24-C23	2.45	104.71	113.62	13	2
4	A	400	PX4	C33-C32-C31	2.45	101.98	114.42	3	1
4	A	412	PX4	C26-C25-C24	2.45	104.38	113.19	2	3
4	A	375	PX4	C16-C15-C14	2.45	101.99	114.42	6	2
4	A	394	PX4	C5-N1-C3	2.45	102.68	108.97	6	5
4	A	388	PX4	C31-C30-C29	2.45	102.00	114.42	14	2
4	A	310	PX4	C29-C28-C27	2.45	102.00	114.42	10	1
4	A	387	PX4	C30-C29-C28	2.45	102.00	114.42	13	1
4	A	403	PX4	O1-P1-O4	2.45	119.11	107.75	6	2
4	A	322	PX4	O1-P1-O3	2.45	119.11	107.75	3	2
4	A	329	PX4	C31-C30-C29	2.45	102.01	114.42	10	3
4	A	342	PX4	C3-N1-C2	2.45	119.92	109.92	3	2
4	A	344	PX4	C12-C11-C10	2.45	104.40	113.19	9	1
4	A	391	PX4	O5-C9-O6	2.45	117.42	123.59	9	2
4	A	342	PX4	O3-C1-C2	2.44	122.01	109.16	8	2
4	A	378	PX4	C20-C19-C18	2.44	102.02	114.42	11	2
4	A	397	PX4	C14-C13-C12	2.44	102.01	114.42	14	1
4	A	355	PX4	C34-C33-C32	2.44	102.02	114.42	2	1
4	A	376	PX4	C25-C24-C23	2.44	104.73	113.62	1	2
4	A	307	PX4	C5-N1-C3	2.44	102.69	108.97	9	3
4	A	307	PX4	C17-C16-C15	2.44	102.03	114.42	12	2
4	A	327	PX4	C5-N1-C2	2.44	119.91	109.92	10	2
4	A	333	PX4	C27-C26-C25	2.44	102.03	114.42	8	1
4	A	336	PX4	O4-P1-O2	2.44	118.61	109.07	3	3
4	A	348	PX4	C32-C31-C30	2.44	102.03	114.42	12	1
4	A	394	PX4	C8-O5-C9	2.44	108.08	117.12	6	2
4	A	310	PX4	C32-C31-C30	2.44	102.03	114.42	9	3
4	A	321	PX4	C33-C32-C31	2.44	102.03	114.42	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	314	PX4	C34-C33-C32	2.44	102.04	114.42	14	1
4	A	362	PX4	C26-C25-C24	2.44	104.42	113.19	13	1
4	A	363	PX4	C31-C30-C29	2.44	102.03	114.42	14	2
4	A	370	PX4	C27-C26-C25	2.44	102.03	114.42	9	1
4	A	372	PX4	C34-C33-C32	2.44	102.03	114.42	10	2
4	A	403	PX4	C26-C25-C24	2.44	104.42	113.19	7	2
4	A	427	PX4	C8-O5-C9	2.44	126.16	117.12	8	4
4	A	313	PX4	C32-C31-C30	2.44	102.05	114.42	3	2
4	A	377	PX4	C31-C30-C29	2.44	102.05	114.42	8	1
4	A	306	PX4	C25-C24-C23	2.44	122.48	113.62	11	1
4	A	347	PX4	C13-C12-C11	2.44	102.06	114.42	4	2
4	A	350	PX4	C11-C10-C9	2.44	104.76	113.62	6	2
4	A	367	PX4	O7-C7-C8	2.44	117.22	108.40	8	2
4	A	410	PX4	C16-C15-C14	2.44	102.05	114.42	12	1
4	A	413	PX4	C26-C25-C24	2.44	104.43	113.19	6	3
4	A	415	PX4	C26-C25-C24	2.44	104.43	113.19	4	1
4	A	415	PX4	C31-C30-C29	2.44	102.05	114.42	10	2
4	A	385	PX4	O3-C1-C2	2.44	121.97	109.16	12	2
4	A	390	PX4	C5-N1-C4	2.44	102.71	108.97	3	1
4	A	319	PX4	C25-C24-C23	2.43	104.77	113.62	13	3
4	A	341	PX4	C18-C17-C16	2.43	102.07	114.42	14	1
4	A	354	PX4	C16-C15-C14	2.43	102.07	114.42	12	1
4	A	410	PX4	C29-C28-C27	2.43	102.06	114.42	4	3
4	A	356	PX4	C28-C27-C26	2.43	102.07	114.42	5	1
4	A	425	PX4	O6-C9-C10	2.43	114.23	123.73	9	2
4	A	363	PX4	C4-N1-C2	2.43	119.87	109.92	3	1
4	A	320	PX4	C27-C26-C25	2.43	102.09	114.42	5	2
4	A	344	PX4	O3-P1-O2	2.43	99.57	109.07	2	3
4	A	345	PX4	C19-C18-C17	2.43	102.08	114.42	12	2
4	A	356	PX4	C5-N1-C3	2.43	115.22	108.97	3	1
4	A	389	PX4	C15-C14-C13	2.43	102.08	114.42	1	2
4	A	347	PX4	C14-C13-C12	2.43	102.09	114.42	7	2
4	A	404	PX4	C12-C11-C10	2.43	104.46	113.19	9	1
4	A	430	PX4	C30-C29-C28	2.43	102.09	114.42	6	2
4	A	320	PX4	O5-C9-C10	2.43	119.52	111.91	13	3
4	A	350	PX4	C29-C28-C27	2.43	102.10	114.42	11	2
4	A	360	PX4	C29-C28-C27	2.43	102.10	114.42	1	1
4	A	405	PX4	O1-P1-O2	2.43	124.24	112.24	9	4
4	A	415	PX4	C32-C31-C30	2.43	102.10	114.42	9	1
4	A	352	PX4	C14-C13-C12	2.43	102.11	114.42	12	1
4	A	373	PX4	C13-C12-C11	2.43	102.11	114.42	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	378	PX4	O8-C23-C24	2.43	114.27	123.73	4	1
4	A	414	PX4	C3-N1-C2	2.43	119.84	109.92	14	3
4	A	422	PX4	C15-C14-C13	2.43	102.11	114.42	6	2
4	A	372	PX4	O3-C1-C2	2.42	121.91	109.16	4	1
4	A	428	PX4	O1-P1-O4	2.43	119.01	107.75	6	2
4	A	331	PX4	C4-N1-C2	2.42	100.00	109.92	5	4
4	A	344	PX4	C5-N1-C2	2.42	119.83	109.92	2	1
4	A	352	PX4	C32-C31-C30	2.42	102.12	114.42	12	1
4	A	356	PX4	C12-C11-C10	2.42	104.48	113.19	12	2
4	A	391	PX4	C30-C29-C28	2.42	102.12	114.42	5	1
4	A	400	PX4	C16-C15-C14	2.42	102.12	114.42	7	2
4	A	417	PX4	C5-N1-C2	2.42	119.83	109.92	14	2
4	A	318	PX4	O4-P1-O2	2.42	118.53	109.07	11	1
4	A	323	PX4	O8-C23-C24	2.42	114.29	123.73	4	1
4	A	358	PX4	C5-N1-C4	2.42	102.75	108.97	12	1
4	A	312	PX4	C4-N1-C2	2.42	119.81	109.92	8	1
4	A	319	PX4	C1-C2-N1	2.42	123.86	115.78	8	1
4	A	334	PX4	O5-C9-O6	2.42	117.48	123.59	14	2
4	A	345	PX4	C5-N1-C2	2.42	119.82	109.92	8	2
4	A	309	PX4	C34-C33-C32	2.42	102.15	114.42	6	2
4	A	313	PX4	C5-N1-C2	2.42	119.81	109.92	2	2
4	A	315	PX4	C30-C29-C28	2.42	102.14	114.42	10	1
4	A	330	PX4	C8-O5-C9	2.42	108.17	117.12	1	1
4	A	364	PX4	O8-C23-C24	2.42	114.30	123.73	11	1
4	A	403	PX4	C33-C32-C31	2.42	102.15	114.42	8	2
4	A	424	PX4	C11-C10-C9	2.42	122.41	113.62	11	1
4	A	425	PX4	C34-C33-C32	2.42	102.14	114.42	7	2
4	A	318	PX4	O3-P1-O2	2.42	99.63	109.07	5	1
4	A	328	PX4	C34-C33-C32	2.42	102.16	114.42	2	2
4	A	330	PX4	O1-P1-O3	2.42	96.52	107.75	3	3
4	A	385	PX4	C34-C33-C32	2.42	102.16	114.42	6	3
4	A	423	PX4	C18-C17-C16	2.42	102.16	114.42	10	1
4	A	424	PX4	C33-C32-C31	2.42	102.16	114.42	13	1
4	A	308	PX4	C1-C2-N1	2.41	123.84	115.78	13	3
4	A	347	PX4	C34-C33-C32	2.41	102.17	114.42	4	3
4	A	353	PX4	C1-C2-N1	2.42	123.84	115.78	4	1
4	A	418	PX4	C26-C25-C24	2.42	104.51	113.19	5	2
4	A	421	PX4	O3-C1-C2	2.42	121.86	109.16	10	1
4	A	308	PX4	C16-C15-C14	2.41	102.17	114.42	3	2
4	A	309	PX4	C27-C26-C25	2.41	102.17	114.42	14	1
4	A	359	PX4	C4-N1-C2	2.41	119.79	109.92	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	362	PX4	C20-C19-C18	2.41	102.17	114.42	6	2
4	A	381	PX4	O8-C23-C24	2.41	114.32	123.73	3	1
4	A	388	PX4	O3-C1-C2	2.41	121.85	109.16	1	3
4	A	423	PX4	C30-C29-C28	2.41	102.17	114.42	4	1
4	A	324	PX4	O5-C9-O6	2.41	117.50	123.59	9	1
4	A	359	PX4	C27-C26-C25	2.41	102.18	114.42	14	2
4	A	364	PX4	C25-C24-C23	2.41	104.85	113.62	2	4
4	A	313	PX4	C13-C12-C11	2.41	102.20	114.42	14	1
4	A	317	PX4	C1-C2-N1	2.41	123.82	115.78	4	3
4	A	338	PX4	C19-C18-C17	2.41	102.19	114.42	8	1
4	A	348	PX4	C27-C26-C25	2.41	102.19	114.42	9	2
4	A	389	PX4	C32-C31-C30	2.41	102.18	114.42	3	1
4	A	408	PX4	C17-C16-C15	2.41	102.18	114.42	4	1
4	A	386	PX4	C18-C17-C16	2.41	102.19	114.42	8	1
4	A	389	PX4	C33-C32-C31	2.41	102.19	114.42	1	1
4	A	412	PX4	C1-C2-N1	2.41	123.83	115.78	11	2
4	A	356	PX4	O5-C9-O6	2.41	117.51	123.59	4	2
4	A	322	PX4	C11-C10-C9	2.41	122.38	113.62	2	2
4	A	322	PX4	C14-C13-C12	2.41	102.20	114.42	10	1
4	A	372	PX4	C16-C15-C14	2.41	102.20	114.42	6	3
4	A	384	PX4	C15-C14-C13	2.41	102.20	114.42	14	1
4	A	337	PX4	C32-C31-C30	2.41	102.20	114.42	12	1
4	A	348	PX4	O3-P1-O2	2.41	99.66	109.07	6	4
4	A	389	PX4	C11-C10-C9	2.41	104.86	113.62	7	1
4	A	403	PX4	C31-C30-C29	2.41	102.20	114.42	10	1
4	A	353	PX4	C25-C24-C23	2.41	104.87	113.62	11	2
4	A	309	PX4	O7-C7-C8	2.40	117.11	108.40	3	1
4	A	317	PX4	C34-C33-C32	2.40	102.22	114.42	9	1
4	A	366	PX4	O4-P1-O2	2.40	118.46	109.07	8	4
4	A	368	PX4	C14-C13-C12	2.41	102.21	114.42	7	1
4	A	384	PX4	C5-N1-C2	2.41	119.76	109.92	5	2
4	A	378	PX4	O3-C1-C2	2.40	121.81	109.16	14	2
4	A	395	PX4	C4-N1-C2	2.41	119.76	109.92	14	1
4	A	409	PX4	C5-N1-C3	2.41	115.16	108.97	12	2
4	A	409	PX4	C29-C28-C27	2.41	102.21	114.42	8	1
4	A	415	PX4	C20-C19-C18	2.41	102.21	114.42	5	1
4	A	369	PX4	C32-C31-C30	2.40	102.22	114.42	5	3
4	A	412	PX4	C3-N1-C2	2.40	119.75	109.92	1	3
4	A	306	PX4	C29-C28-C27	2.40	102.23	114.42	8	1
4	A	428	PX4	C4-N1-C3	2.40	102.79	108.97	10	3
4	A	354	PX4	C11-C10-C9	2.40	104.89	113.62	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	396	PX4	C12-C11-C10	2.40	104.56	113.19	9	2
4	A	397	PX4	C15-C14-C13	2.40	102.23	114.42	2	3
4	A	401	PX4	O3-C1-C2	2.40	121.79	109.16	7	1
4	A	406	PX4	C4-N1-C2	2.40	119.74	109.92	3	2
4	A	414	PX4	O5-C9-O6	2.40	117.53	123.59	9	2
4	A	321	PX4	C14-C13-C12	2.40	102.24	114.42	8	2
4	A	369	PX4	C13-C12-C11	2.40	102.24	114.42	11	1
4	A	307	PX4	C4-N1-C3	2.40	102.81	108.97	12	2
4	A	313	PX4	C26-C25-C24	2.40	104.56	113.19	5	2
4	A	372	PX4	C20-C19-C18	2.40	102.25	114.42	10	1
4	A	382	PX4	C18-C17-C16	2.40	102.24	114.42	7	2
4	A	382	PX4	C5-N1-C2	2.40	119.74	109.92	9	1
4	A	308	PX4	C25-C24-C23	2.40	104.90	113.62	11	3
4	A	362	PX4	C13-C12-C11	2.40	102.25	114.42	7	2
4	A	377	PX4	C7-O7-C23	2.40	111.89	117.79	3	5
4	A	377	PX4	C28-C27-C26	2.40	102.25	114.42	4	1
4	A	385	PX4	C29-C28-C27	2.40	102.25	114.42	9	1
4	A	399	PX4	C17-C16-C15	2.40	102.25	114.42	14	2
4	A	311	PX4	C5-N1-C2	2.40	119.72	109.92	4	1
4	A	317	PX4	C32-C31-C30	2.40	102.26	114.42	7	1
4	A	413	PX4	C16-C15-C14	2.40	102.25	114.42	6	1
4	A	317	PX4	C14-C13-C12	2.40	102.26	114.42	13	1
4	A	342	PX4	C5-N1-C2	2.39	100.12	109.92	14	3
4	A	343	PX4	C15-C14-C13	2.39	102.27	114.42	2	1
4	A	359	PX4	C16-C15-C14	2.39	102.27	114.42	4	1
4	A	366	PX4	C13-C12-C11	2.39	102.27	114.42	3	2
4	A	385	PX4	C15-C14-C13	2.40	102.27	114.42	6	1
4	A	392	PX4	O3-P1-O2	2.39	99.71	109.07	3	3
4	A	331	PX4	C7-O7-C23	2.39	123.68	117.79	2	3
4	A	372	PX4	O5-C9-O6	2.39	129.63	123.59	8	1
4	A	410	PX4	C12-C11-C10	2.39	104.59	113.19	1	2
4	A	343	PX4	C25-C24-C23	2.39	122.32	113.62	1	1
4	A	354	PX4	C1-C2-N1	2.39	123.77	115.78	8	4
4	A	368	PX4	C31-C30-C29	2.39	102.28	114.42	5	2
4	A	424	PX4	C3-N1-C2	2.39	119.71	109.92	9	1
4	A	347	PX4	C16-C15-C14	2.39	102.29	114.42	7	2
4	A	390	PX4	O1-P1-O3	2.39	96.64	107.75	5	1
4	A	398	PX4	O7-C7-C8	2.39	117.06	108.40	7	4
4	A	413	PX4	C32-C31-C30	2.39	102.28	114.42	7	1
4	A	414	PX4	C14-C13-C12	2.39	102.29	114.42	6	1
4	A	430	PX4	C28-C27-C26	2.39	102.29	114.42	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	336	PX4	C1-C2-N1	2.39	123.75	115.78	9	2
4	A	368	PX4	C1-C2-N1	2.39	123.75	115.78	13	2
4	A	342	PX4	O6-C9-C10	2.39	114.42	123.73	2	1
4	A	355	PX4	O5-C9-O6	2.39	117.57	123.59	8	3
4	A	378	PX4	C30-C29-C28	2.39	102.31	114.42	8	2
4	A	420	PX4	C15-C14-C13	2.39	102.31	114.42	7	2
4	A	339	PX4	C12-C11-C10	2.38	104.62	113.19	11	2
4	A	343	PX4	O1-P1-O3	2.38	96.67	107.75	2	1
4	A	390	PX4	C25-C24-C23	2.38	104.95	113.62	4	2
4	A	393	PX4	C29-C28-C27	2.38	102.32	114.42	2	2
4	A	395	PX4	C18-C17-C16	2.38	102.32	114.42	12	1
4	A	421	PX4	C31-C30-C29	2.38	102.32	114.42	14	2
4	A	411	PX4	C18-C17-C16	2.38	102.32	114.42	14	2
4	A	413	PX4	C8-O5-C9	2.38	125.95	117.12	4	3
4	A	319	PX4	C31-C30-C29	2.38	102.34	114.42	6	1
4	A	345	PX4	C31-C30-C29	2.38	102.34	114.42	5	1
4	A	352	PX4	C27-C26-C25	2.38	102.33	114.42	4	1
4	A	356	PX4	C16-C15-C14	2.38	102.33	114.42	11	1
4	A	381	PX4	C4-N1-C2	2.38	100.17	109.92	11	1
4	A	387	PX4	C33-C32-C31	2.38	102.33	114.42	11	2
4	A	319	PX4	C15-C14-C13	2.38	102.35	114.42	10	2
4	A	359	PX4	C18-C17-C16	2.38	102.34	114.42	14	2
4	A	397	PX4	O3-C1-C2	2.38	121.68	109.16	5	3
4	A	417	PX4	C5-N1-C3	2.38	115.09	108.97	3	4
4	A	408	PX4	C32-C31-C30	2.38	102.35	114.42	7	2
4	A	421	PX4	C8-O5-C9	2.38	108.31	117.12	10	1
4	A	345	PX4	C26-C25-C24	2.38	104.65	113.19	1	1
4	A	327	PX4	O3-P1-O2	2.38	99.79	109.07	14	1
4	A	332	PX4	C20-C19-C18	2.38	102.37	114.42	8	1
4	A	398	PX4	C15-C14-C13	2.37	102.37	114.42	1	1
4	A	405	PX4	O7-C7-C8	2.37	117.00	108.40	11	2
4	A	422	PX4	C13-C12-C11	2.38	102.37	114.42	3	1
4	A	426	PX4	C11-C10-C9	2.38	104.98	113.62	7	2
4	A	316	PX4	C14-C13-C12	2.37	102.38	114.42	10	1
4	A	317	PX4	C7-O7-C23	2.37	123.63	117.79	6	1
4	A	325	PX4	C15-C14-C13	2.37	102.38	114.42	2	1
4	A	326	PX4	C17-C16-C15	2.37	102.38	114.42	8	1
4	A	335	PX4	C34-C33-C32	2.37	102.38	114.42	13	1
4	A	345	PX4	C17-C16-C15	2.37	102.38	114.42	7	2
4	A	383	PX4	C13-C12-C11	2.37	102.38	114.42	13	1
4	A	337	PX4	C18-C17-C16	2.37	102.39	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	390	PX4	C5-N1-C2	2.37	119.61	109.92	3	2
4	A	394	PX4	C18-C17-C16	2.37	102.39	114.42	11	1
4	A	413	PX4	C13-C12-C11	2.37	102.39	114.42	3	1
4	A	314	PX4	O4-P1-O2	2.37	99.81	109.07	12	2
4	A	314	PX4	O7-C7-C8	2.37	116.98	108.40	4	6
4	A	324	PX4	O8-C23-C24	2.37	114.49	123.73	5	1
4	A	348	PX4	O6-C9-C10	2.37	114.49	123.73	13	3
4	A	413	PX4	O6-C9-C10	2.37	114.48	123.73	11	1
4	A	382	PX4	C30-C29-C28	2.37	102.40	114.42	11	1
4	A	416	PX4	C17-C16-C15	2.37	102.39	114.42	4	2
4	A	314	PX4	C16-C15-C14	2.37	102.40	114.42	9	2
4	A	325	PX4	O5-C9-O6	2.37	117.61	123.59	11	1
4	A	384	PX4	C28-C27-C26	2.37	102.40	114.42	5	2
4	A	408	PX4	C20-C19-C18	2.37	102.41	114.42	9	1
4	A	415	PX4	C14-C13-C12	2.37	102.40	114.42	13	1
4	A	429	PX4	C5-N1-C3	2.37	102.88	108.97	9	5
4	A	306	PX4	C18-C17-C16	2.37	102.41	114.42	13	1
4	A	321	PX4	C18-C17-C16	2.37	102.41	114.42	1	1
4	A	348	PX4	C5-N1-C2	2.37	119.60	109.92	8	2
4	A	367	PX4	C20-C19-C18	2.37	102.41	114.42	7	2
4	A	381	PX4	C17-C16-C15	2.37	102.41	114.42	12	2
4	A	388	PX4	C26-C25-C24	2.37	121.70	113.19	13	2
4	A	315	PX4	C29-C28-C27	2.36	102.42	114.42	12	3
4	A	362	PX4	C3-N1-C2	2.36	119.59	109.92	7	1
4	A	381	PX4	C18-C17-C16	2.36	102.42	114.42	2	2
4	A	406	PX4	O1-P1-O4	2.36	118.73	107.75	12	1
4	A	428	PX4	C19-C18-C17	2.36	102.42	114.42	14	1
4	A	346	PX4	C28-C27-C26	2.36	102.43	114.42	1	1
4	A	390	PX4	C20-C19-C18	2.36	102.43	114.42	6	2
4	A	406	PX4	C17-C16-C15	2.36	102.44	114.42	11	2
4	A	412	PX4	C8-O5-C9	2.36	125.87	117.12	12	3
4	A	316	PX4	C18-C17-C16	2.36	102.44	114.42	2	1
4	A	339	PX4	C28-C27-C26	2.36	102.44	114.42	12	1
4	A	309	PX4	O5-C9-O6	2.36	117.64	123.59	11	4
4	A	362	PX4	C29-C28-C27	2.36	102.44	114.42	12	2
4	A	417	PX4	C13-C12-C11	2.36	102.44	114.42	9	3
4	A	340	PX4	C28-C27-C26	2.36	102.45	114.42	3	2
4	A	382	PX4	C8-O5-C9	2.36	108.39	117.12	3	4
4	A	389	PX4	O7-C7-C6	2.36	116.94	108.40	7	1
4	A	389	PX4	C17-C16-C15	2.36	102.46	114.42	11	1
4	A	393	PX4	C3-N1-C2	2.36	119.56	109.92	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	C32-C31-C30	2.36	102.45	114.42	5	1
4	A	311	PX4	C5-N1-C3	2.36	102.92	108.97	2	2
4	A	313	PX4	C27-C26-C25	2.36	102.47	114.42	12	2
4	A	359	PX4	C25-C24-C23	2.36	105.05	113.62	11	2
4	A	363	PX4	O5-C9-C10	2.36	119.30	111.91	9	4
4	A	313	PX4	C15-C14-C13	2.35	102.47	114.42	6	1
4	A	342	PX4	C33-C32-C31	2.35	102.47	114.42	3	2
4	A	425	PX4	O8-C23-C24	2.35	114.55	123.73	7	1
4	A	336	PX4	C19-C18-C17	2.35	102.48	114.42	2	2
4	A	405	PX4	C11-C10-C9	2.35	105.06	113.62	5	2
4	A	353	PX4	C15-C14-C13	2.35	102.49	114.42	7	3
4	A	369	PX4	C4-N1-C3	2.35	102.93	108.97	11	4
4	A	417	PX4	C11-C10-C9	2.35	105.07	113.62	14	2
4	A	312	PX4	C13-C12-C11	2.35	102.49	114.42	2	2
4	A	337	PX4	C4-N1-C3	2.35	115.02	108.97	8	2
4	A	371	PX4	C26-C25-C24	2.35	104.74	113.19	6	1
4	A	375	PX4	C5-N1-C2	2.35	119.53	109.92	12	2
4	A	348	PX4	O8-C23-C24	2.35	114.57	123.73	7	1
4	A	353	PX4	C19-C18-C17	2.35	102.50	114.42	6	2
4	A	382	PX4	C4-N1-C2	2.35	119.53	109.92	2	2
4	A	413	PX4	C27-C26-C25	2.35	102.50	114.42	4	1
4	A	415	PX4	C5-N1-C3	2.35	115.01	108.97	10	4
4	A	419	PX4	O5-C9-O6	2.35	117.67	123.59	3	1
4	A	420	PX4	C32-C31-C30	2.35	102.50	114.42	4	2
4	A	429	PX4	C18-C17-C16	2.35	102.50	114.42	6	2
4	A	316	PX4	C5-N1-C2	2.35	119.51	109.92	11	2
4	A	333	PX4	C17-C16-C15	2.35	102.52	114.42	10	2
4	A	370	PX4	C12-C11-C10	2.35	104.75	113.19	5	1
4	A	423	PX4	C34-C33-C32	2.35	102.51	114.42	5	2
4	A	365	PX4	C29-C28-C27	2.34	102.52	114.42	14	2
4	A	372	PX4	C17-C16-C15	2.34	102.52	114.42	5	2
4	A	306	PX4	C11-C10-C9	2.34	105.10	113.62	11	1
4	A	320	PX4	O7-C7-C6	2.34	116.89	108.40	7	4
4	A	421	PX4	C28-C27-C26	2.34	102.52	114.42	13	2
4	A	386	PX4	O4-P1-O2	2.34	118.22	109.07	1	3
4	A	342	PX4	C31-C30-C29	2.34	102.53	114.42	14	1
4	A	346	PX4	C32-C31-C30	2.34	102.53	114.42	4	2
4	A	373	PX4	C18-C17-C16	2.34	102.53	114.42	14	1
4	A	377	PX4	C14-C13-C12	2.34	102.53	114.42	9	1
4	A	396	PX4	C14-C13-C12	2.34	102.53	114.42	5	1
4	A	416	PX4	C16-C15-C14	2.34	102.53	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	343	PX4	O1-P1-O4	2.34	118.62	107.75	12	1
4	A	331	PX4	C26-C25-C24	2.34	104.78	113.19	2	3
4	A	336	PX4	C32-C31-C30	2.34	102.55	114.42	3	2
4	A	341	PX4	C25-C24-C23	2.34	105.11	113.62	1	1
4	A	372	PX4	O1-P1-O4	2.34	118.61	107.75	6	1
4	A	377	PX4	C16-C15-C14	2.34	102.55	114.42	4	1
4	A	393	PX4	C11-C10-C9	2.34	105.11	113.62	11	1
4	A	384	PX4	C31-C30-C29	2.34	102.55	114.42	11	1
4	A	398	PX4	C19-C18-C17	2.34	102.55	114.42	4	1
4	A	411	PX4	O3-C1-C2	2.34	121.47	109.16	3	2
4	A	369	PX4	O7-C7-C6	2.34	116.87	108.40	8	2
4	A	388	PX4	O1-P1-O4	2.34	118.60	107.75	1	1
4	A	411	PX4	C30-C29-C28	2.34	102.55	114.42	3	1
4	A	307	PX4	C18-C17-C16	2.34	102.56	114.42	10	1
4	A	338	PX4	C32-C31-C30	2.34	102.56	114.42	10	1
4	A	347	PX4	O3-C1-C2	2.34	121.45	109.16	7	2
4	A	313	PX4	C14-C13-C12	2.34	102.57	114.42	8	1
4	A	320	PX4	C32-C31-C30	2.34	102.56	114.42	3	2
4	A	336	PX4	C28-C27-C26	2.34	102.56	114.42	12	2
4	A	331	PX4	C27-C26-C25	2.33	102.57	114.42	4	2
4	A	401	PX4	C34-C33-C32	2.34	102.57	114.42	5	2
4	A	368	PX4	C16-C15-C14	2.33	102.58	114.42	8	1
4	A	322	PX4	C28-C27-C26	2.33	102.58	114.42	2	2
4	A	335	PX4	C13-C12-C11	2.33	102.58	114.42	10	1
4	A	352	PX4	O7-C7-C6	2.33	116.85	108.40	3	3
4	A	383	PX4	O3-C1-C2	2.33	121.43	109.16	13	1
4	A	396	PX4	O1-P1-O3	2.33	96.91	107.75	13	1
4	A	410	PX4	O3-P1-O2	2.33	99.95	109.07	2	1
4	A	408	PX4	C34-C33-C32	2.33	102.59	114.42	4	1
4	A	411	PX4	O7-C23-O8	2.33	118.07	123.70	7	2
4	A	345	PX4	C5-N1-C3	2.33	102.98	108.97	12	2
4	A	347	PX4	C7-O7-C23	2.33	123.53	117.79	2	1
4	A	365	PX4	C7-O7-C23	2.33	123.53	117.79	6	2
4	A	389	PX4	C31-C30-C29	2.33	102.61	114.42	9	2
4	A	401	PX4	O8-C23-C24	2.33	114.65	123.73	6	2
4	A	411	PX4	C17-C16-C15	2.33	102.60	114.42	10	1
4	A	324	PX4	C19-C18-C17	2.33	102.61	114.42	12	2
4	A	326	PX4	C1-C2-N1	2.33	123.55	115.78	2	3
4	A	334	PX4	C12-C11-C10	2.33	104.83	113.19	12	2
4	A	338	PX4	C15-C14-C13	2.33	102.61	114.42	8	2
4	A	356	PX4	C14-C13-C12	2.33	102.61	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	404	PX4	C28-C27-C26	2.33	102.61	114.42	14	1
4	A	342	PX4	C14-C13-C12	2.33	102.62	114.42	2	1
4	A	368	PX4	C4-N1-C3	2.33	102.99	108.97	10	3
4	A	343	PX4	C8-O5-C9	2.32	125.73	117.12	7	1
4	A	354	PX4	O6-C9-C10	2.32	114.66	123.73	13	1
4	A	355	PX4	C27-C26-C25	2.33	102.62	114.42	3	2
4	A	362	PX4	C28-C27-C26	2.33	102.62	114.42	6	1
4	A	387	PX4	O1-P1-O4	2.32	118.54	107.75	12	1
4	A	388	PX4	C33-C32-C31	2.32	102.62	114.42	11	2
4	A	391	PX4	C4-N1-C2	2.32	119.42	109.92	13	1
4	A	399	PX4	C26-C25-C24	2.32	121.54	113.19	2	1
4	A	423	PX4	O3-C1-C2	2.32	121.38	109.16	3	1
4	A	426	PX4	O6-C9-C10	2.32	114.67	123.73	3	2
4	A	330	PX4	C31-C30-C29	2.32	102.63	114.42	12	1
4	A	334	PX4	C11-C10-C9	2.32	105.17	113.62	3	1
4	A	323	PX4	C33-C32-C31	2.32	102.64	114.42	7	1
4	A	306	PX4	C4-N1-C3	2.32	103.01	108.97	14	1
4	A	331	PX4	O5-C9-O6	2.32	117.73	123.59	7	4
4	A	353	PX4	O7-C7-C6	2.32	116.81	108.40	7	3
4	A	343	PX4	C34-C33-C32	2.32	102.65	114.42	11	2
4	A	343	PX4	C5-N1-C2	2.32	119.41	109.92	13	1
4	A	359	PX4	C36-C35-C34	2.32	95.81	113.42	14	1
4	A	362	PX4	C15-C14-C13	2.32	102.64	114.42	7	1
4	A	366	PX4	O5-C9-O6	2.32	117.73	123.59	7	2
4	A	425	PX4	C5-N1-C2	2.32	119.42	109.92	10	2
4	A	336	PX4	O3-C1-C2	2.32	121.35	109.16	4	1
4	A	369	PX4	C4-N1-C2	2.32	100.43	109.92	13	1
4	A	419	PX4	C11-C10-C9	2.32	122.06	113.62	3	3
4	A	419	PX4	C25-C24-C23	2.32	105.19	113.62	13	1
4	A	338	PX4	C8-O5-C9	2.32	108.54	117.12	6	2
4	A	347	PX4	C17-C16-C15	2.32	102.66	114.42	7	2
4	A	354	PX4	C32-C31-C30	2.32	102.66	114.42	5	2
4	A	367	PX4	C4-N1-C2	2.32	119.40	109.92	10	1
4	A	368	PX4	C3-N1-C2	2.32	119.40	109.92	14	1
4	A	390	PX4	C18-C17-C16	2.32	102.66	114.42	9	2
4	A	403	PX4	C27-C26-C25	2.32	102.66	114.42	8	1
4	A	315	PX4	C15-C14-C13	2.32	102.67	114.42	4	2
4	A	355	PX4	C29-C28-C27	2.32	102.67	114.42	4	1
4	A	420	PX4	C26-C25-C24	2.32	104.87	113.19	8	2
4	A	426	PX4	C18-C17-C16	2.32	102.67	114.42	13	1
4	A	331	PX4	C11-C10-C9	2.32	105.20	113.62	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	378	PX4	C5-N1-C3	2.31	103.02	108.97	6	1
4	A	429	PX4	C30-C29-C28	2.32	102.67	114.42	1	2
4	A	384	PX4	C27-C26-C25	2.31	102.68	114.42	9	1
4	A	387	PX4	C34-C33-C32	2.31	102.68	114.42	10	2
4	A	408	PX4	C16-C15-C14	2.31	102.68	114.42	9	1
4	A	419	PX4	C18-C17-C16	2.31	102.68	114.42	10	4
4	A	426	PX4	C8-O5-C9	2.31	108.55	117.12	8	2
4	A	316	PX4	C30-C29-C28	2.31	102.69	114.42	1	1
4	A	329	PX4	C13-C12-C11	2.31	102.69	114.42	8	2
4	A	330	PX4	C5-N1-C2	2.31	100.46	109.92	2	2
4	A	352	PX4	O7-C23-O8	2.31	118.11	123.70	10	3
4	A	414	PX4	C19-C18-C17	2.31	102.69	114.42	1	1
4	A	315	PX4	C3-N1-C2	2.31	119.36	109.92	12	2
4	A	360	PX4	C15-C14-C13	2.31	102.70	114.42	12	2
4	A	363	PX4	C4-N1-C3	2.31	114.91	108.97	14	5
4	A	388	PX4	O8-C23-C24	2.31	114.72	123.73	7	3
4	A	367	PX4	C5-N1-C3	2.31	103.04	108.97	2	1
4	A	386	PX4	O1-P1-O4	2.31	118.46	107.75	10	1
4	A	418	PX4	C11-C10-C9	2.31	105.23	113.62	4	2
4	A	313	PX4	O5-C9-O6	2.31	117.77	123.59	1	3
4	A	319	PX4	C29-C28-C27	2.31	102.72	114.42	3	1
4	A	344	PX4	O5-C9-C10	2.30	119.14	111.91	11	2
4	A	320	PX4	C34-C33-C32	2.30	102.73	114.42	2	1
4	A	365	PX4	C16-C15-C14	2.30	102.73	114.42	11	1
4	A	368	PX4	C15-C14-C13	2.31	102.72	114.42	12	2
4	A	388	PX4	C3-N1-C2	2.31	100.48	109.92	8	1
4	A	386	PX4	C34-C33-C32	2.30	102.73	114.42	13	2
4	A	309	PX4	C14-C13-C12	2.30	102.74	114.42	3	1
4	A	329	PX4	C27-C26-C25	2.30	126.11	114.42	13	1
4	A	403	PX4	C28-C27-C26	2.30	102.73	114.42	1	1
4	A	430	PX4	O1-P1-O3	2.30	97.05	107.75	14	1
4	A	333	PX4	O1-P1-O3	2.30	97.05	107.75	8	2
4	A	405	PX4	C32-C31-C30	2.30	102.74	114.42	5	1
4	A	370	PX4	C25-C24-C23	2.30	121.98	113.62	9	2
4	A	374	PX4	O4-P1-O2	2.30	118.06	109.07	5	1
4	A	381	PX4	C27-C26-C25	2.30	102.74	114.42	2	2
4	A	413	PX4	O3-C1-C2	2.30	121.26	109.16	12	1
4	A	306	PX4	C17-C16-C15	2.30	102.76	114.42	10	1
4	A	326	PX4	C8-O5-C9	2.30	108.61	117.12	13	1
4	A	355	PX4	C19-C18-C17	2.30	102.75	114.42	12	1
4	A	357	PX4	C19-C18-C17	2.30	102.75	114.42	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	406	PX4	C29-C28-C27	2.30	102.75	114.42	3	1
4	A	319	PX4	C32-C31-C30	2.30	102.76	114.42	10	1
4	A	314	PX4	C13-C12-C11	2.30	102.77	114.42	4	1
4	A	347	PX4	C25-C24-C23	2.30	105.27	113.62	14	3
4	A	401	PX4	O7-C7-C6	2.30	116.72	108.40	1	3
4	A	421	PX4	C20-C19-C18	2.30	102.76	114.42	11	1
4	A	422	PX4	C28-C27-C26	2.30	102.77	114.42	14	1
4	A	423	PX4	C1-C2-N1	2.30	123.45	115.78	12	2
4	A	325	PX4	C33-C32-C31	2.30	102.77	114.42	10	1
4	A	373	PX4	C3-N1-C2	2.30	100.52	109.92	2	1
4	A	375	PX4	C29-C28-C27	2.30	102.77	114.42	11	1
4	A	403	PX4	C15-C14-C13	2.30	102.77	114.42	13	3
4	A	410	PX4	C30-C29-C28	2.30	102.77	114.42	3	1
4	A	422	PX4	C26-C25-C24	2.30	104.94	113.19	13	1
4	A	424	PX4	C1-C2-N1	2.30	123.44	115.78	10	2
4	A	309	PX4	C19-C18-C17	2.29	102.78	114.42	5	1
4	A	313	PX4	C30-C29-C28	2.29	102.78	114.42	4	1
4	A	344	PX4	C32-C31-C30	2.29	102.78	114.42	13	1
4	A	361	PX4	C13-C12-C11	2.29	102.78	114.42	2	1
4	A	373	PX4	C19-C18-C17	2.29	102.78	114.42	7	1
4	A	398	PX4	C31-C30-C29	2.29	102.78	114.42	2	1
4	A	325	PX4	C30-C29-C28	2.29	102.79	114.42	3	1
4	A	329	PX4	C5-N1-C2	2.29	100.54	109.92	9	1
4	A	357	PX4	C28-C27-C26	2.29	102.79	114.42	13	1
4	A	386	PX4	C27-C26-C25	2.29	102.80	114.42	9	2
4	A	333	PX4	C26-C25-C24	2.29	104.96	113.19	14	3
4	A	381	PX4	C11-C10-C9	2.29	105.29	113.62	4	2
4	A	390	PX4	C1-C2-N1	2.29	123.42	115.78	8	1
4	A	415	PX4	C13-C12-C11	2.29	102.80	114.42	6	2
4	A	306	PX4	C30-C29-C28	2.29	102.81	114.42	6	1
4	A	339	PX4	C26-C25-C24	2.29	104.97	113.19	9	2
4	A	346	PX4	C18-C17-C16	2.29	102.81	114.42	11	2
4	A	347	PX4	C1-C2-N1	2.29	123.42	115.78	1	2
4	A	381	PX4	C3-N1-C2	2.29	119.28	109.92	5	2
4	A	412	PX4	C33-C32-C31	2.29	102.81	114.42	11	2
4	A	425	PX4	C17-C16-C15	2.29	102.81	114.42	9	2
4	A	337	PX4	C20-C19-C18	2.29	102.82	114.42	14	1
4	A	348	PX4	O5-C9-O6	2.29	117.82	123.59	5	1
4	A	339	PX4	C32-C31-C30	2.29	102.82	114.42	5	1
4	A	358	PX4	C1-C2-N1	2.29	123.41	115.78	6	1
4	A	355	PX4	C13-C12-C11	2.28	102.83	114.42	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	363	PX4	C34-C33-C32	2.29	102.82	114.42	9	2
4	A	368	PX4	O6-C9-C10	2.29	114.82	123.73	8	2
4	A	426	PX4	C32-C31-C30	2.29	102.82	114.42	6	2
4	A	401	PX4	C1-C2-N1	2.28	123.41	115.78	8	2
4	A	417	PX4	C26-C25-C24	2.29	104.98	113.19	13	2
4	A	359	PX4	C3-N1-C2	2.28	119.26	109.92	11	1
4	A	381	PX4	O3-C1-C2	2.28	121.17	109.16	5	1
4	A	410	PX4	C4-N1-C3	2.28	103.10	108.97	9	1
4	A	426	PX4	C4-N1-C2	2.28	100.57	109.92	12	1
4	A	421	PX4	C12-C11-C10	2.28	121.39	113.19	7	2
4	A	340	PX4	C16-C15-C14	2.28	102.84	114.42	12	1
4	A	320	PX4	C30-C29-C28	2.28	102.85	114.42	8	2
4	A	332	PX4	C5-N1-C2	2.28	100.59	109.92	5	1
4	A	426	PX4	O1-P1-O4	2.28	118.34	107.75	8	1
4	A	339	PX4	C16-C15-C14	2.28	102.86	114.42	9	1
4	A	372	PX4	C15-C14-C13	2.28	102.86	114.42	5	1
4	A	390	PX4	C15-C14-C13	2.28	102.85	114.42	5	1
4	A	337	PX4	C11-C10-C9	2.28	105.34	113.62	4	2
4	A	422	PX4	C4-N1-C2	2.28	100.60	109.92	6	1
4	A	341	PX4	C11-C10-C9	2.27	105.35	113.62	10	1
4	A	409	PX4	C4-N1-C2	2.27	100.61	109.92	13	1
4	A	318	PX4	O1-P1-O3	2.27	97.19	107.75	4	1
4	A	341	PX4	C32-C31-C30	2.27	102.89	114.42	10	1
4	A	358	PX4	C8-O5-C9	2.27	108.71	117.12	7	2
4	A	388	PX4	C34-C33-C32	2.27	102.89	114.42	9	2
4	A	309	PX4	C29-C28-C27	2.27	102.90	114.42	6	2
4	A	345	PX4	C29-C28-C27	2.27	102.90	114.42	1	1
4	A	308	PX4	C4-N1-C2	2.27	119.20	109.92	6	3
4	A	314	PX4	O3-P1-O2	2.27	117.93	109.07	7	2
4	A	345	PX4	C33-C32-C31	2.27	102.90	114.42	8	1
4	A	350	PX4	C5-N1-C2	2.27	100.62	109.92	6	1
4	A	411	PX4	C19-C18-C17	2.27	102.90	114.42	1	2
4	A	390	PX4	O8-C23-C24	2.27	114.88	123.73	6	1
4	A	309	PX4	C12-C11-C10	2.27	105.04	113.19	1	1
4	A	355	PX4	C33-C32-C31	2.27	102.91	114.42	8	3
4	A	327	PX4	C19-C18-C17	2.27	102.92	114.42	10	1
4	A	346	PX4	C5-N1-C2	2.27	119.19	109.92	4	2
4	A	349	PX4	C30-C29-C28	2.27	102.92	114.42	10	1
4	A	357	PX4	O3-P1-O2	2.27	100.21	109.07	4	1
4	A	362	PX4	C5-N1-C2	2.27	100.64	109.92	6	1
4	A	404	PX4	C26-C25-C24	2.27	105.04	113.19	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	409	PX4	C28-C27-C26	2.27	102.92	114.42	3	1
4	A	424	PX4	C5-N1-C4	2.27	103.15	108.97	10	3
4	A	427	PX4	C11-C10-C9	2.27	105.38	113.62	11	1
4	A	319	PX4	C13-C12-C11	2.26	102.94	114.42	3	1
4	A	345	PX4	C15-C14-C13	2.26	102.93	114.42	4	1
4	A	407	PX4	C30-C29-C28	2.26	102.93	114.42	9	3
4	A	352	PX4	C8-O5-C9	2.26	108.74	117.12	7	2
4	A	356	PX4	C15-C14-C13	2.26	102.94	114.42	4	2
4	A	315	PX4	C19-C18-C17	2.26	102.94	114.42	12	1
4	A	328	PX4	C5-N1-C2	2.26	119.17	109.92	3	1
4	A	371	PX4	C30-C29-C28	2.26	125.91	114.42	9	1
4	A	406	PX4	C7-O7-C23	2.26	123.36	117.79	5	1
4	A	329	PX4	C16-C15-C14	2.26	102.94	114.42	5	2
4	A	331	PX4	C20-C19-C18	2.26	102.94	114.42	6	1
4	A	357	PX4	O1-P1-O4	2.26	118.25	107.75	11	2
4	A	394	PX4	C1-C2-N1	2.26	123.33	115.78	10	1
4	A	423	PX4	C5-N1-C2	2.26	119.17	109.92	5	1
4	A	351	PX4	O7-C23-O8	2.26	129.16	123.70	4	1
4	A	314	PX4	C29-C28-C27	2.26	102.96	114.42	8	2
4	A	340	PX4	O3-C1-C2	2.26	121.04	109.16	6	1
4	A	349	PX4	C33-C32-C31	2.26	102.96	114.42	14	1
4	A	366	PX4	C15-C14-C13	2.26	102.95	114.42	4	1
4	A	374	PX4	O7-C7-C6	2.26	116.58	108.40	1	3
4	A	377	PX4	C3-N1-C2	2.26	119.16	109.92	13	2
4	A	382	PX4	O3-C1-C2	2.26	121.04	109.16	12	2
4	A	341	PX4	C20-C19-C18	2.26	102.97	114.42	2	3
4	A	404	PX4	C8-O5-C9	2.26	108.76	117.12	5	2
4	A	417	PX4	C12-C11-C10	2.26	105.08	113.19	8	1
4	A	310	PX4	O1-P1-O3	2.26	97.27	107.75	7	3
4	A	364	PX4	C17-C16-C15	2.26	102.97	114.42	13	2
4	A	372	PX4	C30-C29-C28	2.26	102.97	114.42	10	1
4	A	375	PX4	C4-N1-C2	2.26	119.15	109.92	3	1
4	A	385	PX4	C20-C19-C18	2.26	102.97	114.42	7	1
4	A	385	PX4	C28-C27-C26	2.26	102.97	114.42	8	1
4	A	387	PX4	O7-C7-C8	2.26	116.57	108.40	7	1
4	A	425	PX4	O3-P1-O2	2.26	100.25	109.07	14	2
4	A	312	PX4	C33-C32-C31	2.25	102.98	114.42	12	2
4	A	323	PX4	C4-N1-C2	2.25	119.14	109.92	3	2
4	A	409	PX4	C5-N1-C2	2.25	119.14	109.92	13	2
4	A	315	PX4	C16-C15-C14	2.25	102.99	114.42	11	1
4	A	351	PX4	C3-N1-C2	2.25	119.13	109.92	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	C26-C25-C24	2.25	105.09	113.19	9	3
4	A	371	PX4	C28-C27-C26	2.25	102.99	114.42	1	2
4	A	396	PX4	C30-C29-C28	2.25	102.99	114.42	6	1
4	A	401	PX4	C13-C12-C11	2.25	102.99	114.42	7	4
4	A	310	PX4	C30-C29-C28	2.25	103.01	114.42	3	2
4	A	310	PX4	C31-C30-C29	2.25	103.01	114.42	13	1
4	A	333	PX4	C3-N1-C2	2.25	100.71	109.92	4	1
4	A	335	PX4	C33-C32-C31	2.25	103.00	114.42	7	1
4	A	358	PX4	C32-C31-C30	2.25	103.00	114.42	13	1
4	A	364	PX4	C12-C11-C10	2.25	105.10	113.19	12	1
4	A	409	PX4	C8-O5-C9	2.25	108.79	117.12	4	1
4	A	422	PX4	O3-C1-C2	2.25	120.99	109.16	5	1
4	A	342	PX4	C11-C10-C9	2.25	105.44	113.62	1	1
4	A	383	PX4	C28-C27-C26	2.25	103.01	114.42	11	1
4	A	396	PX4	C15-C14-C13	2.25	103.02	114.42	4	1
4	A	396	PX4	C11-C10-C9	2.25	121.80	113.62	14	1
4	A	347	PX4	C20-C19-C18	2.25	103.02	114.42	1	1
4	A	358	PX4	C25-C24-C23	2.25	105.45	113.62	5	2
4	A	363	PX4	C15-C14-C13	2.25	103.02	114.42	12	1
4	A	400	PX4	C34-C33-C32	2.25	103.02	114.42	4	3
4	A	419	PX4	C19-C18-C17	2.25	103.02	114.42	9	2
4	A	411	PX4	C5-N1-C2	2.25	119.10	109.92	13	1
4	A	423	PX4	C16-C15-C14	2.25	103.02	114.42	6	2
4	A	309	PX4	O3-C1-C2	2.24	120.96	109.16	5	1
4	A	311	PX4	C31-C30-C29	2.24	103.03	114.42	2	2
4	A	349	PX4	O5-C9-C10	2.24	118.95	111.91	4	2
4	A	396	PX4	C16-C15-C14	2.24	103.03	114.42	9	2
4	A	321	PX4	C4-N1-C2	2.24	119.09	109.92	1	1
4	A	321	PX4	C16-C15-C14	2.24	103.04	114.42	3	1
4	A	417	PX4	C16-C15-C14	2.24	103.04	114.42	6	1
4	A	421	PX4	C29-C28-C27	2.24	103.03	114.42	12	3
4	A	328	PX4	C31-C30-C29	2.24	103.05	114.42	8	2
4	A	363	PX4	C7-O7-C23	2.24	123.31	117.79	1	2
4	A	378	PX4	C16-C15-C14	2.24	103.04	114.42	5	2
4	A	386	PX4	C29-C28-C27	2.24	103.05	114.42	13	1
4	A	417	PX4	C32-C31-C30	2.24	103.05	114.42	8	2
4	A	316	PX4	O7-C7-C6	2.24	116.51	108.40	1	2
4	A	322	PX4	C27-C26-C25	2.24	103.06	114.42	4	1
4	A	333	PX4	C11-C10-C9	2.24	121.76	113.62	1	1
4	A	373	PX4	C4-N1-C2	2.24	119.08	109.92	13	1
4	A	408	PX4	C8-O5-C9	2.24	108.83	117.12	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	306	PX4	C34-C33-C32	2.24	103.06	114.42	6	1
4	A	346	PX4	C20-C19-C18	2.24	103.06	114.42	14	3
4	A	347	PX4	C29-C28-C27	2.24	103.06	114.42	14	1
4	A	386	PX4	C8-O5-C9	2.24	108.83	117.12	3	1
4	A	393	PX4	C14-C13-C12	2.24	103.06	114.42	8	2
4	A	311	PX4	C19-C18-C17	2.24	103.07	114.42	6	3
4	A	334	PX4	C5-N1-C2	2.24	100.76	109.92	1	2
4	A	346	PX4	C12-C11-C10	2.24	105.15	113.19	9	1
4	A	360	PX4	C28-C27-C26	2.24	103.07	114.42	2	2
4	A	360	PX4	C32-C31-C30	2.24	103.07	114.42	3	1
4	A	369	PX4	C34-C33-C32	2.24	103.07	114.42	11	1
4	A	392	PX4	C5-N1-C2	2.24	119.07	109.92	6	1
4	A	407	PX4	O8-C23-C24	2.24	115.01	123.73	9	1
4	A	411	PX4	C11-C10-C9	2.24	105.49	113.62	10	2
4	A	425	PX4	C3-N1-C2	2.24	119.07	109.92	7	1
4	A	311	PX4	O6-C9-C10	2.24	115.01	123.73	3	3
4	A	427	PX4	C15-C14-C13	2.24	103.07	114.42	13	3
4	A	335	PX4	C14-C13-C12	2.23	103.08	114.42	7	1
4	A	361	PX4	C27-C26-C25	2.23	103.08	114.42	3	2
4	A	391	PX4	O8-C23-C24	2.23	115.01	123.73	12	1
4	A	400	PX4	C20-C19-C18	2.23	103.08	114.42	4	2
4	A	374	PX4	C29-C28-C27	2.23	103.09	114.42	6	1
4	A	381	PX4	C16-C15-C14	2.23	103.08	114.42	9	1
4	A	383	PX4	C15-C14-C13	2.23	103.08	114.42	8	1
4	A	323	PX4	O1-P1-O4	2.23	118.11	107.75	8	2
4	A	376	PX4	C1-C2-N1	2.23	123.24	115.78	11	2
4	A	400	PX4	O1-P1-O4	2.23	118.12	107.75	3	3
4	A	400	PX4	O3-C1-C2	2.23	120.91	109.16	14	1
4	A	329	PX4	C1-C2-N1	2.23	123.23	115.78	7	2
4	A	395	PX4	C30-C29-C28	2.23	103.09	114.42	3	2
4	A	402	PX4	C4-N1-C3	2.23	103.23	108.97	9	3
4	A	310	PX4	C20-C19-C18	2.23	103.10	114.42	14	2
4	A	312	PX4	O8-C23-C24	2.23	115.03	123.73	9	1
4	A	314	PX4	C11-C10-C9	2.23	105.51	113.62	13	2
4	A	374	PX4	C5-N1-C2	2.23	119.04	109.92	1	1
4	A	389	PX4	C16-C15-C14	2.23	103.10	114.42	9	1
4	A	430	PX4	C33-C32-C31	2.23	103.10	114.42	3	1
4	A	329	PX4	C35-C34-C33	2.23	94.61	115.30	11	1
4	A	334	PX4	C13-C12-C11	2.23	103.11	114.42	9	3
4	A	357	PX4	C32-C31-C30	2.23	103.11	114.42	14	1
4	A	364	PX4	C16-C15-C14	2.23	103.11	114.42	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	368	PX4	C18-C17-C16	2.23	103.10	114.42	5	2
4	A	400	PX4	C27-C26-C25	2.23	103.11	114.42	7	4
4	A	367	PX4	C29-C28-C27	2.23	103.11	114.42	7	2
4	A	378	PX4	C5-N1-C2	2.23	119.02	109.92	10	1
4	A	395	PX4	C13-C12-C11	2.23	103.13	114.42	14	1
4	A	398	PX4	C14-C13-C12	2.23	103.12	114.42	7	1
4	A	411	PX4	O8-C23-C24	2.23	115.04	123.73	8	2
4	A	360	PX4	O8-C23-C24	2.23	115.05	123.73	10	1
4	A	311	PX4	C3-N1-C2	2.22	119.02	109.92	12	3
4	A	388	PX4	C20-C19-C18	2.22	103.13	114.42	6	1
4	A	309	PX4	C8-O5-C9	2.22	108.89	117.12	6	2
4	A	326	PX4	C16-C15-C14	2.22	103.14	114.42	10	1
4	A	380	PX4	C19-C18-C17	2.22	103.14	114.42	4	1
4	A	385	PX4	C14-C13-C12	2.22	103.14	114.42	5	1
4	A	351	PX4	C28-C27-C26	2.22	103.15	114.42	14	1
4	A	392	PX4	C19-C18-C17	2.22	103.15	114.42	11	2
4	A	374	PX4	C26-C25-C24	2.22	121.17	113.19	13	1
4	A	397	PX4	O3-P1-O2	2.22	100.39	109.07	6	4
4	A	401	PX4	C20-C19-C18	2.22	103.14	114.42	7	1
4	A	368	PX4	C19-C18-C17	2.22	103.15	114.42	13	1
4	A	412	PX4	C27-C26-C25	2.22	103.15	114.42	11	1
4	A	310	PX4	C17-C16-C15	2.22	103.16	114.42	3	1
4	A	329	PX4	C19-C18-C17	2.22	103.16	114.42	14	1
4	A	376	PX4	C15-C14-C13	2.22	103.16	114.42	2	1
4	A	384	PX4	O5-C9-O6	2.22	117.99	123.59	5	1
4	A	416	PX4	C30-C29-C28	2.22	103.15	114.42	10	1
4	A	346	PX4	C29-C28-C27	2.22	103.16	114.42	11	1
4	A	321	PX4	C8-O5-C9	2.22	125.33	117.12	10	3
4	A	333	PX4	C13-C12-C11	2.22	103.17	114.42	4	1
4	A	339	PX4	O8-C23-C24	2.22	115.08	123.73	9	1
4	A	339	PX4	C5-N1-C2	2.22	118.99	109.92	13	1
4	A	342	PX4	C4-N1-C2	2.22	118.99	109.92	8	3
4	A	358	PX4	C11-C10-C9	2.22	121.69	113.62	8	1
4	A	369	PX4	C20-C19-C18	2.22	103.16	114.42	9	1
4	A	310	PX4	C5-N1-C2	2.21	118.98	109.92	11	1
4	A	379	PX4	C7-O7-C23	2.21	123.24	117.79	9	1
4	A	397	PX4	C4-N1-C2	2.21	100.85	109.92	4	1
4	A	339	PX4	C14-C13-C12	2.21	103.19	114.42	1	1
4	A	356	PX4	C25-C24-C23	2.21	105.57	113.62	12	1
4	A	309	PX4	C17-C16-C15	2.21	103.20	114.42	7	2
4	A	326	PX4	C3-N1-C2	2.21	118.96	109.92	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	355	PX4	C28-C27-C26	2.21	103.20	114.42	1	1
4	A	368	PX4	C12-C11-C10	2.21	105.24	113.19	7	2
4	A	371	PX4	C12-C11-C10	2.21	105.23	113.19	10	1
4	A	414	PX4	C4-N1-C2	2.21	100.86	109.92	9	2
4	A	332	PX4	C8-O5-C9	2.21	108.94	117.12	3	2
4	A	375	PX4	C13-C12-C11	2.21	103.20	114.42	1	1
4	A	379	PX4	C17-C16-C15	2.21	103.20	114.42	10	1
4	A	406	PX4	C13-C12-C11	2.21	103.20	114.42	6	1
4	A	332	PX4	C13-C12-C11	2.21	103.21	114.42	3	1
4	A	357	PX4	C8-O5-C9	2.21	125.31	117.12	11	2
4	A	370	PX4	C17-C16-C15	2.21	103.20	114.42	3	2
4	A	401	PX4	O3-P1-O2	2.21	100.43	109.07	3	2
4	A	373	PX4	O7-C7-C8	2.21	116.40	108.40	4	3
4	A	307	PX4	C5-N1-C4	2.21	103.30	108.97	13	2
4	A	349	PX4	C32-C31-C30	2.21	103.22	114.42	2	1
4	A	365	PX4	C3-N1-C2	2.21	100.89	109.92	5	2
4	A	379	PX4	C16-C15-C14	2.21	103.22	114.42	11	2
4	A	381	PX4	C5-N1-C2	2.21	100.89	109.92	7	1
4	A	382	PX4	C13-C12-C11	2.21	103.22	114.42	7	2
4	A	385	PX4	C30-C29-C28	2.21	103.22	114.42	5	1
4	A	366	PX4	O3-C1-C2	2.21	120.76	109.16	8	1
4	A	369	PX4	C25-C24-C23	2.21	105.60	113.62	3	2
4	A	373	PX4	C26-C25-C24	2.20	105.26	113.19	7	1
4	A	385	PX4	C4-N1-C2	2.21	118.94	109.92	13	1
4	A	418	PX4	O6-C9-C10	2.21	115.13	123.73	7	1
4	A	421	PX4	O5-C9-O6	2.21	118.03	123.59	14	4
4	A	372	PX4	C8-O5-C9	2.20	108.96	117.12	12	1
4	A	376	PX4	C17-C16-C15	2.20	103.24	114.42	11	2
4	A	314	PX4	C30-C29-C28	2.20	103.25	114.42	6	1
4	A	323	PX4	O4-P1-O2	2.20	117.67	109.07	12	1
4	A	332	PX4	C33-C32-C31	2.20	103.24	114.42	2	1
4	A	311	PX4	C8-O5-C9	2.20	108.97	117.12	6	3
4	A	315	PX4	C34-C33-C32	2.20	103.25	114.42	10	2
4	A	385	PX4	C33-C32-C31	2.20	103.25	114.42	6	2
4	A	388	PX4	C13-C12-C11	2.20	103.25	114.42	4	1
4	A	398	PX4	C32-C31-C30	2.20	103.25	114.42	12	2
4	A	403	PX4	C12-C11-C10	2.20	105.28	113.19	12	1
4	A	413	PX4	C14-C13-C12	2.20	103.25	114.42	4	1
4	A	362	PX4	C25-C24-C23	2.20	121.62	113.62	11	3
4	A	318	PX4	C19-C18-C17	2.20	103.26	114.42	11	1
4	A	356	PX4	C20-C19-C18	2.20	103.26	114.42	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	C17-C16-C15	2.20	103.26	114.42	7	1
4	A	367	PX4	C32-C31-C30	2.20	125.59	114.42	6	2
4	A	393	PX4	O7-C7-C6	2.20	116.36	108.40	14	1
4	A	313	PX4	O3-P1-O2	2.20	100.48	109.07	14	2
4	A	322	PX4	C34-C33-C32	2.20	103.27	114.42	2	1
4	A	343	PX4	C16-C15-C14	2.20	103.27	114.42	9	2
4	A	391	PX4	O5-C9-C10	2.20	118.80	111.91	8	1
4	A	306	PX4	C5-N1-C3	2.19	103.33	108.97	4	1
4	A	329	PX4	C8-O5-C9	2.20	108.99	117.12	6	2
4	A	368	PX4	C26-C25-C24	2.20	105.30	113.19	1	1
4	A	379	PX4	O6-C9-C10	2.20	115.17	123.73	2	1
4	A	404	PX4	O8-C23-C24	2.20	115.17	123.73	9	1
4	A	410	PX4	O5-C9-O6	2.20	118.05	123.59	10	3
4	A	415	PX4	C33-C32-C31	2.20	103.28	114.42	9	1
4	A	338	PX4	C5-N1-C2	2.19	118.89	109.92	10	1
4	A	361	PX4	C28-C27-C26	2.19	103.29	114.42	3	1
4	A	412	PX4	C16-C15-C14	2.19	103.29	114.42	1	2
4	A	322	PX4	C20-C19-C18	2.19	103.29	114.42	8	1
4	A	326	PX4	C32-C31-C30	2.19	103.29	114.42	8	1
4	A	358	PX4	C14-C13-C12	2.19	103.29	114.42	3	1
4	A	361	PX4	O6-C9-C10	2.19	115.18	123.73	6	2
4	A	400	PX4	C11-C10-C9	2.19	105.65	113.62	5	1
4	A	311	PX4	C29-C28-C27	2.19	103.30	114.42	3	1
4	A	328	PX4	C33-C32-C31	2.19	103.30	114.42	4	1
4	A	329	PX4	O8-C23-C24	2.19	115.19	123.73	6	1
4	A	407	PX4	C3-N1-C2	2.19	100.95	109.92	7	2
4	A	410	PX4	C20-C19-C18	2.19	103.30	114.42	4	1
4	A	313	PX4	O7-C23-O8	2.19	118.41	123.70	10	1
4	A	376	PX4	C27-C26-C25	2.19	103.31	114.42	7	1
4	A	419	PX4	C29-C28-C27	2.19	103.31	114.42	11	1
4	A	317	PX4	C28-C27-C26	2.19	103.31	114.42	12	2
4	A	383	PX4	C29-C28-C27	2.19	103.32	114.42	11	1
4	A	402	PX4	O6-C9-C10	2.19	115.19	123.73	8	1
4	A	405	PX4	C33-C32-C31	2.19	103.32	114.42	6	2
4	A	425	PX4	C28-C27-C26	2.19	103.31	114.42	6	1
4	A	315	PX4	C13-C12-C11	2.19	103.32	114.42	5	2
4	A	347	PX4	C31-C30-C29	2.19	103.32	114.42	8	1
4	A	369	PX4	C18-C17-C16	2.19	103.32	114.42	4	1
4	A	389	PX4	C8-O5-C9	2.19	109.02	117.12	9	1
4	A	347	PX4	C28-C27-C26	2.19	103.33	114.42	11	1
4	A	327	PX4	O1-P1-O4	2.18	117.89	107.75	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	348	PX4	O1-P1-O4	2.18	117.89	107.75	2	3
4	A	356	PX4	C8-O5-C9	2.19	109.03	117.12	10	1
4	A	393	PX4	C32-C31-C30	2.19	103.33	114.42	10	1
4	A	371	PX4	C4-N1-C2	2.18	118.86	109.92	12	2
4	A	427	PX4	C30-C29-C28	2.19	103.33	114.42	9	1
4	A	338	PX4	O6-C9-C10	2.18	115.22	123.73	8	1
4	A	348	PX4	C28-C27-C26	2.18	103.35	114.42	12	2
4	A	355	PX4	C3-N1-C2	2.18	100.98	109.92	12	1
4	A	364	PX4	C11-C10-C9	2.18	105.68	113.62	6	2
4	A	357	PX4	C16-C15-C14	2.18	103.35	114.42	11	1
4	A	385	PX4	C4-N1-C3	2.18	114.58	108.97	9	1
4	A	422	PX4	O1-P1-O4	2.18	117.88	107.75	5	4
4	A	425	PX4	C32-C31-C30	2.18	103.35	114.42	4	1
4	A	354	PX4	C3-N1-C2	2.18	118.84	109.92	1	1
4	A	366	PX4	C4-N1-C2	2.18	118.84	109.92	7	2
4	A	377	PX4	C32-C31-C30	2.18	103.36	114.42	7	2
4	A	396	PX4	C4-N1-C2	2.18	118.83	109.92	14	2
4	A	402	PX4	C34-C33-C32	2.18	103.36	114.42	8	1
4	A	332	PX4	C25-C24-C23	2.18	105.70	113.62	3	2
4	A	351	PX4	C19-C18-C17	2.18	103.37	114.42	2	1
4	A	393	PX4	C8-O5-C9	2.18	109.06	117.12	4	1
4	A	407	PX4	C13-C12-C11	2.18	103.37	114.42	13	1
4	A	421	PX4	C36-C35-C34	2.18	96.89	113.42	6	2
4	A	393	PX4	O8-C23-C24	2.18	115.24	123.73	7	1
4	A	402	PX4	C5-N1-C3	2.18	103.38	108.97	7	2
4	A	427	PX4	C19-C18-C17	2.18	103.37	114.42	6	1
4	A	376	PX4	C4-N1-C2	2.17	118.81	109.92	14	1
4	A	380	PX4	C1-C2-N1	2.18	123.04	115.78	3	2
4	A	408	PX4	C25-C24-C23	2.18	105.71	113.62	11	1
4	A	306	PX4	C32-C31-C30	2.17	103.39	114.42	7	1
4	A	320	PX4	O5-C9-O6	2.17	118.10	123.59	11	2
4	A	384	PX4	O1-P1-O3	2.17	97.65	107.75	7	1
4	A	395	PX4	C16-C15-C14	2.17	103.39	114.42	13	1
4	A	396	PX4	O5-C9-C10	2.17	118.73	111.91	6	1
4	A	418	PX4	C28-C27-C26	2.18	103.38	114.42	14	2
4	A	310	PX4	O4-P1-O2	2.17	117.56	109.07	4	1
4	A	325	PX4	C16-C15-C14	2.17	103.39	114.42	13	1
4	A	332	PX4	C14-C13-C12	2.17	103.39	114.42	9	1
4	A	335	PX4	O8-C23-C24	2.17	115.25	123.73	9	1
4	A	398	PX4	C28-C27-C26	2.17	103.39	114.42	7	1
4	A	402	PX4	C33-C32-C31	2.17	103.39	114.42	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C29-C28-C27	2.17	103.39	114.42	13	2
4	A	357	PX4	O1-P1-O3	2.17	97.66	107.75	4	2
4	A	318	PX4	C30-C29-C28	2.17	103.40	114.42	14	1
4	A	346	PX4	C30-C29-C28	2.17	103.40	114.42	14	1
4	A	361	PX4	C12-C11-C10	2.17	105.38	113.19	14	1
4	A	403	PX4	C18-C17-C16	2.17	103.40	114.42	1	1
4	A	420	PX4	C33-C32-C31	2.17	103.40	114.42	10	1
4	A	308	PX4	C15-C14-C13	2.17	103.41	114.42	10	1
4	A	328	PX4	C8-O5-C9	2.17	109.09	117.12	1	1
4	A	332	PX4	C34-C33-C32	2.17	103.41	114.42	4	1
4	A	363	PX4	C16-C15-C14	2.17	103.41	114.42	9	2
4	A	392	PX4	C27-C26-C25	2.17	103.41	114.42	2	1
4	A	394	PX4	C17-C16-C15	2.17	103.41	114.42	2	1
4	A	399	PX4	C4-N1-C2	2.17	118.80	109.92	12	1
4	A	382	PX4	C1-C2-N1	2.17	123.02	115.78	3	2
4	A	383	PX4	C8-O5-C9	2.17	109.09	117.12	6	2
4	A	407	PX4	C31-C30-C29	2.17	103.41	114.42	11	1
4	A	415	PX4	C19-C18-C17	2.17	103.41	114.42	1	2
4	A	313	PX4	O1-P1-O3	2.17	97.68	107.75	11	3
4	A	332	PX4	C28-C27-C26	2.17	103.42	114.42	8	1
4	A	349	PX4	C25-C24-C23	2.17	121.50	113.62	1	1
4	A	425	PX4	C18-C17-C16	2.17	103.42	114.42	4	1
4	A	428	PX4	O7-C7-C6	2.17	116.25	108.40	11	3
4	A	348	PX4	C34-C33-C32	2.17	103.42	114.42	11	1
4	A	355	PX4	C14-C13-C12	2.17	103.42	114.42	6	1
4	A	332	PX4	C12-C11-C10	2.17	120.97	113.19	11	1
4	A	343	PX4	C3-N1-C2	2.17	118.78	109.92	14	1
4	A	357	PX4	C3-N1-C2	2.17	118.78	109.92	1	1
4	A	359	PX4	C30-C29-C28	2.17	103.42	114.42	6	1
4	A	389	PX4	O6-C9-C10	2.17	115.27	123.73	4	1
4	A	382	PX4	C31-C30-C29	2.17	103.43	114.42	1	1
4	A	414	PX4	O3-C1-C2	2.17	120.55	109.16	3	2
4	A	310	PX4	C4-N1-C2	2.16	118.77	109.92	7	2
4	A	314	PX4	C8-O5-C9	2.16	109.11	117.12	7	1
4	A	328	PX4	C12-C11-C10	2.16	105.42	113.19	10	1
4	A	369	PX4	C27-C26-C25	2.16	103.44	114.42	2	1
4	A	371	PX4	C17-C16-C15	2.16	103.44	114.42	8	1
4	A	387	PX4	C19-C18-C17	2.16	103.44	114.42	12	1
4	A	395	PX4	O3-C1-C2	2.16	120.54	109.16	14	2
4	A	376	PX4	C14-C13-C12	2.16	103.45	114.42	5	1
4	A	397	PX4	C29-C28-C27	2.16	103.45	114.42	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	387	PX4	C5-N1-C2	2.16	118.76	109.92	14	2
4	A	391	PX4	O7-C7-C8	2.16	116.23	108.40	2	1
4	A	399	PX4	C25-C24-C23	2.16	105.76	113.62	2	2
4	A	401	PX4	O6-C9-C10	2.16	115.30	123.73	4	2
4	A	414	PX4	C34-C33-C32	2.16	125.40	114.42	5	1
4	A	308	PX4	C27-C26-C25	2.16	103.46	114.42	1	1
4	A	408	PX4	C13-C12-C11	2.16	103.46	114.42	1	3
4	A	423	PX4	C13-C12-C11	2.16	103.46	114.42	9	1
4	A	340	PX4	O4-P1-O2	2.16	100.63	109.07	11	2
4	A	321	PX4	C32-C31-C30	2.16	103.47	114.42	10	1
4	A	338	PX4	C28-C27-C26	2.16	103.47	114.42	6	1
4	A	349	PX4	C8-O5-C9	2.16	109.13	117.12	3	2
4	A	350	PX4	C25-C24-C23	2.16	105.77	113.62	6	1
4	A	398	PX4	C33-C32-C31	2.16	103.47	114.42	11	1
4	A	408	PX4	C31-C30-C29	2.16	103.47	114.42	8	1
4	A	417	PX4	C33-C32-C31	2.16	103.47	114.42	5	1
4	A	419	PX4	C28-C27-C26	2.16	103.47	114.42	10	2
4	A	385	PX4	C13-C12-C11	2.16	103.48	114.42	9	1
4	A	393	PX4	C33-C32-C31	2.16	103.48	114.42	7	1
4	A	418	PX4	C5-N1-C4	2.16	114.52	108.97	14	2
4	A	338	PX4	C17-C16-C15	2.15	103.49	114.42	13	1
4	A	355	PX4	C16-C15-C14	2.15	103.49	114.42	13	2
4	A	380	PX4	C3-N1-C2	2.15	101.10	109.92	6	1
4	A	381	PX4	C30-C29-C28	2.15	103.49	114.42	1	2
4	A	405	PX4	C5-N1-C2	2.15	118.73	109.92	4	1
4	A	319	PX4	C17-C16-C15	2.15	103.50	114.42	12	1
4	A	355	PX4	O1-P1-O3	2.15	97.75	107.75	2	2
4	A	365	PX4	O6-C9-C10	2.15	115.34	123.73	6	2
4	A	392	PX4	C13-C12-C11	2.15	103.50	114.42	1	3
4	A	362	PX4	C33-C32-C31	2.15	103.51	114.42	2	1
4	A	376	PX4	C13-C12-C11	2.15	103.51	114.42	7	1
4	A	309	PX4	C3-N1-C2	2.15	118.71	109.92	12	1
4	A	324	PX4	C17-C16-C15	2.15	103.51	114.42	14	1
4	A	325	PX4	O5-C9-C10	2.15	118.65	111.91	11	3
4	A	395	PX4	C8-O5-C9	2.15	109.16	117.12	12	1
4	A	308	PX4	C29-C28-C27	2.15	103.52	114.42	2	1
4	A	334	PX4	O8-C23-C24	2.15	132.12	123.73	11	1
4	A	330	PX4	O8-C23-C24	2.15	115.35	123.73	11	1
4	A	348	PX4	C18-C17-C16	2.15	103.52	114.42	4	1
4	A	382	PX4	C16-C15-C14	2.15	103.52	114.42	13	1
4	A	358	PX4	O5-C9-O6	2.15	118.17	123.59	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	362	PX4	O5-C9-O6	2.15	118.17	123.59	8	2
4	A	319	PX4	C11-C10-C9	2.15	105.82	113.62	1	1
4	A	330	PX4	O3-C1-C2	2.14	120.44	109.16	10	1
4	A	338	PX4	C5-N1-C3	2.15	103.46	108.97	9	1
4	A	342	PX4	C30-C29-C28	2.15	103.53	114.42	11	1
4	A	344	PX4	C29-C28-C27	2.15	103.53	114.42	11	1
4	A	392	PX4	O8-C23-C24	2.15	115.35	123.73	5	1
4	A	394	PX4	C5-N1-C2	2.15	118.70	109.92	7	1
4	A	395	PX4	C28-C27-C26	2.15	103.53	114.42	4	1
4	A	426	PX4	C27-C26-C25	2.15	103.52	114.42	4	1
4	A	353	PX4	O3-C1-C2	2.14	120.44	109.16	6	2
4	A	371	PX4	C20-C19-C18	2.14	103.54	114.42	4	1
4	A	374	PX4	C3-N1-C2	2.14	118.69	109.92	10	1
4	A	403	PX4	C17-C16-C15	2.14	103.54	114.42	11	1
4	A	326	PX4	C28-C27-C26	2.14	103.54	114.42	1	1
4	A	412	PX4	C32-C31-C30	2.14	103.54	114.42	3	1
4	A	419	PX4	O1-P1-O4	2.14	117.70	107.75	2	1
4	A	314	PX4	O8-C23-C24	2.14	115.37	123.73	13	1
4	A	334	PX4	C4-N1-C2	2.14	101.15	109.92	14	1
4	A	352	PX4	C20-C19-C18	2.14	103.55	114.42	13	1
4	A	383	PX4	C3-N1-C2	2.14	101.15	109.92	10	1
4	A	404	PX4	C3-N1-C2	2.14	118.68	109.92	1	1
4	A	406	PX4	C31-C30-C29	2.14	103.55	114.42	1	1
4	A	338	PX4	O4-P1-O2	2.14	100.70	109.07	10	1
4	A	394	PX4	C29-C28-C27	2.14	103.56	114.42	3	1
4	A	397	PX4	C8-O5-C9	2.14	109.19	117.12	9	1
4	A	404	PX4	O6-C9-C10	2.14	115.38	123.73	7	1
4	A	343	PX4	C31-C30-C29	2.14	103.56	114.42	12	1
4	A	419	PX4	C33-C32-C31	2.14	103.56	114.42	8	1
4	A	328	PX4	C32-C31-C30	2.14	103.57	114.42	8	1
4	A	344	PX4	C4-N1-C2	2.14	118.67	109.92	9	1
4	A	346	PX4	C17-C16-C15	2.14	103.57	114.42	13	1
4	A	350	PX4	C27-C26-C25	2.14	103.57	114.42	8	1
4	A	353	PX4	C18-C17-C16	2.14	103.57	114.42	2	1
4	A	361	PX4	O8-C23-C24	2.14	115.39	123.73	8	1
4	A	374	PX4	O5-C9-C10	2.14	118.62	111.91	3	2
4	A	400	PX4	C4-N1-C2	2.14	118.67	109.92	7	3
4	A	408	PX4	O3-C1-C2	2.14	120.40	109.16	9	1
4	A	424	PX4	C8-O5-C9	2.14	109.20	117.12	6	1
4	A	319	PX4	O6-C9-C10	2.14	115.39	123.73	5	1
4	A	320	PX4	O6-C9-C10	2.14	115.39	123.73	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	334	PX4	C16-C15-C14	2.14	103.57	114.42	1	3
4	A	363	PX4	O1-P1-O4	2.14	117.67	107.75	3	1
4	A	324	PX4	C4-N1-C3	2.14	103.48	108.97	9	2
4	A	357	PX4	C34-C33-C32	2.14	103.58	114.42	4	1
4	A	323	PX4	O5-C9-C10	2.13	118.61	111.91	2	2
4	A	384	PX4	C17-C16-C15	2.13	103.60	114.42	6	1
4	A	391	PX4	C20-C19-C18	2.13	103.59	114.42	1	1
4	A	403	PX4	O6-C9-C10	2.13	115.41	123.73	10	2
4	A	408	PX4	C15-C14-C13	2.13	103.59	114.42	6	1
4	A	423	PX4	C32-C31-C30	2.13	103.59	114.42	2	1
4	A	350	PX4	C5-N1-C4	2.13	103.49	108.97	10	3
4	A	308	PX4	O3-C1-C2	2.13	120.37	109.16	5	1
4	A	317	PX4	C5-N1-C2	2.13	101.19	109.92	2	1
4	A	360	PX4	C19-C18-C17	2.13	103.60	114.42	1	1
4	A	424	PX4	C18-C17-C16	2.13	103.60	114.42	11	1
4	A	400	PX4	O3-P1-O2	2.13	117.39	109.07	10	1
4	A	323	PX4	C25-C24-C23	2.13	105.88	113.62	9	1
4	A	337	PX4	C3-N1-C2	2.13	101.20	109.92	11	1
4	A	370	PX4	C11-C10-C9	2.13	121.36	113.62	9	1
4	A	382	PX4	C3-N1-C2	2.13	118.63	109.92	1	1
4	A	382	PX4	C20-C19-C18	2.13	103.61	114.42	4	1
4	A	391	PX4	C16-C15-C14	2.13	103.61	114.42	11	1
4	A	408	PX4	C33-C32-C31	2.13	103.61	114.42	14	2
4	A	373	PX4	C32-C31-C30	2.13	103.62	114.42	5	1
4	A	376	PX4	C29-C28-C27	2.13	103.62	114.42	13	1
4	A	421	PX4	C13-C12-C11	2.13	103.61	114.42	9	1
4	A	342	PX4	C34-C33-C32	2.13	103.62	114.42	5	1
4	A	356	PX4	O1-P1-O3	2.13	117.63	107.75	11	2
4	A	398	PX4	O8-C23-C24	2.13	115.43	123.73	12	1
4	A	327	PX4	C16-C15-C14	2.13	103.63	114.42	12	1
4	A	341	PX4	O8-C23-C24	2.13	115.43	123.73	7	1
4	A	369	PX4	C33-C32-C31	2.13	103.62	114.42	10	1
4	A	374	PX4	C13-C12-C11	2.13	103.63	114.42	7	2
4	A	324	PX4	C25-C24-C23	2.13	105.89	113.62	12	1
4	A	344	PX4	O1-P1-O3	2.13	97.87	107.75	6	1
4	A	344	PX4	C19-C18-C17	2.13	103.63	114.42	8	1
4	A	353	PX4	C20-C19-C18	2.13	103.64	114.42	10	2
4	A	359	PX4	O3-C1-C2	2.13	120.34	109.16	3	1
4	A	363	PX4	O3-C1-C2	2.13	120.34	109.16	2	1
4	A	398	PX4	C27-C26-C25	2.13	103.63	114.42	5	1
4	A	402	PX4	C5-N1-C2	2.13	118.61	109.92	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PX4	O1-P1-O4	2.13	117.62	107.75	1	1
4	A	422	PX4	C11-C10-C9	2.13	105.89	113.62	11	1
4	A	306	PX4	O3-C1-C2	2.12	120.33	109.16	2	1
4	A	350	PX4	C18-C17-C16	2.12	103.64	114.42	3	1
4	A	362	PX4	C19-C18-C17	2.12	103.64	114.42	7	1
4	A	394	PX4	C13-C12-C11	2.12	103.64	114.42	7	1
4	A	320	PX4	C28-C27-C26	2.12	103.65	114.42	11	1
4	A	350	PX4	C12-C11-C10	2.12	105.56	113.19	13	1
4	A	354	PX4	C34-C33-C32	2.12	103.65	114.42	1	1
4	A	406	PX4	C18-C17-C16	2.12	103.65	114.42	3	1
4	A	410	PX4	C27-C26-C25	2.12	103.65	114.42	6	1
4	A	411	PX4	C26-C25-C24	2.12	120.82	113.19	7	2
4	A	371	PX4	O3-C1-C2	2.12	120.32	109.16	2	1
4	A	412	PX4	C29-C28-C27	2.12	103.66	114.42	14	1
4	A	379	PX4	C5-N1-C2	2.12	101.25	109.92	3	1
4	A	381	PX4	O5-C9-C10	2.12	118.56	111.91	10	1
4	A	397	PX4	C33-C32-C31	2.12	103.67	114.42	14	2
4	A	418	PX4	O1-P1-O4	2.12	117.59	107.75	1	1
4	A	362	PX4	C12-C11-C10	2.12	105.57	113.19	1	1
4	A	365	PX4	O5-C9-O6	2.12	118.24	123.59	3	1
4	A	386	PX4	C19-C18-C17	2.12	103.67	114.42	12	1
4	A	371	PX4	C18-C17-C16	2.12	103.68	114.42	2	1
4	A	422	PX4	C34-C33-C32	2.12	103.67	114.42	9	1
4	A	348	PX4	O4-P1-O2	2.12	100.80	109.07	13	1
4	A	390	PX4	O4-P1-O2	2.12	117.33	109.07	9	1
4	A	414	PX4	C29-C28-C27	2.12	103.69	114.42	4	1
4	A	415	PX4	C27-C26-C25	2.12	103.68	114.42	13	1
4	A	424	PX4	C13-C12-C11	2.12	103.68	114.42	11	2
4	A	336	PX4	O7-C7-C6	2.11	116.05	108.40	1	2
4	A	354	PX4	C4-N1-C2	2.11	118.57	109.92	10	1
4	A	357	PX4	C27-C26-C25	2.11	103.69	114.42	5	1
4	A	361	PX4	C16-C15-C14	2.11	103.70	114.42	6	1
4	A	366	PX4	O6-C9-C10	2.11	115.48	123.73	10	1
4	A	378	PX4	C28-C27-C26	2.11	103.69	114.42	8	1
4	A	387	PX4	O8-C23-C24	2.11	115.48	123.73	3	1
4	A	378	PX4	O6-C9-C10	2.11	115.49	123.73	1	2
4	A	306	PX4	C28-C27-C26	2.11	103.71	114.42	4	2
4	A	353	PX4	C11-C10-C9	2.11	105.94	113.62	2	2
4	A	371	PX4	C13-C12-C11	2.11	103.71	114.42	13	1
4	A	372	PX4	C32-C31-C30	2.11	103.70	114.42	13	1
4	A	426	PX4	C5-N1-C2	2.11	118.56	109.92	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	429	PX4	C11-C10-C9	2.11	105.94	113.62	9	1
4	A	427	PX4	C3-N1-C2	2.11	118.55	109.92	2	1
4	A	317	PX4	C19-C18-C17	2.11	103.72	114.42	5	1
4	A	330	PX4	O3-P1-O2	2.11	100.83	109.07	3	1
4	A	381	PX4	C28-C27-C26	2.11	103.71	114.42	1	1
4	A	330	PX4	C18-C17-C16	2.11	103.72	114.42	12	1
4	A	373	PX4	C31-C30-C29	2.11	103.72	114.42	1	1
4	A	384	PX4	C3-N1-C2	2.11	118.55	109.92	2	1
4	A	331	PX4	C12-C11-C10	2.11	105.61	113.19	8	2
4	A	389	PX4	C34-C33-C32	2.11	103.72	114.42	6	1
4	A	391	PX4	O1-P1-O4	2.11	117.54	107.75	8	2
4	A	341	PX4	C19-C18-C17	2.11	103.72	114.42	5	1
4	A	426	PX4	O3-C1-C2	2.11	120.25	109.16	2	1
4	A	429	PX4	C29-C28-C27	2.11	103.72	114.42	2	1
4	A	360	PX4	C34-C33-C32	2.11	103.73	114.42	3	1
4	A	316	PX4	C8-O5-C9	2.11	109.33	117.12	6	1
4	A	331	PX4	O4-P1-O2	2.11	117.29	109.07	4	1
4	A	320	PX4	C1-C2-N1	2.10	122.81	115.78	6	1
4	A	365	PX4	C5-N1-C4	2.10	103.56	108.97	3	2
4	A	370	PX4	O8-C23-C24	2.11	115.52	123.73	5	1
4	A	401	PX4	C32-C31-C30	2.11	103.74	114.42	12	2
4	A	426	PX4	C3-N1-C2	2.11	118.53	109.92	9	1
4	A	323	PX4	C17-C16-C15	2.10	103.75	114.42	8	1
4	A	339	PX4	C15-C14-C13	2.10	103.75	114.42	6	1
4	A	350	PX4	C8-O5-C9	2.10	109.33	117.12	12	1
4	A	375	PX4	C31-C30-C29	2.10	103.75	114.42	1	1
4	A	388	PX4	C18-C17-C16	2.10	103.75	114.42	3	1
4	A	362	PX4	C31-C30-C29	2.10	103.75	114.42	11	2
4	A	379	PX4	C33-C32-C31	2.10	103.76	114.42	2	1
4	A	346	PX4	C22-C21-C20	2.10	97.48	113.42	14	1
4	A	360	PX4	O1-P1-O4	2.10	117.50	107.75	6	1
4	A	381	PX4	C31-C30-C29	2.10	103.76	114.42	14	2
4	A	381	PX4	C15-C14-C13	2.10	103.76	114.42	11	1
4	A	405	PX4	O1-P1-O4	2.10	117.50	107.75	14	2
4	A	342	PX4	C20-C19-C18	2.10	103.77	114.42	13	1
4	A	320	PX4	C20-C19-C18	2.10	103.78	114.42	9	1
4	A	354	PX4	C33-C32-C31	2.10	103.78	114.42	14	1
4	A	357	PX4	C13-C12-C11	2.10	103.78	114.42	1	1
4	A	405	PX4	C26-C25-C24	2.10	105.65	113.19	4	2
4	A	419	PX4	C14-C13-C12	2.10	103.78	114.42	11	2
4	A	310	PX4	C14-C13-C12	2.10	103.79	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	331	PX4	C30-C29-C28	2.10	103.78	114.42	13	1
4	A	341	PX4	C33-C32-C31	2.10	103.79	114.42	4	1
4	A	410	PX4	O1-P1-O3	2.10	117.48	107.75	14	1
4	A	323	PX4	C15-C14-C13	2.09	103.80	114.42	4	1
4	A	323	PX4	C19-C18-C17	2.09	103.80	114.42	6	2
4	A	375	PX4	C32-C31-C30	2.09	103.79	114.42	3	1
4	A	393	PX4	O5-C9-C10	2.09	118.48	111.91	14	1
4	A	397	PX4	C19-C18-C17	2.09	103.79	114.42	11	1
4	A	311	PX4	C22-C21-C20	2.09	97.54	113.42	5	1
4	A	343	PX4	O3-P1-O2	2.09	100.89	109.07	12	1
4	A	371	PX4	C5-N1-C2	2.09	118.48	109.92	9	1
4	A	314	PX4	C14-C13-C12	2.09	103.81	114.42	9	1
4	A	318	PX4	C11-C10-C9	2.09	106.01	113.62	8	1
4	A	422	PX4	C17-C16-C15	2.09	103.80	114.42	11	1
4	A	319	PX4	O1-P1-O4	2.09	117.46	107.75	8	1
4	A	321	PX4	C20-C19-C18	2.09	103.81	114.42	2	1
4	A	324	PX4	C26-C25-C24	2.09	120.70	113.19	1	1
4	A	311	PX4	C33-C32-C31	2.09	103.82	114.42	13	1
4	A	411	PX4	C3-N1-C2	2.09	118.47	109.92	1	1
4	A	417	PX4	C30-C29-C28	2.09	103.81	114.42	7	1
4	A	426	PX4	C33-C32-C31	2.09	103.81	114.42	14	1
4	A	328	PX4	C13-C12-C11	2.09	103.82	114.42	3	1
4	A	361	PX4	C20-C19-C18	2.09	103.83	114.42	7	2
4	A	364	PX4	C30-C29-C28	2.09	103.82	114.42	6	1
4	A	370	PX4	C16-C15-C14	2.09	103.82	114.42	12	1
4	A	405	PX4	C18-C17-C16	2.09	103.82	114.42	5	1
4	A	416	PX4	C29-C28-C27	2.09	103.83	114.42	2	2
4	A	425	PX4	C33-C32-C31	2.09	103.83	114.42	9	1
4	A	413	PX4	C19-C18-C17	2.09	103.83	114.42	13	2
4	A	337	PX4	C16-C15-C14	2.09	103.84	114.42	1	1
4	A	352	PX4	C18-C17-C16	2.09	103.84	114.42	2	1
4	A	401	PX4	O1-P1-O3	2.09	98.06	107.75	10	1
4	A	425	PX4	C20-C19-C18	2.09	103.83	114.42	14	1
4	A	322	PX4	O3-C1-C2	2.08	120.11	109.16	1	1
4	A	356	PX4	C17-C16-C15	2.08	103.84	114.42	6	1
4	A	407	PX4	C14-C13-C12	2.08	103.85	114.42	14	1
4	A	412	PX4	C19-C18-C17	2.08	103.84	114.42	1	1
4	A	358	PX4	O7-C23-O8	2.08	118.67	123.70	9	1
4	A	317	PX4	O3-C1-C2	2.08	120.11	109.16	10	1
4	A	327	PX4	C13-C12-C11	2.08	103.86	114.42	5	2
4	A	333	PX4	C15-C14-C13	2.08	103.85	114.42	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	377	PX4	C20-C19-C18	2.08	103.85	114.42	13	1
4	A	399	PX4	O3-C1-C2	2.08	120.11	109.16	2	1
4	A	413	PX4	C15-C14-C13	2.08	103.85	114.42	13	1
4	A	348	PX4	O1-P1-O3	2.08	98.08	107.75	5	1
4	A	314	PX4	C3-N1-C2	2.08	101.41	109.92	5	1
4	A	317	PX4	C13-C12-C11	2.08	103.87	114.42	10	2
4	A	322	PX4	C31-C30-C29	2.08	103.86	114.42	13	2
4	A	351	PX4	C8-O5-C9	2.08	109.42	117.12	13	1
4	A	378	PX4	C25-C24-C23	2.08	106.06	113.62	4	1
4	A	307	PX4	O1-P1-O3	2.08	98.10	107.75	2	1
4	A	367	PX4	O4-P1-O2	2.08	117.19	109.07	6	2
4	A	372	PX4	C3-N1-C2	2.08	118.42	109.92	3	1
4	A	410	PX4	C36-C35-C34	2.08	97.64	113.42	4	1
4	A	372	PX4	O6-C9-C10	2.08	115.62	123.73	8	2
4	A	381	PX4	O1-P1-O4	2.08	117.40	107.75	6	1
4	A	412	PX4	O8-C23-C24	2.08	115.62	123.73	4	1
4	A	317	PX4	C18-C17-C16	2.08	103.88	114.42	10	1
4	A	336	PX4	C14-C13-C12	2.08	103.88	114.42	5	2
4	A	347	PX4	O6-C9-C10	2.08	115.63	123.73	14	1
4	A	383	PX4	C27-C26-C25	2.08	103.89	114.42	2	1
4	A	412	PX4	C36-C35-C34	2.08	97.67	113.42	5	1
4	A	414	PX4	C27-C26-C25	2.08	103.89	114.42	9	1
4	A	327	PX4	C34-C33-C32	2.07	103.89	114.42	5	1
4	A	369	PX4	C15-C14-C13	2.07	103.89	114.42	3	1
4	A	429	PX4	C20-C19-C18	2.08	103.89	114.42	1	1
4	A	325	PX4	C29-C28-C27	2.07	103.90	114.42	3	1
4	A	369	PX4	C14-C13-C12	2.07	103.90	114.42	14	1
4	A	371	PX4	C11-C10-C9	2.07	106.09	113.62	10	1
4	A	412	PX4	C15-C14-C13	2.07	103.90	114.42	10	1
4	A	307	PX4	C29-C28-C27	2.07	103.91	114.42	7	1
4	A	315	PX4	C4-N1-C2	2.07	101.44	109.92	9	1
4	A	323	PX4	C29-C28-C27	2.07	103.91	114.42	10	1
4	A	390	PX4	C33-C32-C31	2.07	103.91	114.42	4	1
4	A	306	PX4	O1-P1-O3	2.07	117.36	107.75	12	1
4	A	329	PX4	C15-C14-C13	2.07	103.92	114.42	6	1
4	A	342	PX4	C13-C12-C11	2.07	103.92	114.42	8	1
4	A	330	PX4	C5-N1-C4	2.07	114.29	108.97	6	1
4	A	341	PX4	C26-C25-C24	2.07	105.75	113.19	14	1
4	A	359	PX4	O8-C23-C24	2.07	115.66	123.73	1	2
4	A	364	PX4	C3-N1-C2	2.07	101.45	109.92	5	2
4	A	366	PX4	C27-C26-C25	2.07	103.92	114.42	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PX4	C20-C19-C18	2.07	103.92	114.42	5	1
4	A	412	PX4	C28-C27-C26	2.07	103.92	114.42	14	1
4	A	318	PX4	C33-C32-C31	2.07	103.93	114.42	13	1
4	A	321	PX4	C13-C12-C11	2.07	103.93	114.42	10	2
4	A	377	PX4	C29-C28-C27	2.07	124.92	114.42	5	1
4	A	392	PX4	C34-C33-C32	2.07	103.93	114.42	6	1
4	A	394	PX4	C16-C15-C14	2.07	103.92	114.42	8	1
4	A	410	PX4	C17-C16-C15	2.07	103.92	114.42	8	1
4	A	412	PX4	C31-C30-C29	2.07	103.93	114.42	5	1
4	A	430	PX4	C18-C17-C16	2.07	103.92	114.42	8	1
4	A	339	PX4	C18-C17-C16	2.07	103.93	114.42	5	1
4	A	346	PX4	C31-C30-C29	2.07	103.93	114.42	9	1
4	A	374	PX4	C16-C15-C14	2.07	103.94	114.42	4	1
4	A	380	PX4	C5-N1-C2	2.07	118.37	109.92	6	1
4	A	406	PX4	C3-N1-C2	2.07	118.37	109.92	12	1
4	A	408	PX4	C30-C29-C28	2.07	103.94	114.42	14	1
4	A	410	PX4	C15-C14-C13	2.07	103.94	114.42	3	1
4	A	424	PX4	O3-C1-C2	2.07	120.03	109.16	8	2
4	A	412	PX4	C4-N1-C2	2.07	118.37	109.92	13	1
4	A	429	PX4	C4-N1-C2	2.07	118.37	109.92	6	1
4	A	315	PX4	C18-C17-C16	2.06	103.94	114.42	2	1
4	A	346	PX4	C13-C12-C11	2.06	103.95	114.42	12	1
4	A	351	PX4	C4-N1-C2	2.06	101.47	109.92	5	1
4	A	357	PX4	C14-C13-C12	2.06	103.94	114.42	10	1
4	A	366	PX4	C5-N1-C2	2.06	101.47	109.92	5	1
4	A	426	PX4	C34-C33-C32	2.07	103.94	114.42	5	1
4	A	383	PX4	C5-N1-C2	2.06	118.36	109.92	11	1
4	A	384	PX4	C16-C15-C14	2.06	103.95	114.42	1	3
4	A	394	PX4	C25-C24-C23	2.06	106.12	113.62	3	1
4	A	402	PX4	C18-C17-C16	2.06	103.96	114.42	13	1
4	A	408	PX4	C28-C27-C26	2.06	103.95	114.42	14	1
4	A	414	PX4	C11-C10-C9	2.06	106.12	113.62	2	2
4	A	419	PX4	C20-C19-C18	2.06	103.95	114.42	13	1
4	A	420	PX4	C13-C12-C11	2.06	103.95	114.42	1	1
4	A	422	PX4	C5-N1-C2	2.06	118.36	109.92	5	1
4	A	330	PX4	C15-C14-C13	2.06	103.95	114.42	4	1
4	A	338	PX4	O3-P1-O2	2.06	101.01	109.07	11	1
4	A	339	PX4	C20-C19-C18	2.06	103.96	114.42	1	2
4	A	367	PX4	C14-C13-C12	2.06	103.96	114.42	1	1
4	A	374	PX4	C14-C13-C12	2.06	103.96	114.42	3	1
4	A	382	PX4	O6-C9-C10	2.06	115.69	123.73	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	C15-C14-C13	2.06	103.96	114.42	12	1
4	A	311	PX4	C34-C33-C32	2.06	103.97	114.42	12	1
4	A	346	PX4	O1-P1-O3	2.06	117.31	107.75	6	1
4	A	319	PX4	C33-C32-C31	2.06	103.97	114.42	11	1
4	A	327	PX4	O1-P1-O3	2.06	117.31	107.75	13	1
4	A	331	PX4	C16-C15-C14	2.06	103.97	114.42	10	1
4	A	398	PX4	C8-O5-C9	2.06	109.49	117.12	7	1
4	A	414	PX4	C32-C31-C30	2.06	103.97	114.42	11	1
4	A	347	PX4	C4-N1-C2	2.06	101.49	109.92	14	1
4	A	365	PX4	C27-C26-C25	2.06	103.98	114.42	6	1
4	A	387	PX4	C20-C19-C18	2.06	103.98	114.42	5	1
4	A	330	PX4	C4-N1-C2	2.06	101.50	109.92	6	1
4	A	362	PX4	O1-P1-O4	2.06	117.30	107.75	2	1
4	A	376	PX4	O8-C23-C24	2.06	115.71	123.73	12	1
4	A	322	PX4	C3-N1-C2	2.06	118.33	109.92	13	1
4	A	323	PX4	O1-P1-O3	2.06	98.20	107.75	2	1
4	A	382	PX4	C34-C33-C32	2.05	104.00	114.42	2	1
4	A	383	PX4	C31-C30-C29	2.05	104.00	114.42	12	2
4	A	416	PX4	C28-C27-C26	2.06	103.99	114.42	10	1
4	A	347	PX4	C11-C10-C9	2.05	121.09	113.62	9	1
4	A	356	PX4	O3-C1-C2	2.05	119.96	109.16	7	1
4	A	357	PX4	C18-C17-C16	2.05	104.00	114.42	6	1
4	A	379	PX4	O8-C23-C24	2.05	115.72	123.73	5	1
4	A	425	PX4	C31-C30-C29	2.05	104.00	114.42	7	1
4	A	315	PX4	C5-N1-C3	2.05	103.70	108.97	12	1
4	A	339	PX4	O6-C9-C10	2.05	115.73	123.73	12	1
4	A	349	PX4	C28-C27-C26	2.05	104.01	114.42	14	1
4	A	372	PX4	C26-C25-C24	2.05	105.82	113.19	6	1
4	A	375	PX4	C15-C14-C13	2.05	104.01	114.42	5	1
4	A	409	PX4	C31-C30-C29	2.05	104.01	114.42	14	3
4	A	411	PX4	C4-N1-C2	2.05	118.31	109.92	3	1
4	A	321	PX4	C30-C29-C28	2.05	104.02	114.42	1	1
4	A	327	PX4	O5-C9-C10	2.05	118.34	111.91	6	1
4	A	317	PX4	C27-C26-C25	2.05	104.03	114.42	8	1
4	A	324	PX4	C31-C30-C29	2.05	104.03	114.42	6	2
4	A	329	PX4	C33-C32-C31	2.05	104.02	114.42	4	1
4	A	380	PX4	C15-C14-C13	2.05	104.02	114.42	4	1
4	A	345	PX4	C4-N1-C2	2.05	118.30	109.92	12	2
4	A	361	PX4	C25-C24-C23	2.05	106.17	113.62	4	1
4	A	414	PX4	C13-C12-C11	2.05	104.03	114.42	10	1
4	A	423	PX4	C33-C32-C31	2.05	104.02	114.42	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	426	PX4	C13-C12-C11	2.05	104.03	114.42	1	1
4	A	395	PX4	C11-C10-C9	2.05	106.18	113.62	3	1
4	A	374	PX4	C32-C31-C30	2.05	104.04	114.42	3	1
4	A	375	PX4	C34-C33-C32	2.05	104.04	114.42	1	1
4	A	419	PX4	O6-C9-C10	2.05	115.75	123.73	1	1
4	A	311	PX4	C14-C13-C12	2.04	104.05	114.42	11	1
4	A	320	PX4	C17-C16-C15	2.04	104.05	114.42	1	1
4	A	377	PX4	C27-C26-C25	2.04	104.05	114.42	3	1
4	A	396	PX4	C32-C31-C30	2.04	104.05	114.42	5	1
4	A	398	PX4	C16-C15-C14	2.05	104.04	114.42	7	1
4	A	333	PX4	C18-C17-C16	2.04	104.05	114.42	12	1
4	A	334	PX4	O3-C1-C2	2.04	119.91	109.16	3	1
4	A	404	PX4	C11-C10-C9	2.04	106.19	113.62	10	1
4	A	312	PX4	C32-C31-C30	2.04	104.07	114.42	13	1
4	A	343	PX4	C18-C17-C16	2.04	104.06	114.42	8	1
4	A	391	PX4	C8-O5-C9	2.04	109.56	117.12	1	1
4	A	385	PX4	O1-P1-O3	2.04	98.27	107.75	9	1
4	A	393	PX4	C30-C29-C28	2.04	104.07	114.42	8	1
4	A	401	PX4	C29-C28-C27	2.04	104.07	114.42	14	1
4	A	419	PX4	C13-C12-C11	2.04	104.07	114.42	3	1
4	A	307	PX4	O3-C1-C2	2.04	119.88	109.16	2	1
4	A	312	PX4	C5-N1-C2	2.04	101.58	109.92	13	1
4	A	316	PX4	C4-N1-C2	2.04	101.58	109.92	11	1
4	A	346	PX4	C14-C13-C12	2.04	104.08	114.42	12	1
4	A	366	PX4	C14-C13-C12	2.04	104.07	114.42	5	1
4	A	372	PX4	C19-C18-C17	2.04	104.08	114.42	8	1
4	A	383	PX4	C25-C24-C23	2.04	121.03	113.62	3	1
4	A	419	PX4	C27-C26-C25	2.04	104.08	114.42	7	1
4	A	309	PX4	C11-C10-C9	2.04	106.22	113.62	13	1
4	A	340	PX4	C32-C31-C30	2.04	104.09	114.42	8	1
4	A	345	PX4	O4-P1-O2	2.04	101.11	109.07	1	1
4	A	405	PX4	O8-C23-C24	2.04	115.78	123.73	10	1
4	A	311	PX4	C32-C31-C30	2.03	104.09	114.42	14	1
4	A	355	PX4	C30-C29-C28	2.04	104.09	114.42	1	1
4	A	388	PX4	C30-C29-C28	2.04	104.09	114.42	12	1
4	A	308	PX4	C3-N1-C2	2.03	118.24	109.92	3	1
4	A	324	PX4	O5-C9-C10	2.03	118.29	111.91	12	1
4	A	352	PX4	C12-C11-C10	2.03	105.88	113.19	14	1
4	A	309	PX4	C5-N1-C2	2.03	118.23	109.92	7	1
4	A	318	PX4	C4-N1-C2	2.03	118.23	109.92	9	1
4	A	355	PX4	C31-C30-C29	2.03	104.10	114.42	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	362	PX4	C36-C35-C34	2.03	128.87	113.42	4	1
4	A	388	PX4	C4-N1-C2	2.03	118.24	109.92	13	1
4	A	424	PX4	C19-C18-C17	2.04	104.09	114.42	4	1
4	A	399	PX4	C16-C15-C14	2.03	104.10	114.42	3	1
4	A	411	PX4	C27-C26-C25	2.03	104.10	114.42	11	1
4	A	418	PX4	C33-C32-C31	2.03	104.10	114.42	10	1
4	A	429	PX4	O7-C7-C8	2.03	115.77	108.40	12	1
4	A	329	PX4	C25-C24-C23	2.03	106.23	113.62	2	1
4	A	336	PX4	C20-C19-C18	2.03	104.11	114.42	5	1
4	A	351	PX4	C17-C16-C15	2.03	104.11	114.42	8	2
4	A	364	PX4	C19-C18-C17	2.03	104.11	114.42	10	1
4	A	423	PX4	C27-C26-C25	2.03	104.10	114.42	13	1
4	A	374	PX4	C17-C16-C15	2.03	104.11	114.42	4	1
4	A	389	PX4	C13-C12-C11	2.03	104.11	114.42	10	1
4	A	430	PX4	O6-C9-C10	2.03	115.81	123.73	9	1
4	A	312	PX4	O1-P1-O4	2.03	117.17	107.75	6	1
4	A	315	PX4	C36-C35-C34	2.03	98.01	113.42	4	1
4	A	328	PX4	C27-C26-C25	2.03	104.12	114.42	2	1
4	A	337	PX4	C30-C29-C28	2.03	104.12	114.42	4	1
4	A	365	PX4	C30-C29-C28	2.03	104.12	114.42	2	1
4	A	368	PX4	C32-C31-C30	2.03	104.12	114.42	12	1
4	A	400	PX4	O8-C23-C24	2.03	115.81	123.73	9	1
4	A	403	PX4	C13-C12-C11	2.03	104.12	114.42	3	1
4	A	405	PX4	C25-C24-C23	2.03	106.24	113.62	4	1
4	A	417	PX4	O3-C1-C2	2.03	119.84	109.16	12	1
4	A	419	PX4	C31-C30-C29	2.03	104.12	114.42	10	2
4	A	395	PX4	C32-C31-C30	2.03	104.12	114.42	8	1
4	A	426	PX4	C35-C34-C33	2.03	96.47	115.30	8	1
4	A	314	PX4	O1-P1-O3	2.03	98.33	107.75	8	1
4	A	323	PX4	C31-C30-C29	2.03	104.14	114.42	14	1
4	A	353	PX4	C27-C26-C25	2.03	104.14	114.42	13	1
4	A	368	PX4	C34-C33-C32	2.03	104.13	114.42	2	1
4	A	401	PX4	O4-P1-O2	2.03	116.99	109.07	13	1
4	A	429	PX4	O1-P1-O4	2.03	117.16	107.75	7	1
4	A	375	PX4	C18-C17-C16	2.03	104.14	114.42	9	1
4	A	333	PX4	C16-C15-C14	2.02	104.15	114.42	8	1
4	A	340	PX4	O6-C9-C10	2.02	115.83	123.73	8	1
4	A	361	PX4	C1-C2-N1	2.03	122.54	115.78	12	1
4	A	404	PX4	O1-P1-O4	2.03	117.15	107.75	11	1
4	A	405	PX4	C4-N1-C2	2.02	118.20	109.92	5	1
4	A	418	PX4	C12-C11-C10	2.02	105.92	113.19	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	423	PX4	C7-O7-C23	2.02	112.81	117.79	13	2
4	A	346	PX4	C8-O5-C9	2.02	109.63	117.12	4	1
4	A	330	PX4	C32-C31-C30	2.02	104.17	114.42	3	1
4	A	353	PX4	O1-P1-O3	2.02	117.14	107.75	10	1
4	A	370	PX4	C8-O5-C9	2.02	109.63	117.12	12	1
4	A	373	PX4	C28-C27-C26	2.02	104.16	114.42	12	1
4	A	376	PX4	O3-C1-C2	2.02	119.79	109.16	2	1
4	A	405	PX4	C28-C27-C26	2.02	104.16	114.42	3	1
4	A	373	PX4	O5-C9-C10	2.02	118.25	111.91	14	1
4	A	374	PX4	C18-C17-C16	2.02	104.17	114.42	7	1
4	A	387	PX4	C3-N1-C2	2.02	101.65	109.92	3	1
4	A	397	PX4	C30-C29-C28	2.02	104.17	114.42	3	1
4	A	401	PX4	O1-P1-O4	2.02	117.12	107.75	12	1
4	A	401	PX4	C30-C29-C28	2.02	104.17	114.42	12	1
4	A	407	PX4	C27-C26-C25	2.02	104.17	114.42	12	1
4	A	414	PX4	C12-C11-C10	2.02	105.93	113.19	2	1
4	A	427	PX4	C14-C13-C12	2.02	104.17	114.42	8	1
4	A	321	PX4	C19-C18-C17	2.02	104.18	114.42	11	1
4	A	338	PX4	C20-C19-C18	2.02	104.18	114.42	3	1
4	A	369	PX4	C26-C25-C24	2.02	105.93	113.19	11	1
4	A	386	PX4	C13-C12-C11	2.02	104.18	114.42	13	1
4	A	363	PX4	C28-C27-C26	2.02	104.19	114.42	13	1
4	A	375	PX4	O1-P1-O4	2.02	117.11	107.75	14	1
4	A	395	PX4	C15-C14-C13	2.02	104.19	114.42	3	1
4	A	335	PX4	C20-C19-C18	2.01	104.20	114.42	4	1
4	A	382	PX4	C29-C28-C27	2.02	124.66	114.42	4	1
4	A	383	PX4	C14-C13-C12	2.02	104.19	114.42	10	1
4	A	312	PX4	C16-C15-C14	2.01	104.21	114.42	8	1
4	A	376	PX4	C7-O7-C23	2.01	122.75	117.79	1	1
4	A	332	PX4	C29-C28-C27	2.01	104.22	114.42	9	1
4	A	389	PX4	C30-C29-C28	2.01	104.21	114.42	5	1
4	A	391	PX4	C5-N1-C4	2.01	114.15	108.97	6	1
4	A	398	PX4	C5-N1-C2	2.01	118.15	109.92	4	1
4	A	318	PX4	C20-C19-C18	2.01	104.22	114.42	2	1
4	A	319	PX4	C14-C13-C12	2.01	104.22	114.42	1	1
4	A	332	PX4	C31-C30-C29	2.01	104.23	114.42	13	1
4	A	346	PX4	C3-N1-C2	2.01	118.14	109.92	3	1
4	A	342	PX4	C8-O5-C9	2.01	109.69	117.12	4	1
4	A	349	PX4	C14-C13-C12	2.01	104.23	114.42	12	1
4	A	371	PX4	C3-N1-C2	2.01	101.70	109.92	7	1
4	A	392	PX4	C16-C15-C14	2.01	104.23	114.42	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C17-C16-C15	2.01	104.23	114.42	8	1
4	A	420	PX4	C3-N1-C2	2.01	118.14	109.92	9	1
4	A	429	PX4	C17-C16-C15	2.01	104.23	114.42	8	1
4	A	430	PX4	O1-P1-O4	2.01	117.08	107.75	9	1
4	A	313	PX4	O1-P1-O4	2.01	117.06	107.75	1	1
4	A	317	PX4	C33-C32-C31	2.01	104.23	114.42	8	1
4	A	331	PX4	C15-C14-C13	2.01	104.24	114.42	5	1
4	A	340	PX4	C18-C17-C16	2.01	104.24	114.42	4	1
4	A	322	PX4	O1-P1-O4	2.00	117.06	107.75	4	1
4	A	418	PX4	C13-C12-C11	2.01	104.24	114.42	1	1
4	A	325	PX4	C12-C11-C10	2.00	105.99	113.19	6	1
4	A	331	PX4	C5-N1-C2	2.00	118.12	109.92	13	1
4	A	333	PX4	C32-C31-C30	2.00	104.25	114.42	8	1
4	A	338	PX4	C3-N1-C2	2.00	101.72	109.92	3	1
4	A	337	PX4	C15-C14-C13	2.00	104.25	114.42	7	1
4	A	341	PX4	C17-C16-C15	2.00	104.25	114.42	14	1
4	A	393	PX4	C34-C33-C32	2.00	104.25	114.42	2	1
4	A	352	PX4	C19-C18-C17	2.00	104.25	114.42	7	1
4	A	413	PX4	C5-N1-C2	2.00	118.12	109.92	1	1
4	A	423	PX4	C29-C28-C27	2.00	104.25	114.42	11	1
4	A	428	PX4	C18-C17-C16	2.00	104.25	114.42	4	1
4	A	312	PX4	C34-C33-C32	2.00	104.27	114.42	12	1
4	A	329	PX4	C28-C27-C26	2.00	104.26	114.42	1	1
4	A	384	PX4	C19-C18-C17	2.00	104.26	114.42	9	1
4	A	415	PX4	C18-C17-C16	2.00	104.26	114.42	10	1
4	A	356	PX4	C3-N1-C2	2.00	118.10	109.92	2	1
4	A	359	PX4	C14-C13-C12	2.00	104.27	114.42	13	1

There are no chirality outliers.

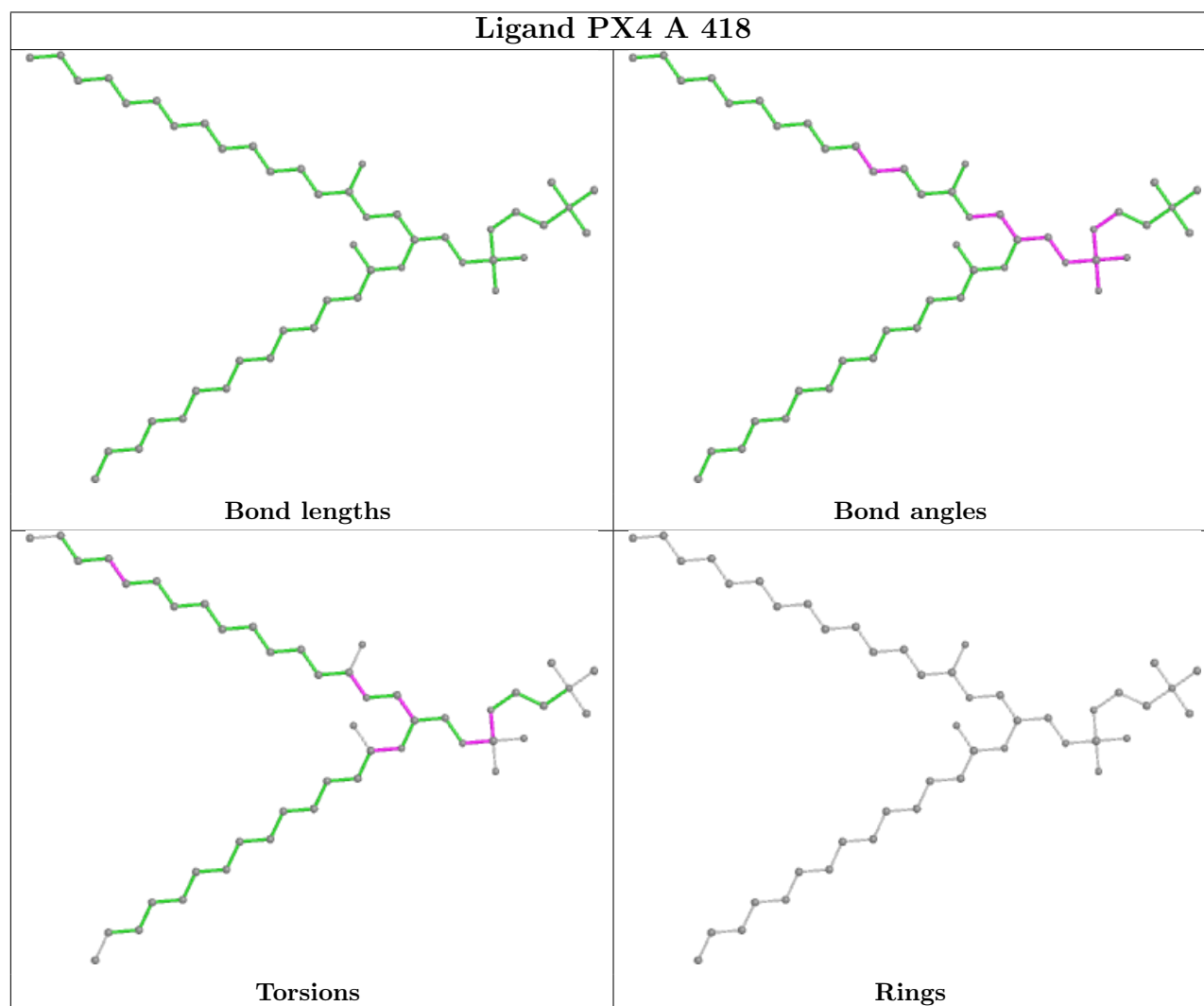
All unique torsion outliers are listed below.

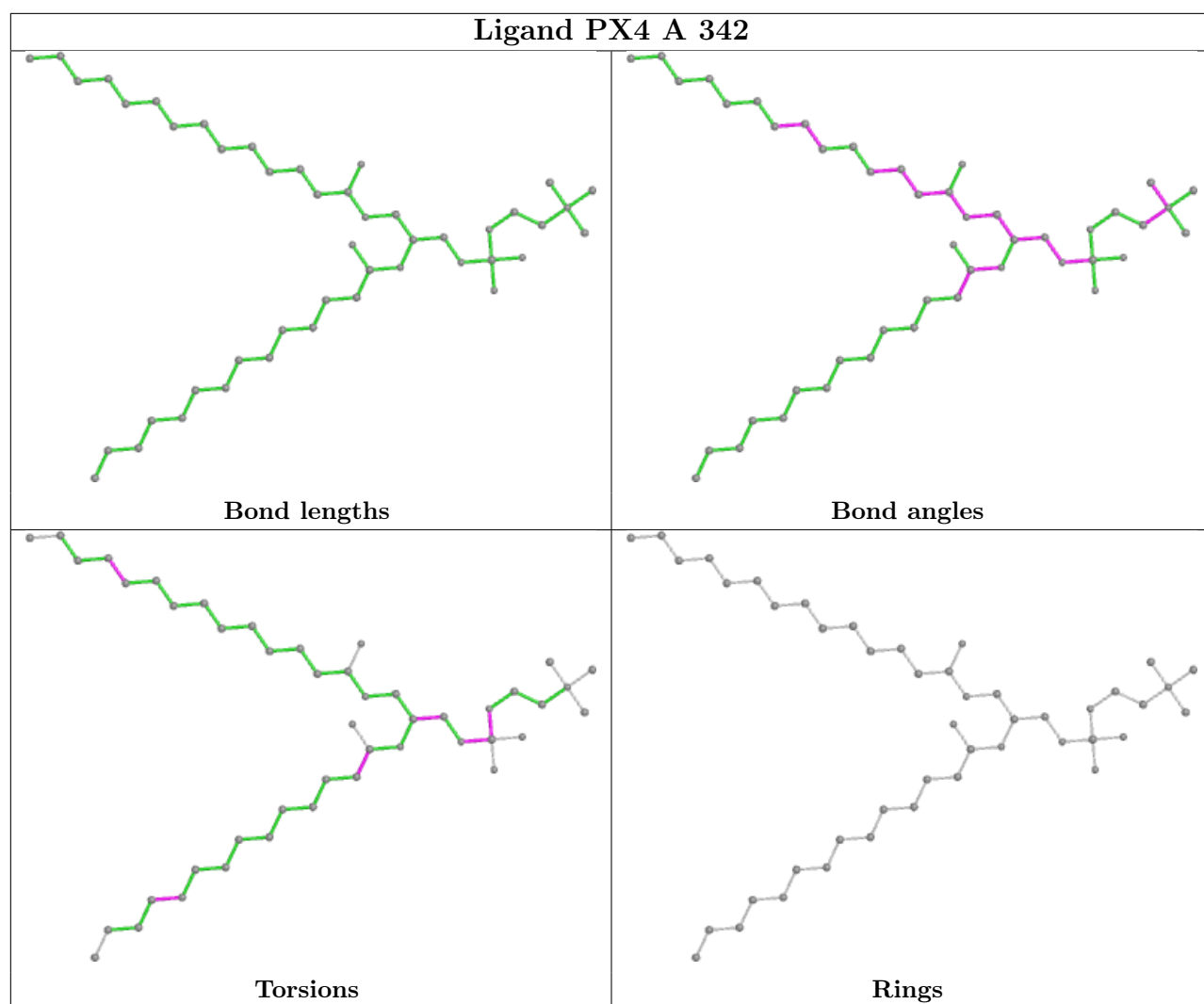
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	335	PX4	O8-C23-O7-C7	2

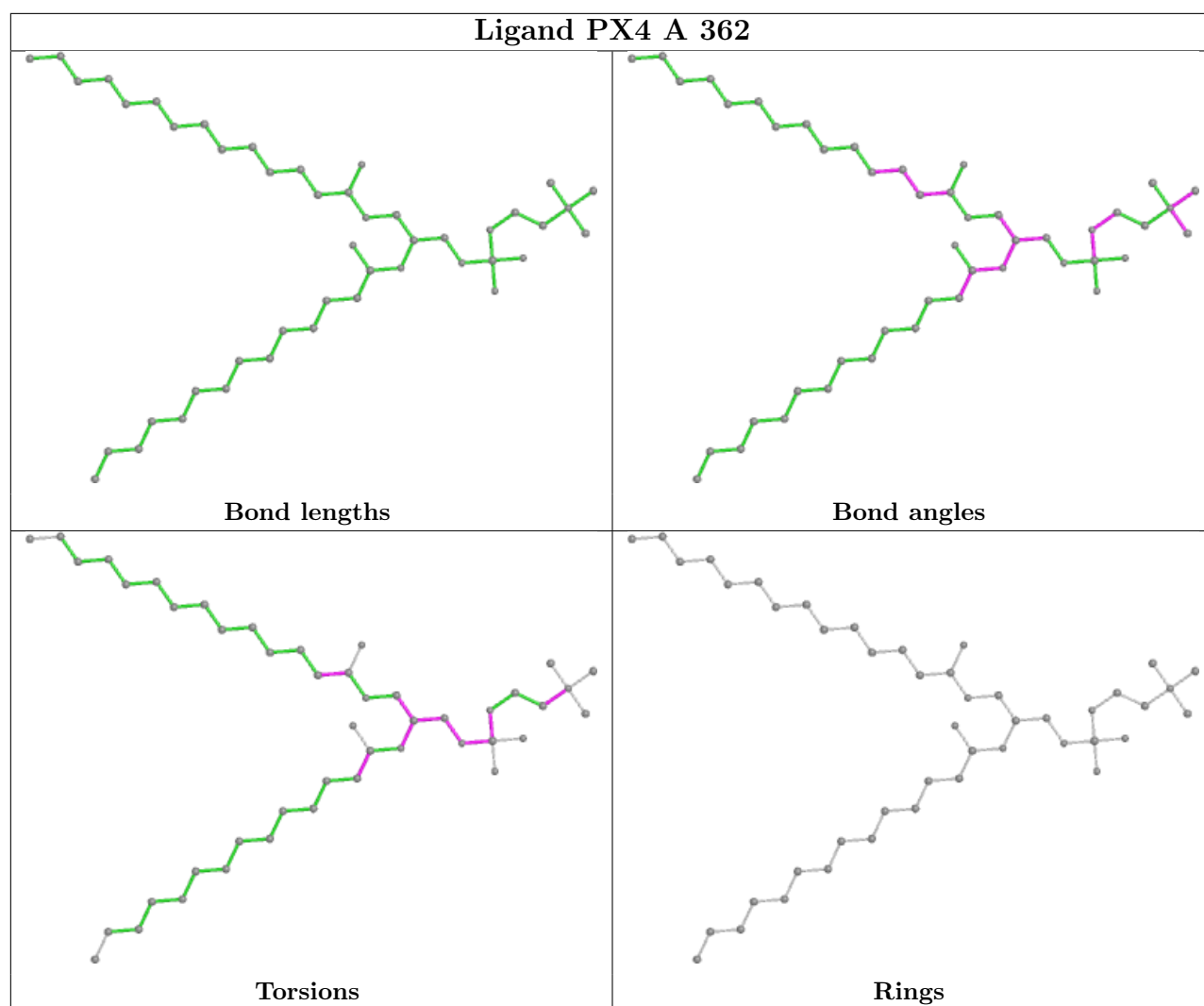
There are no ring outliers.

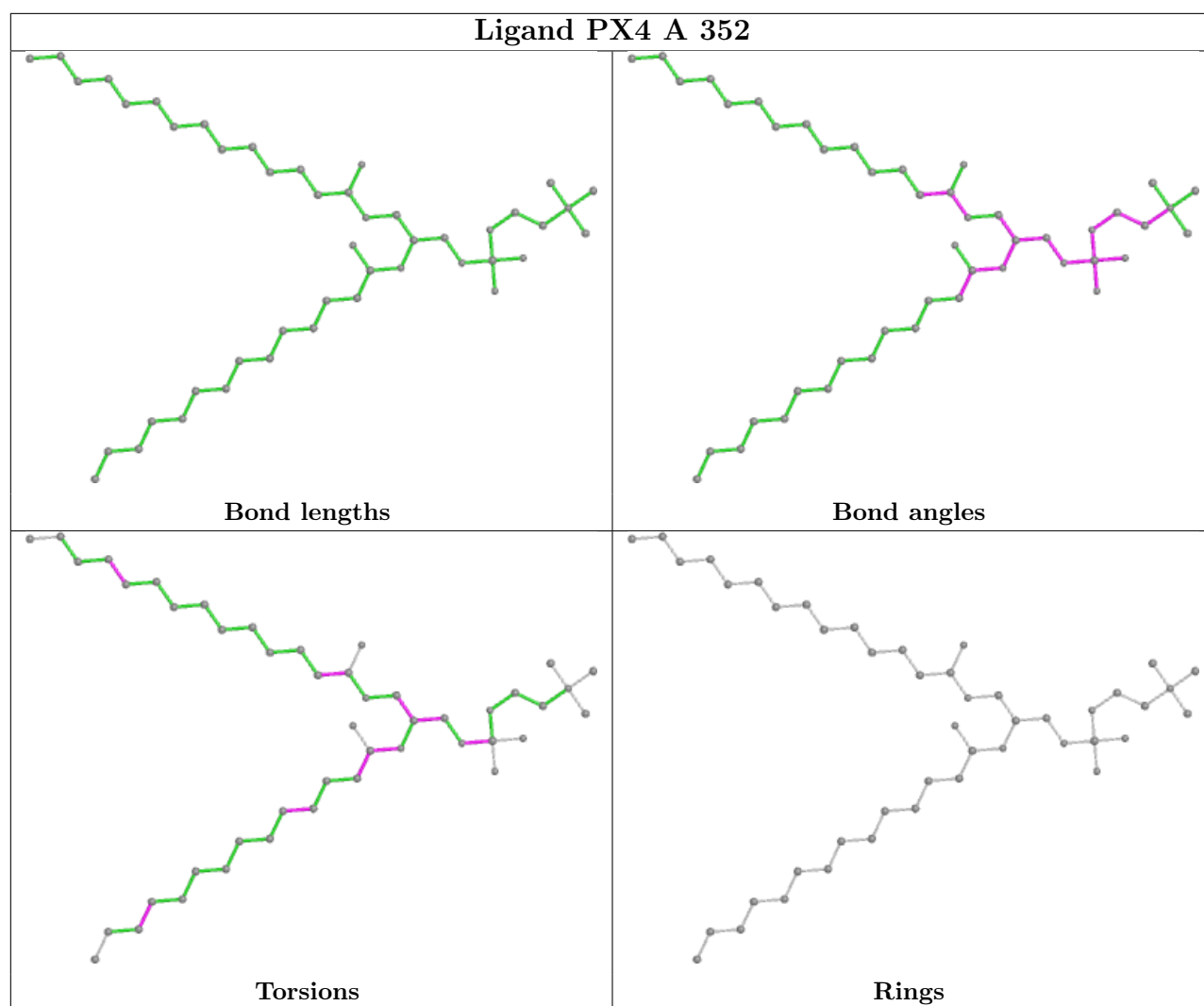
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

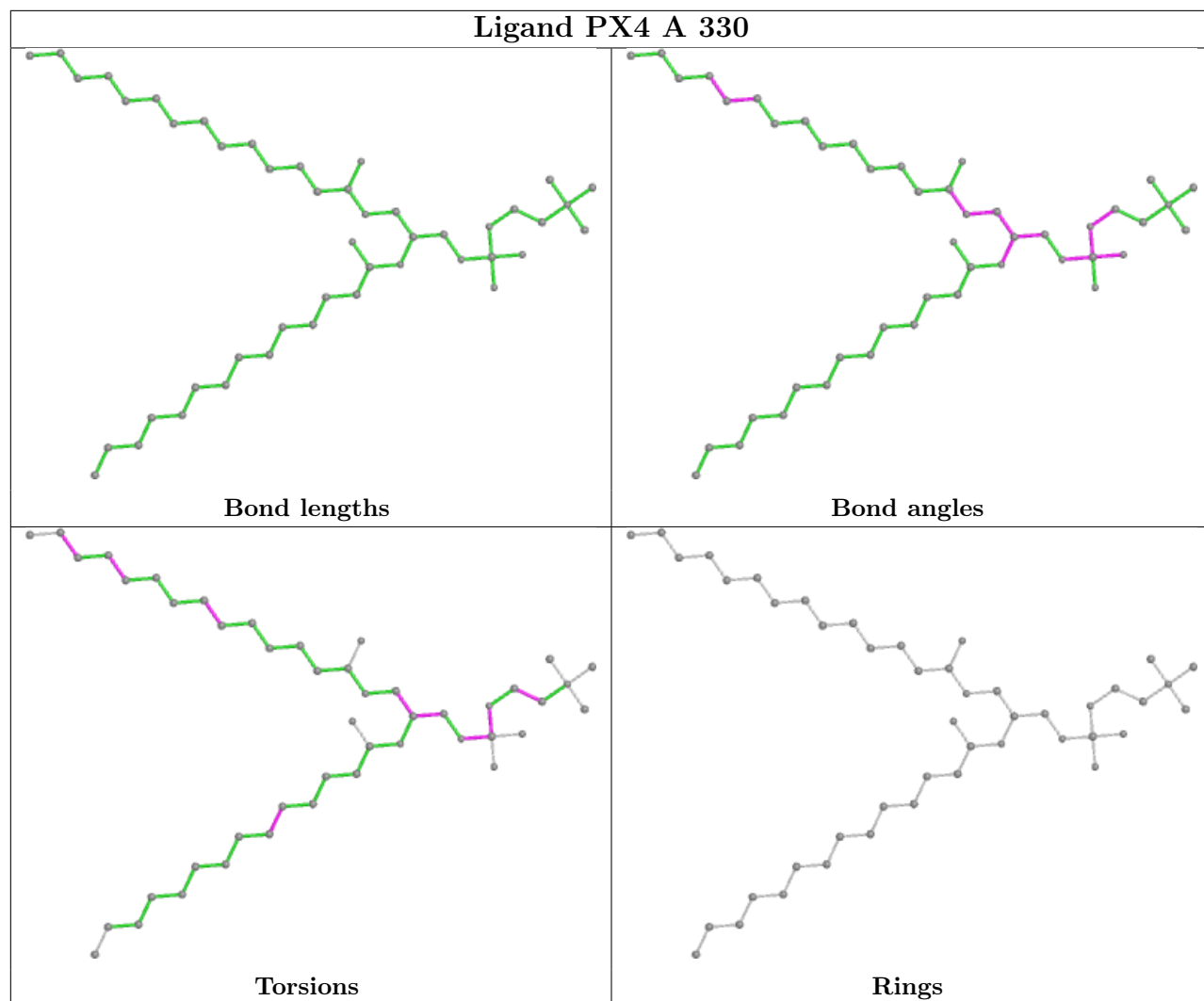
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

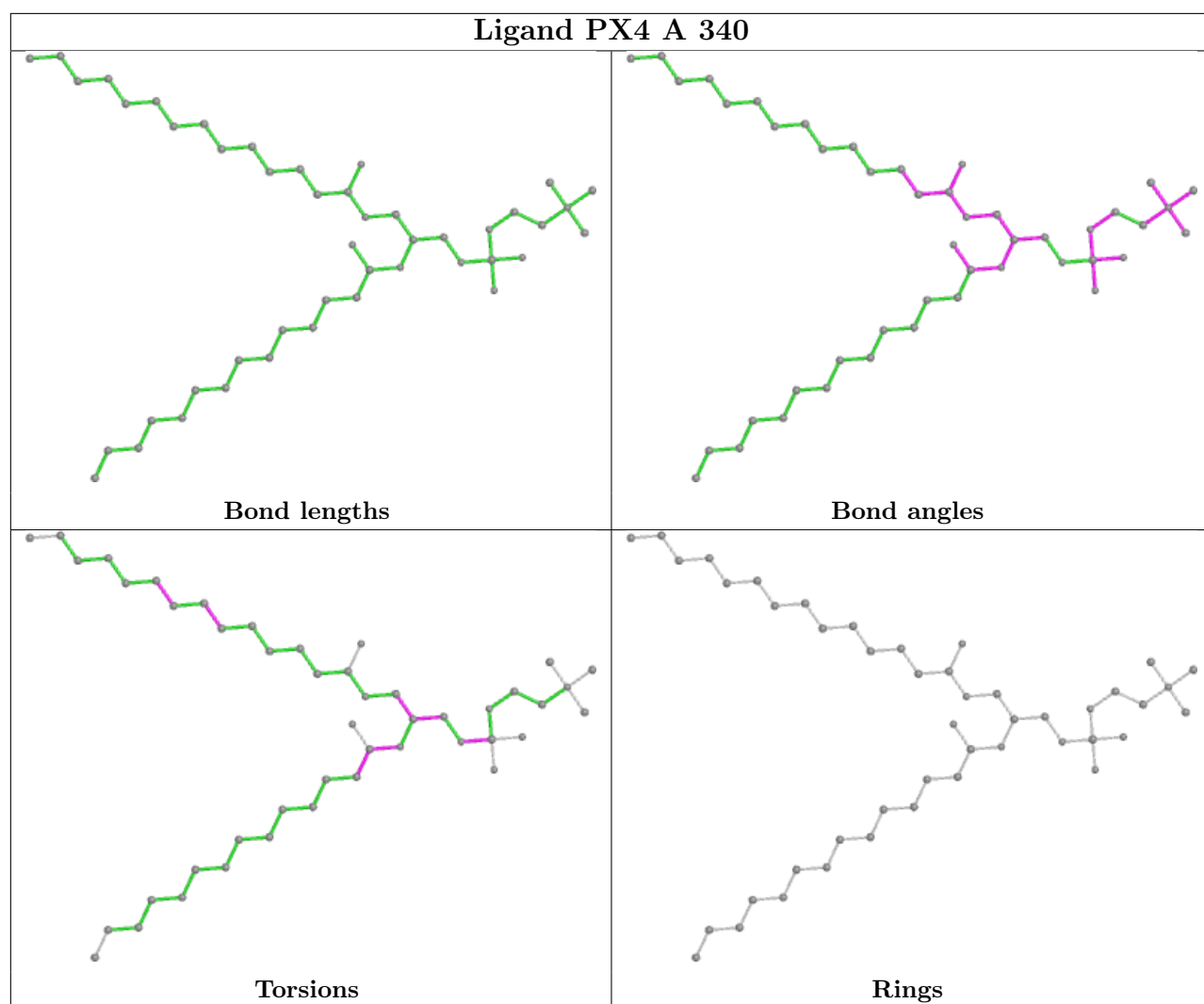


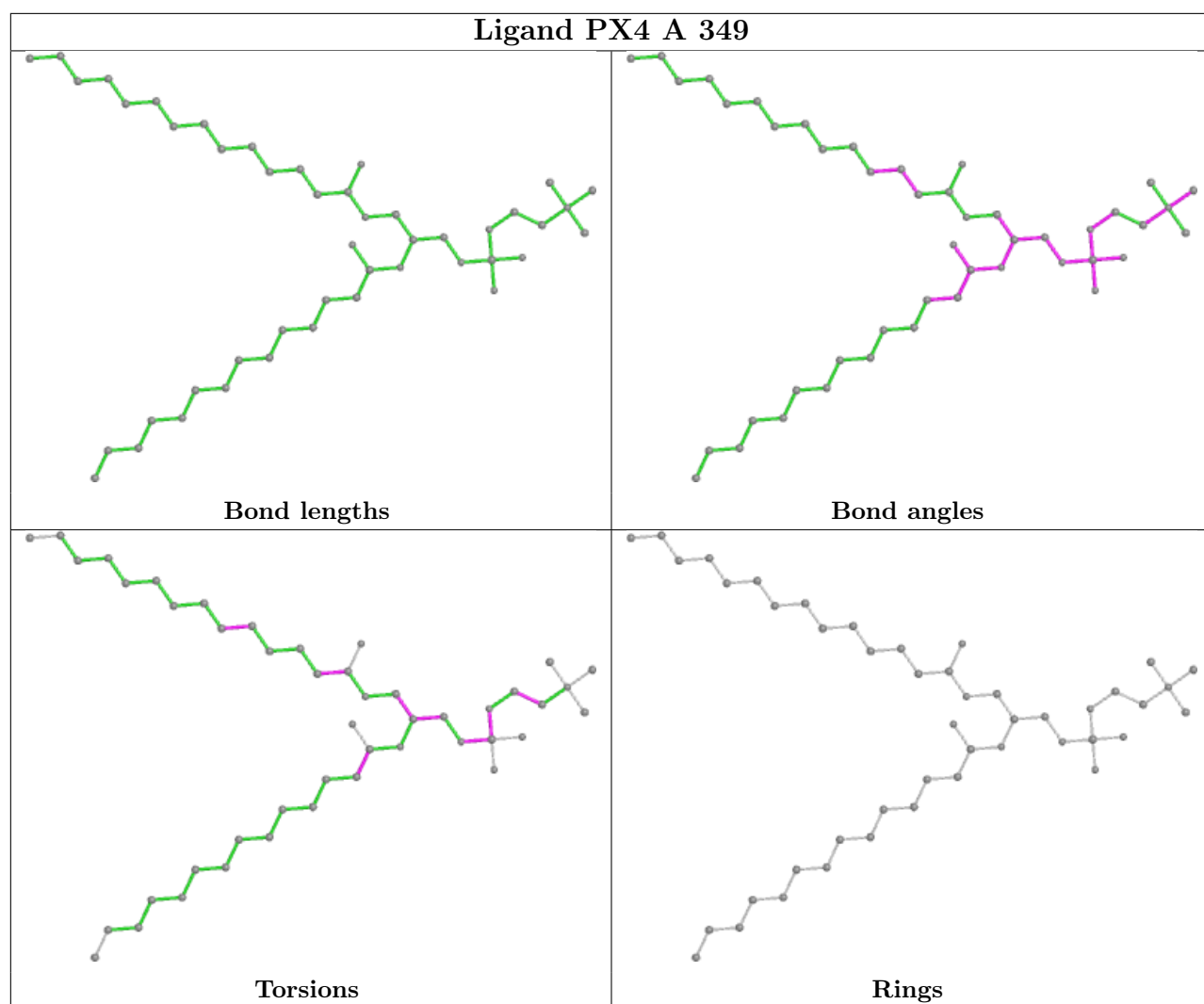


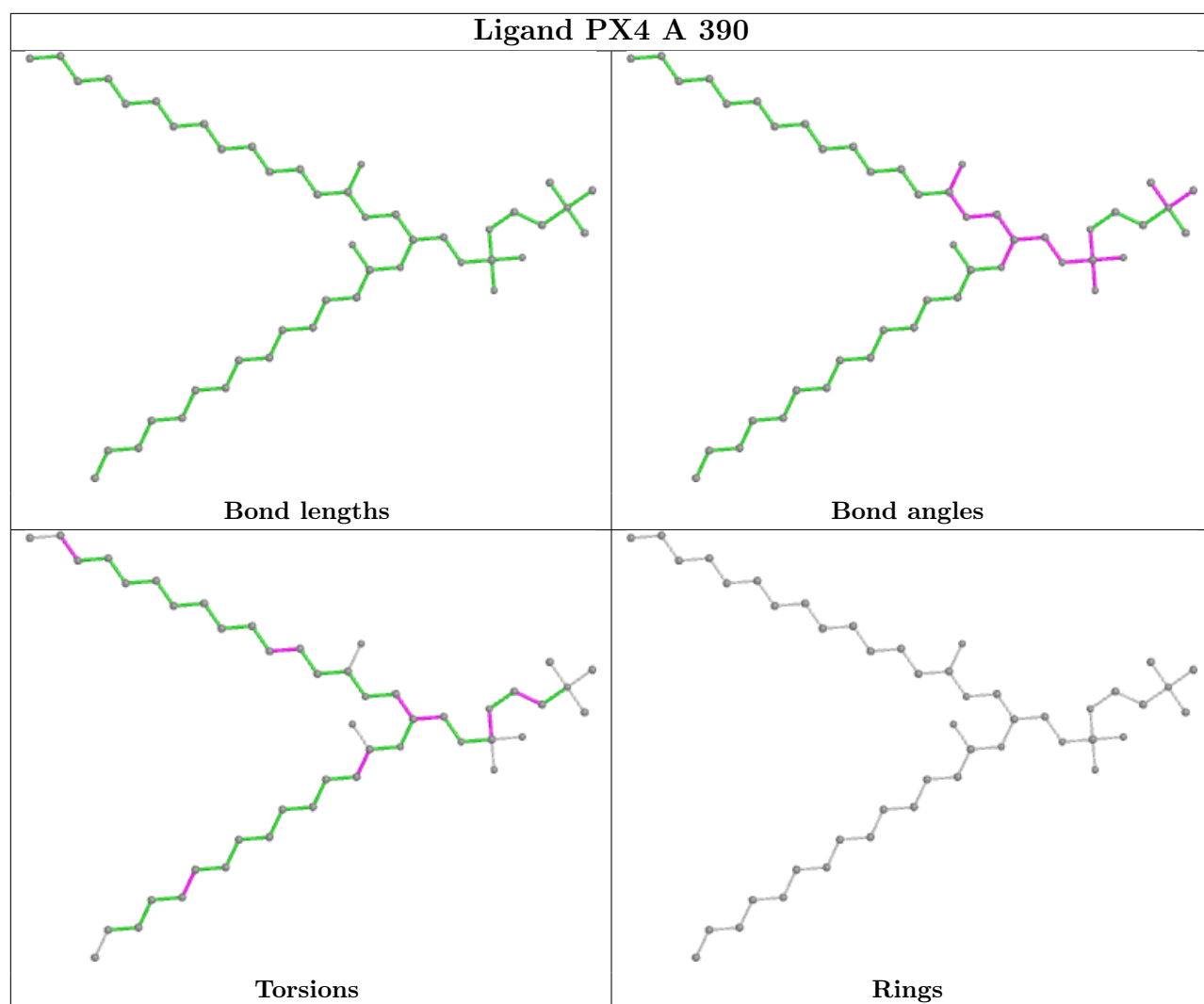


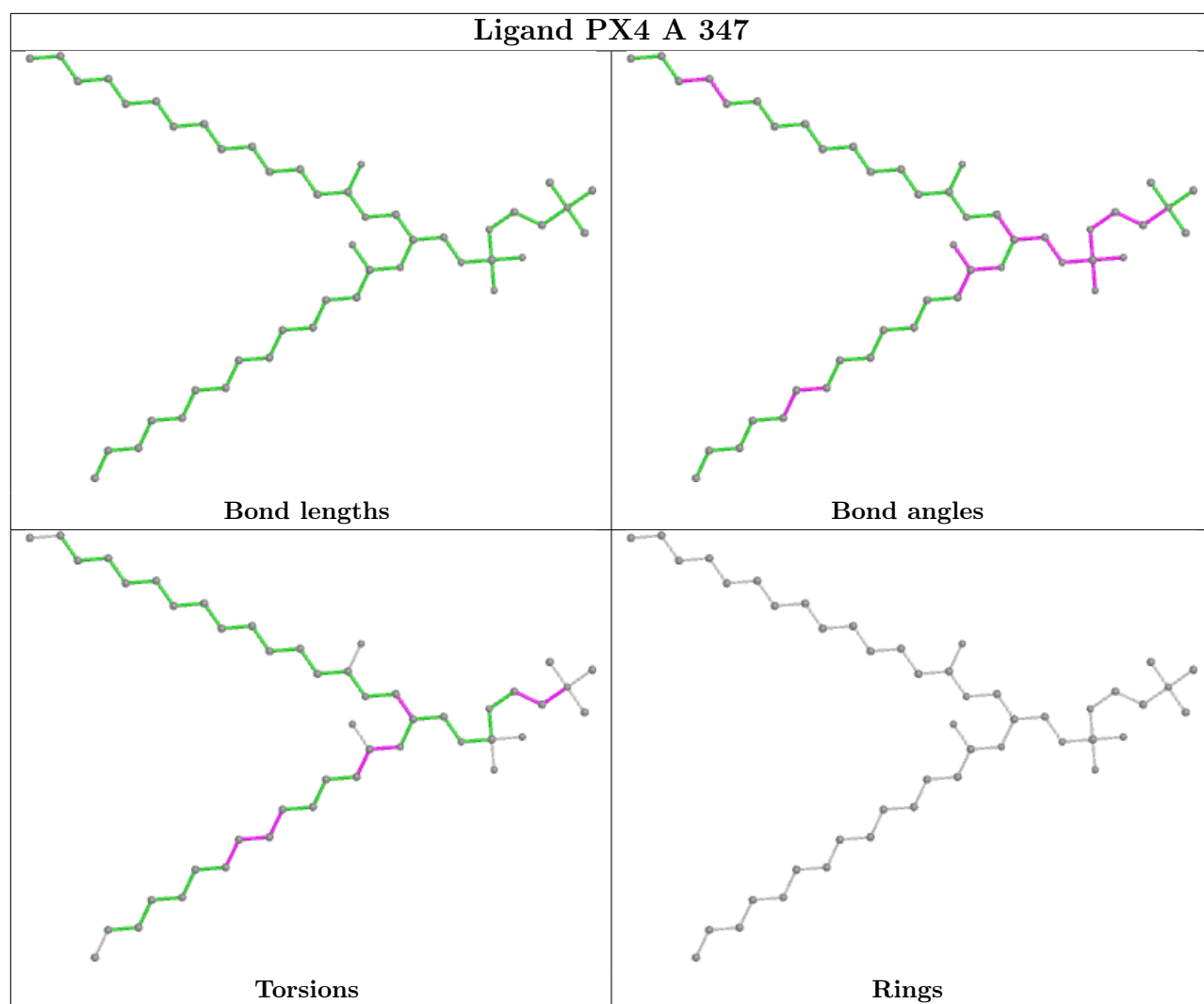


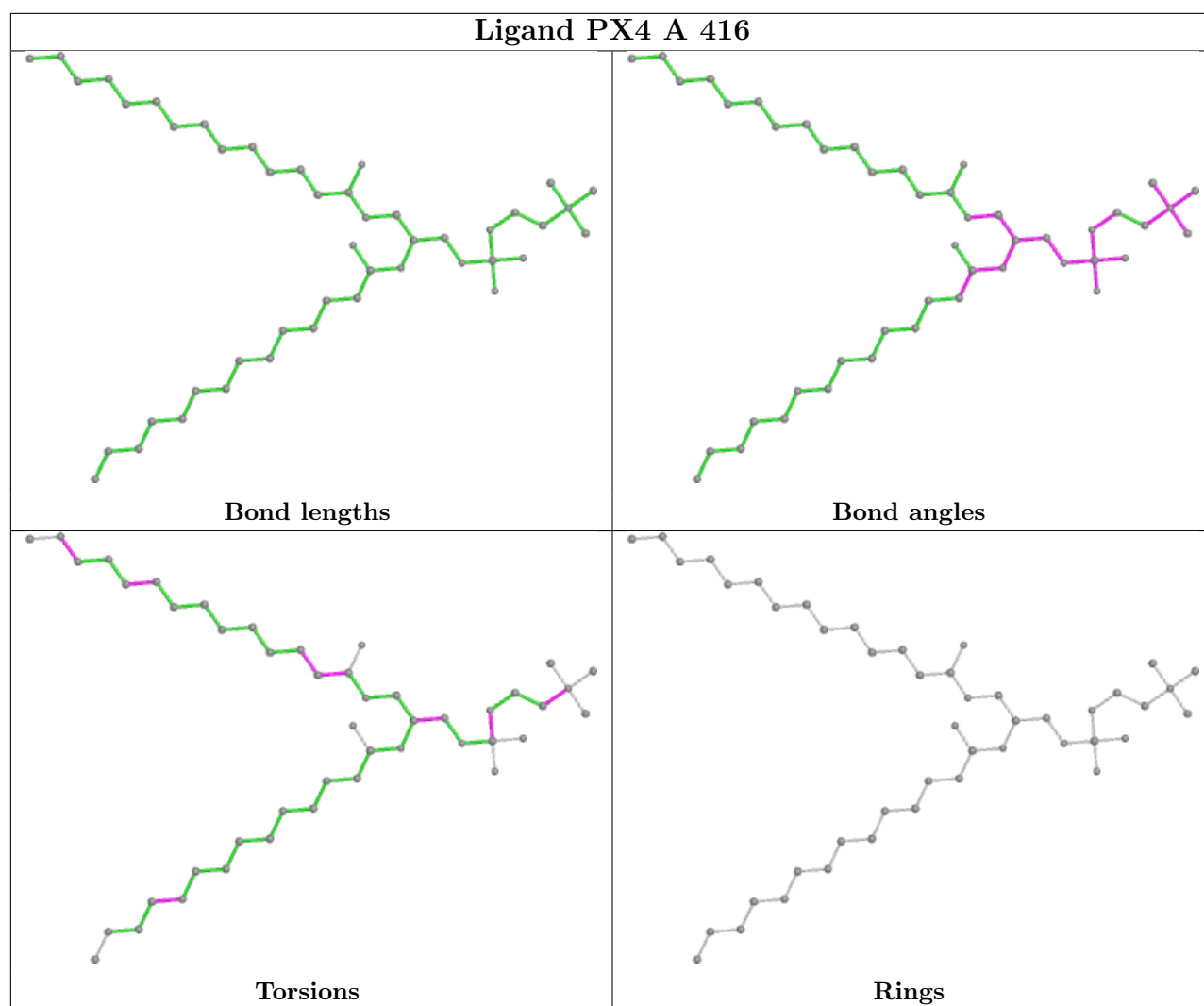


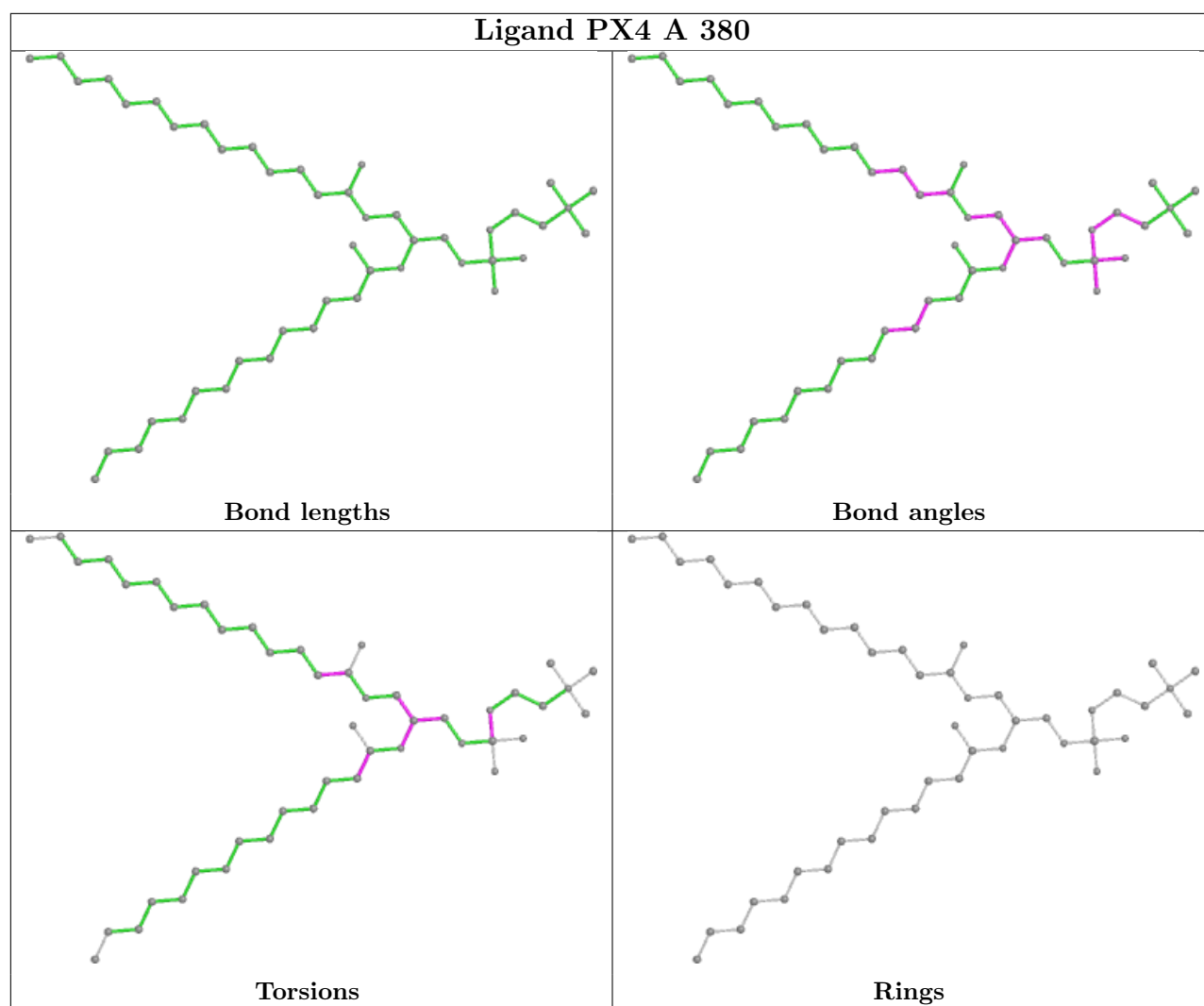


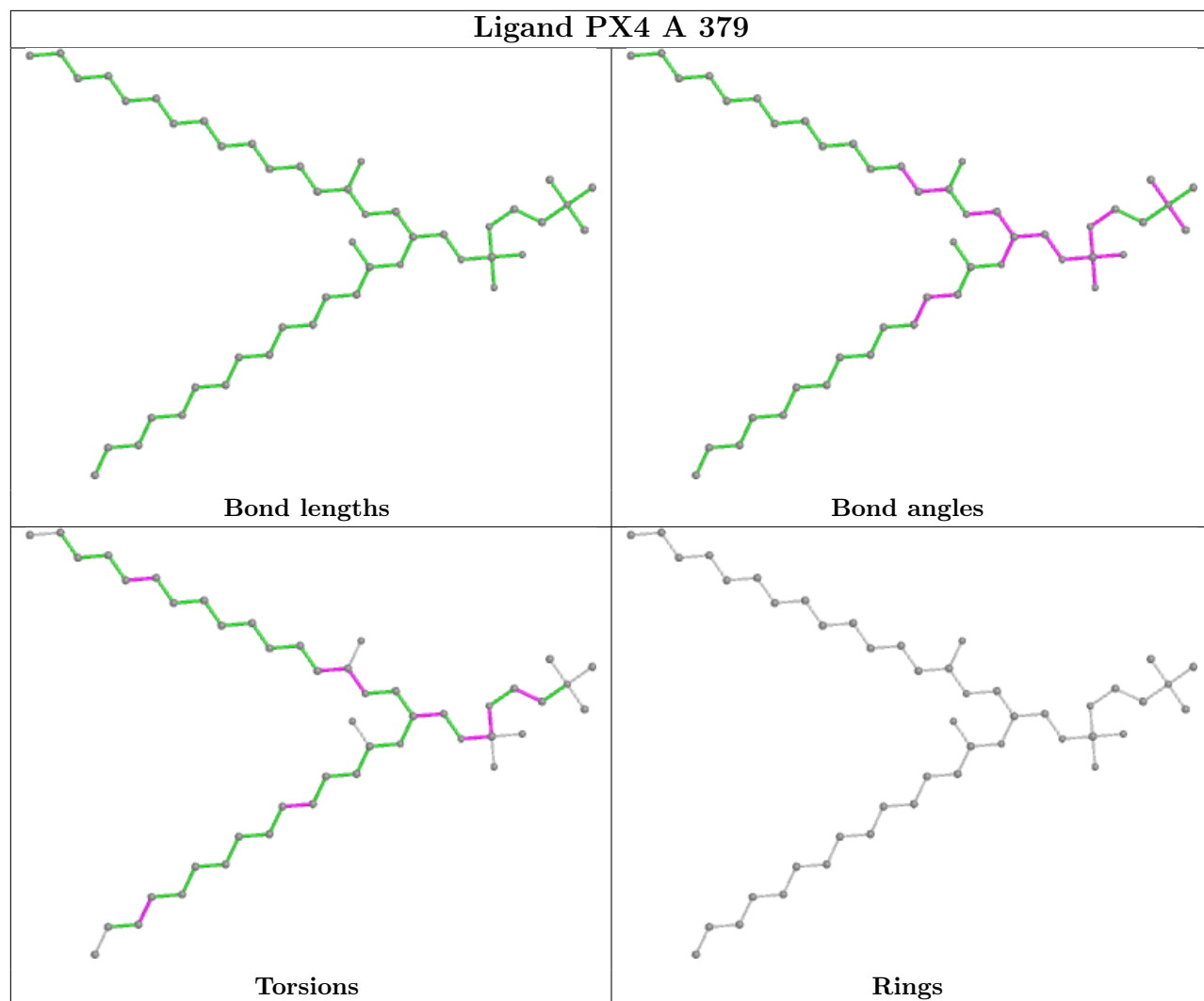


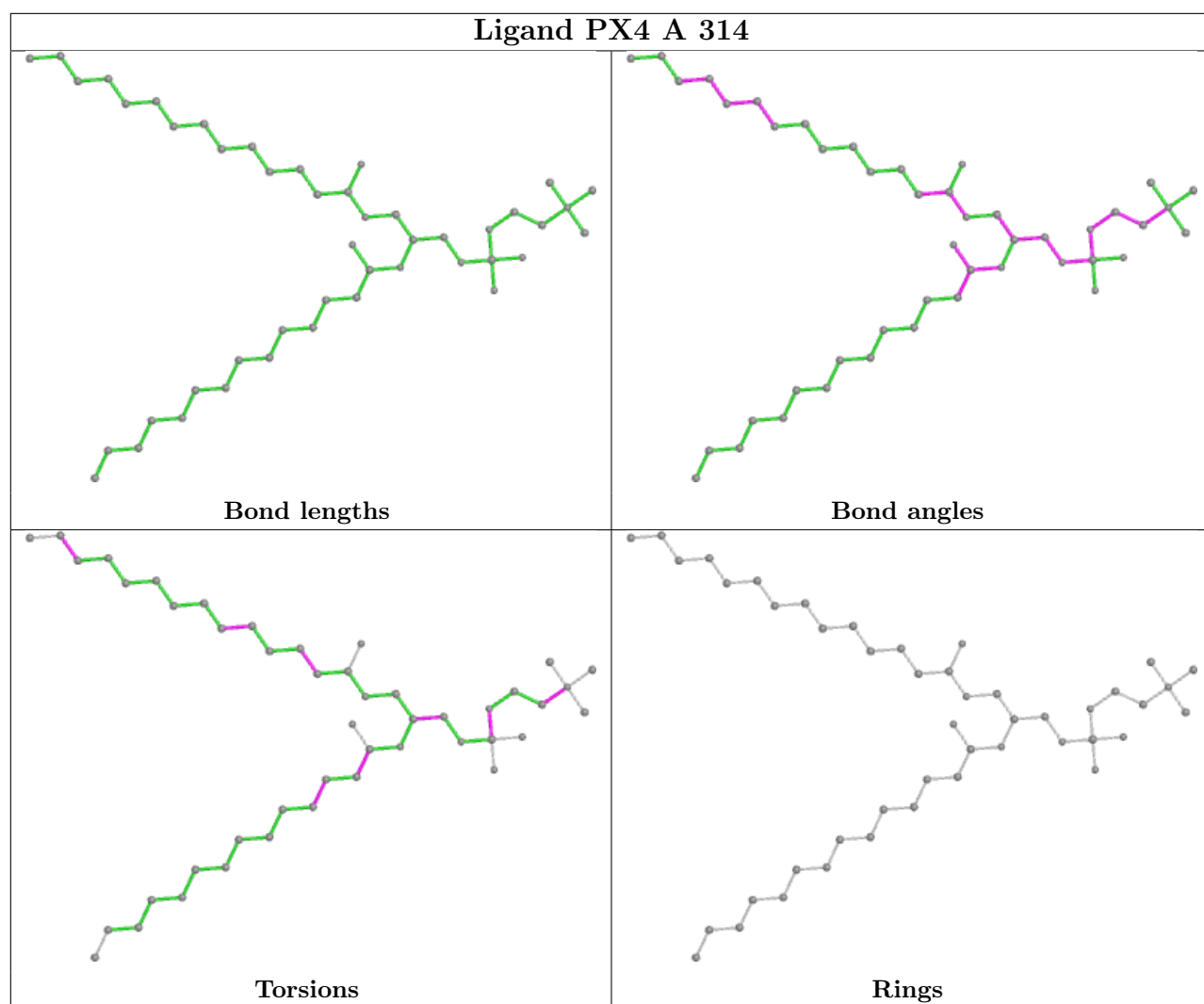


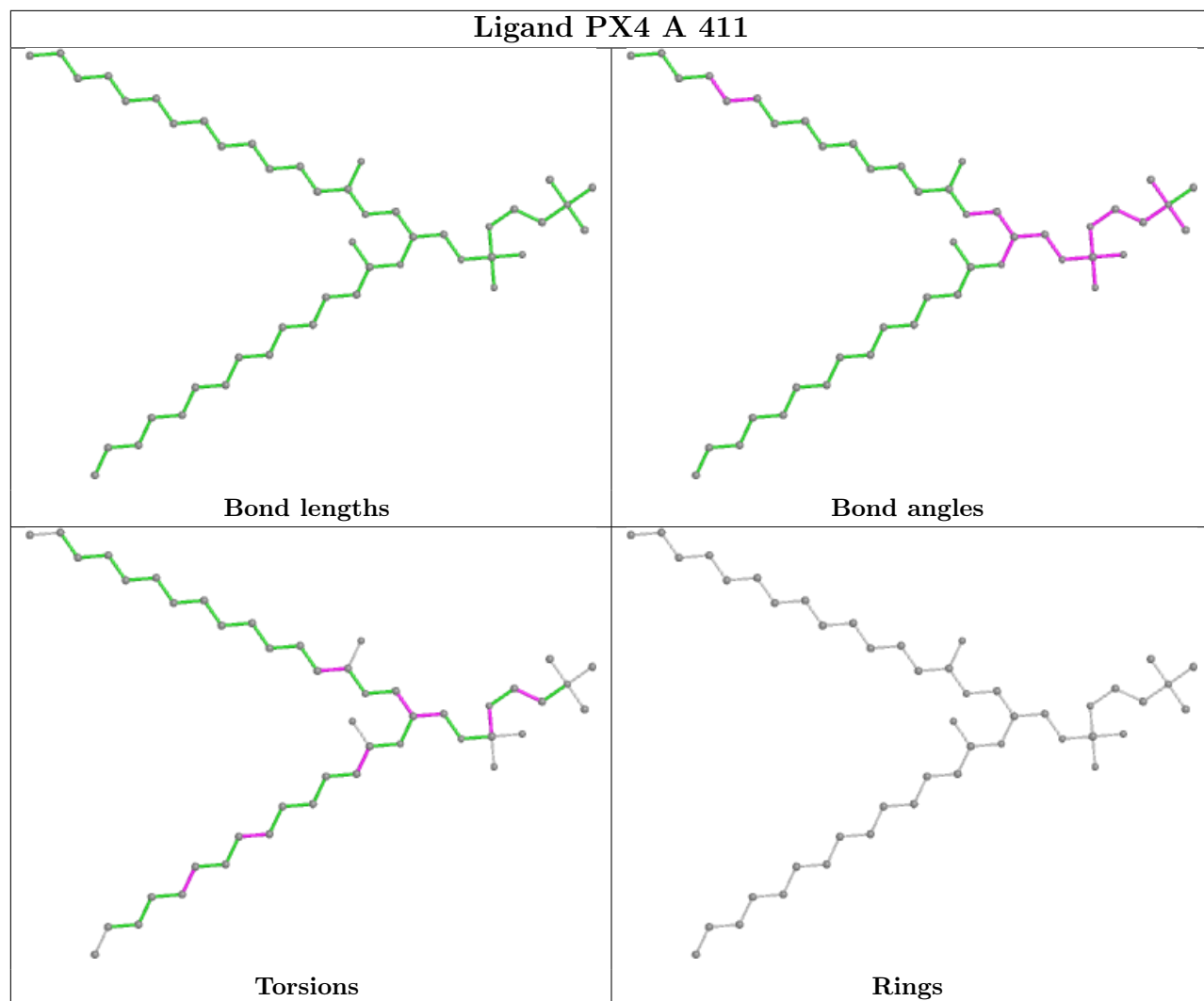


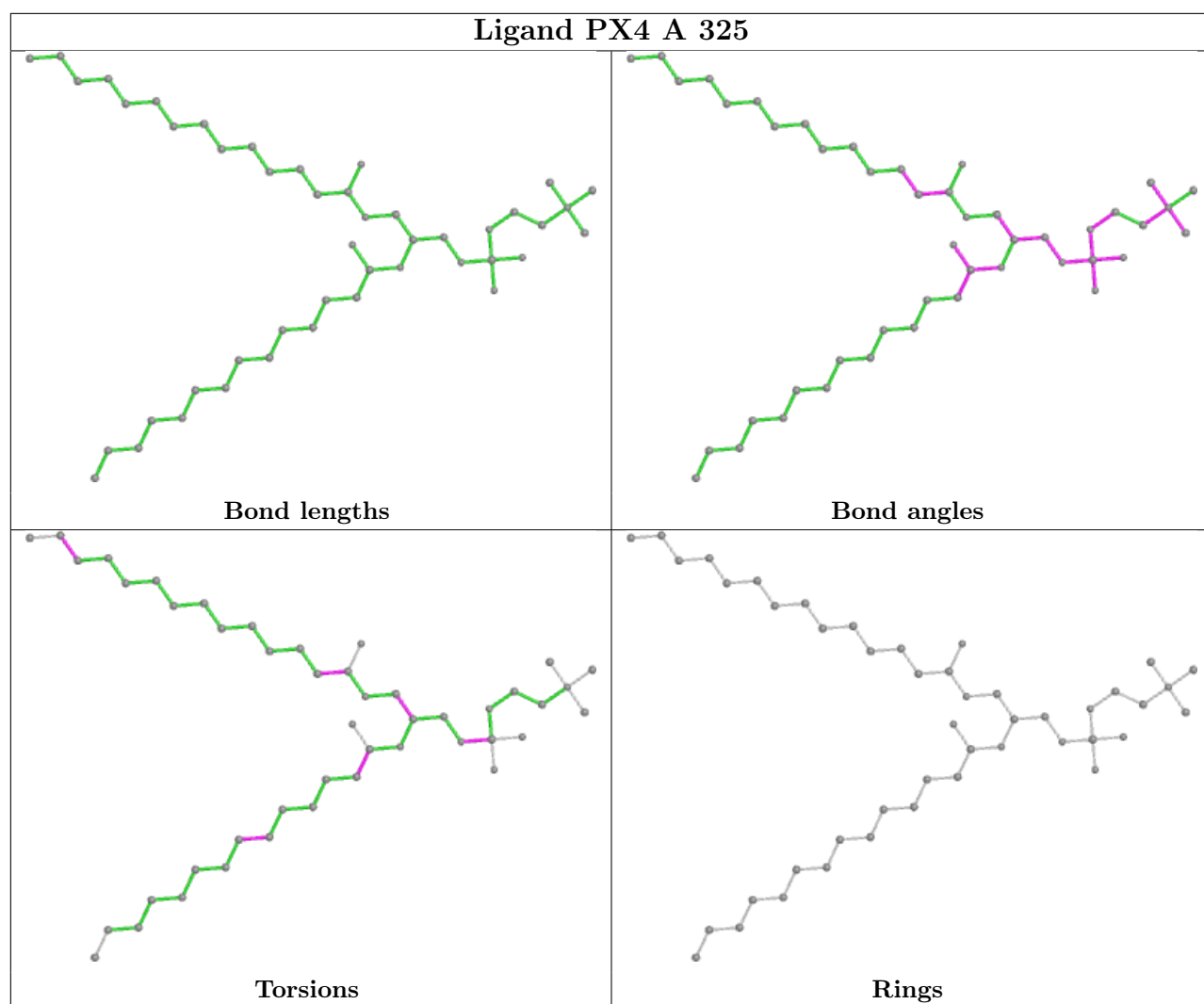


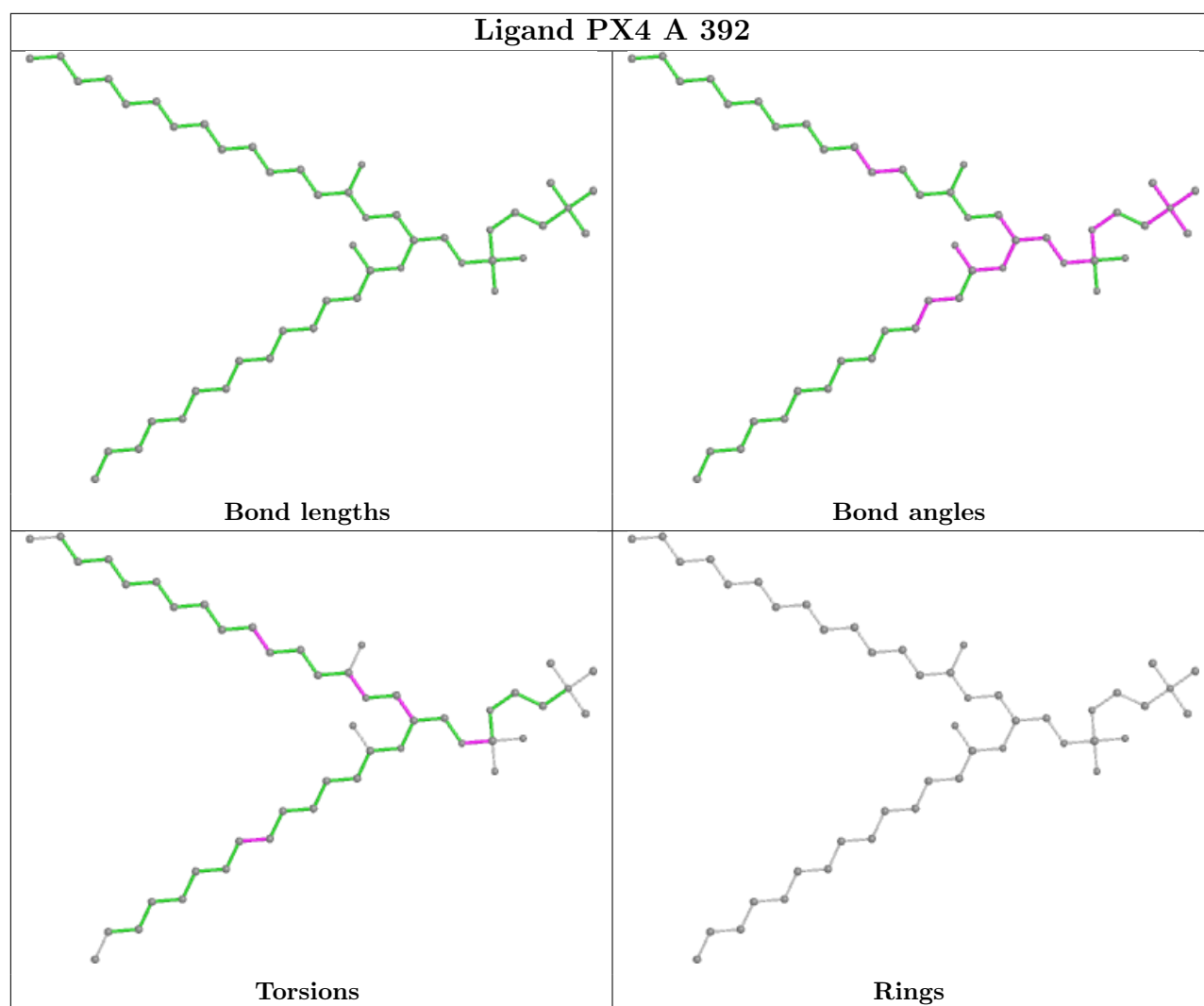


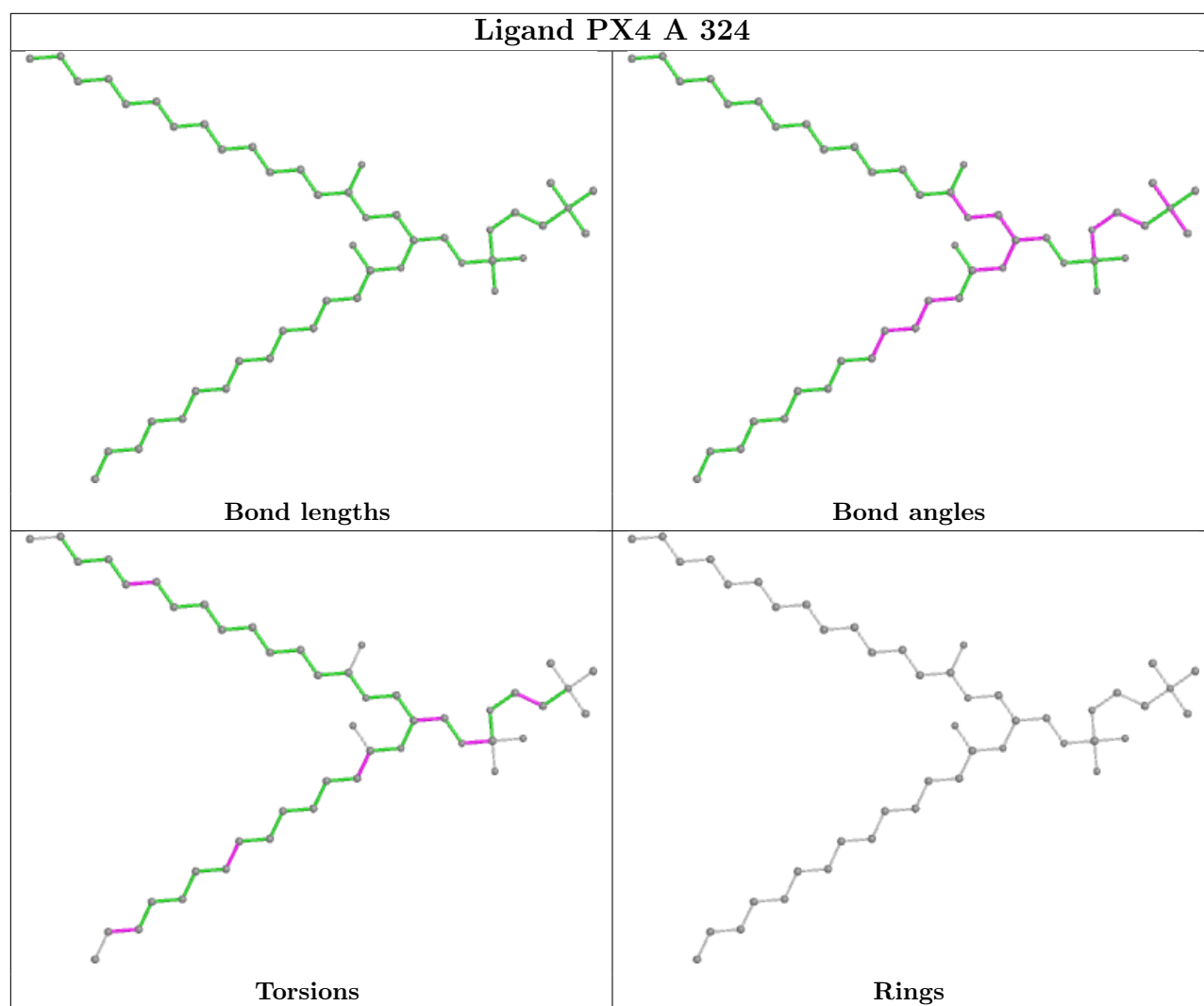


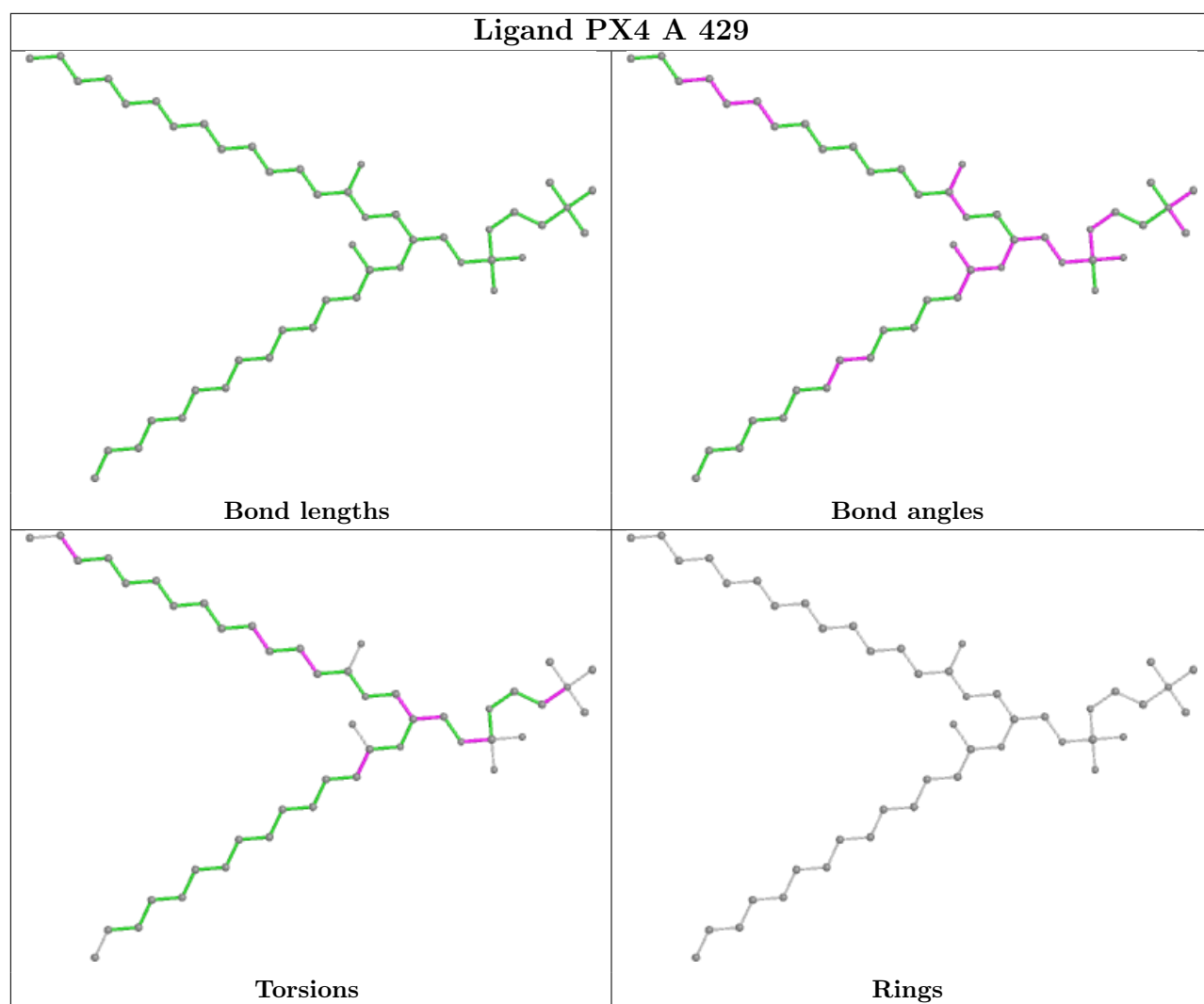


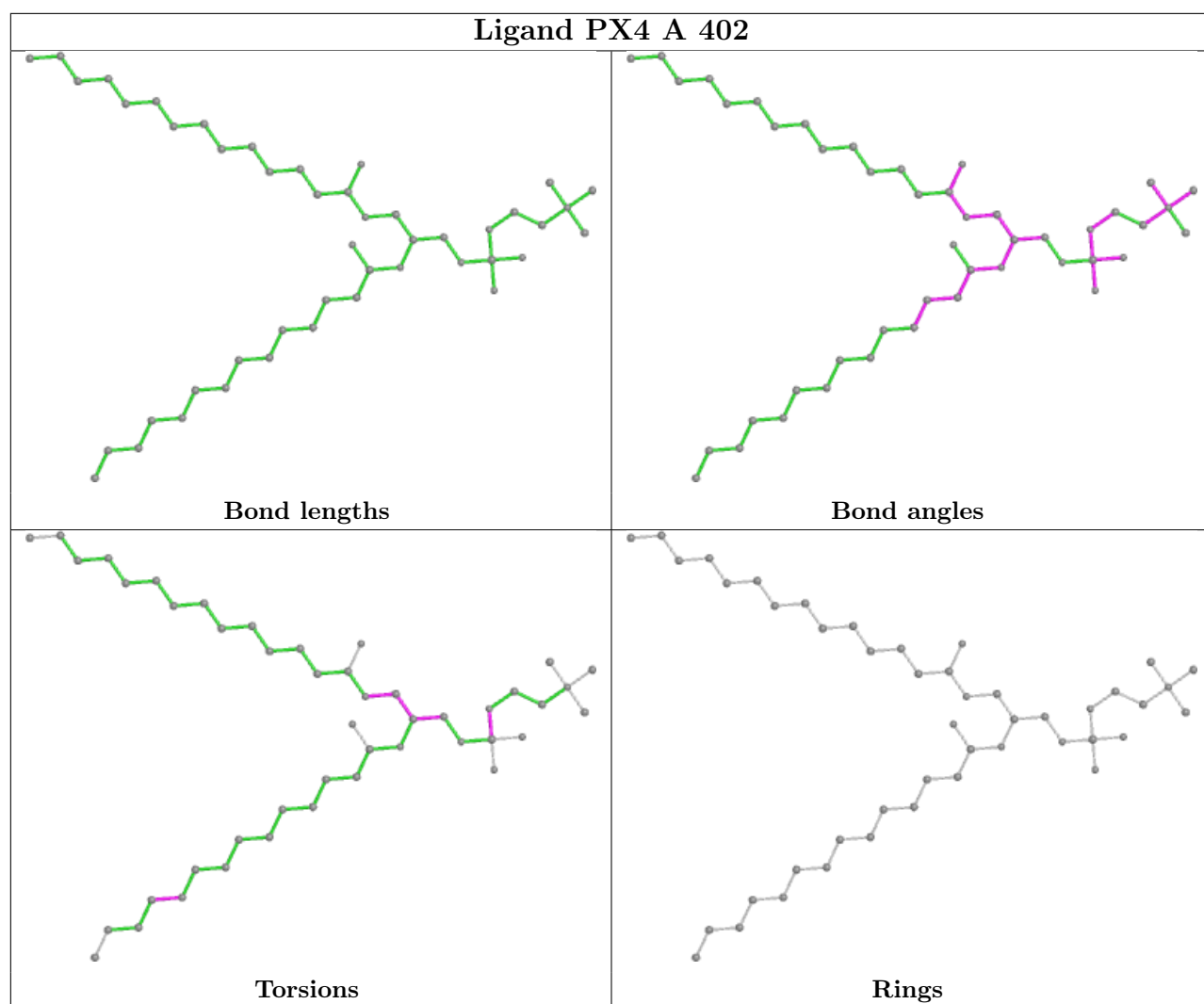


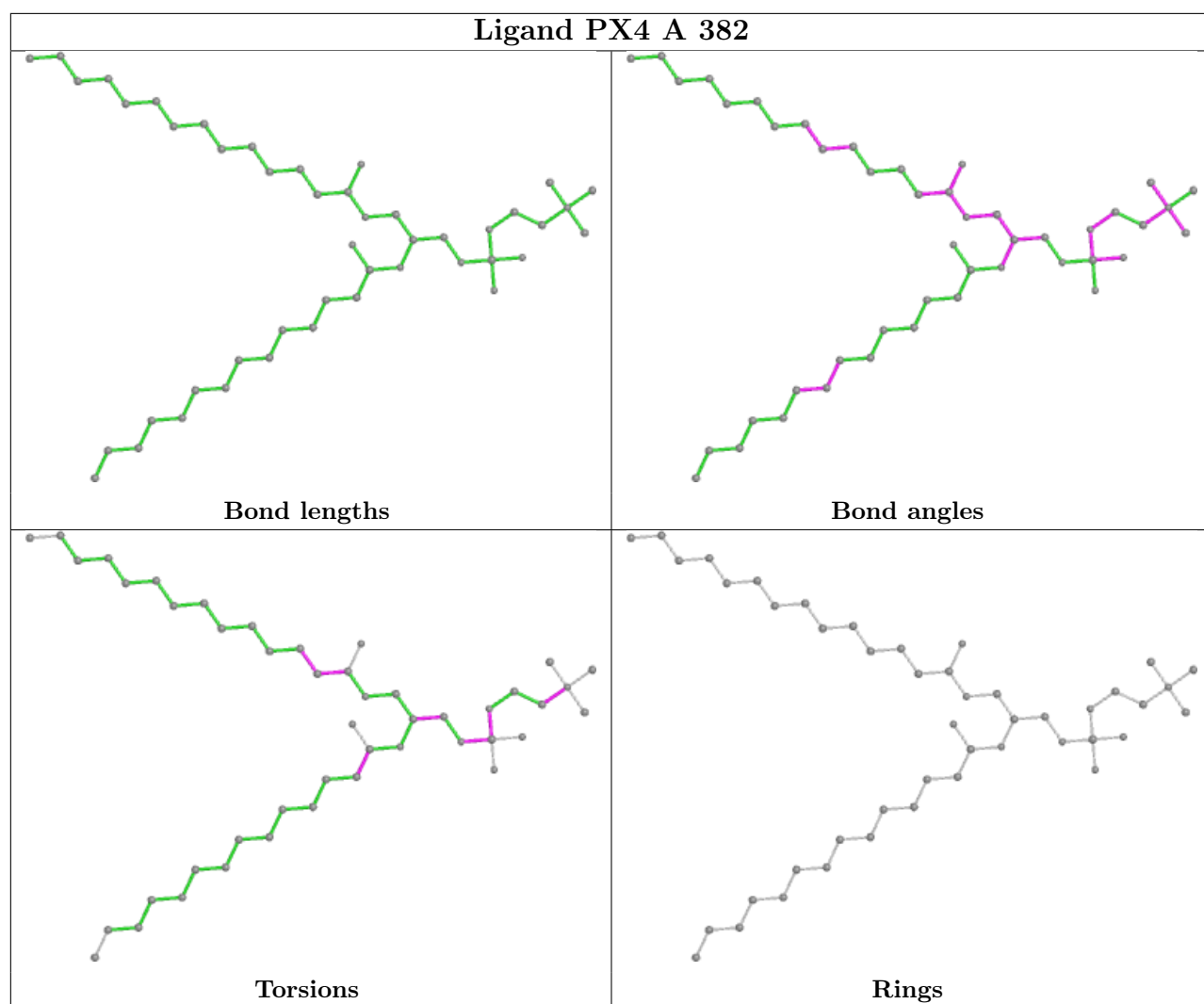


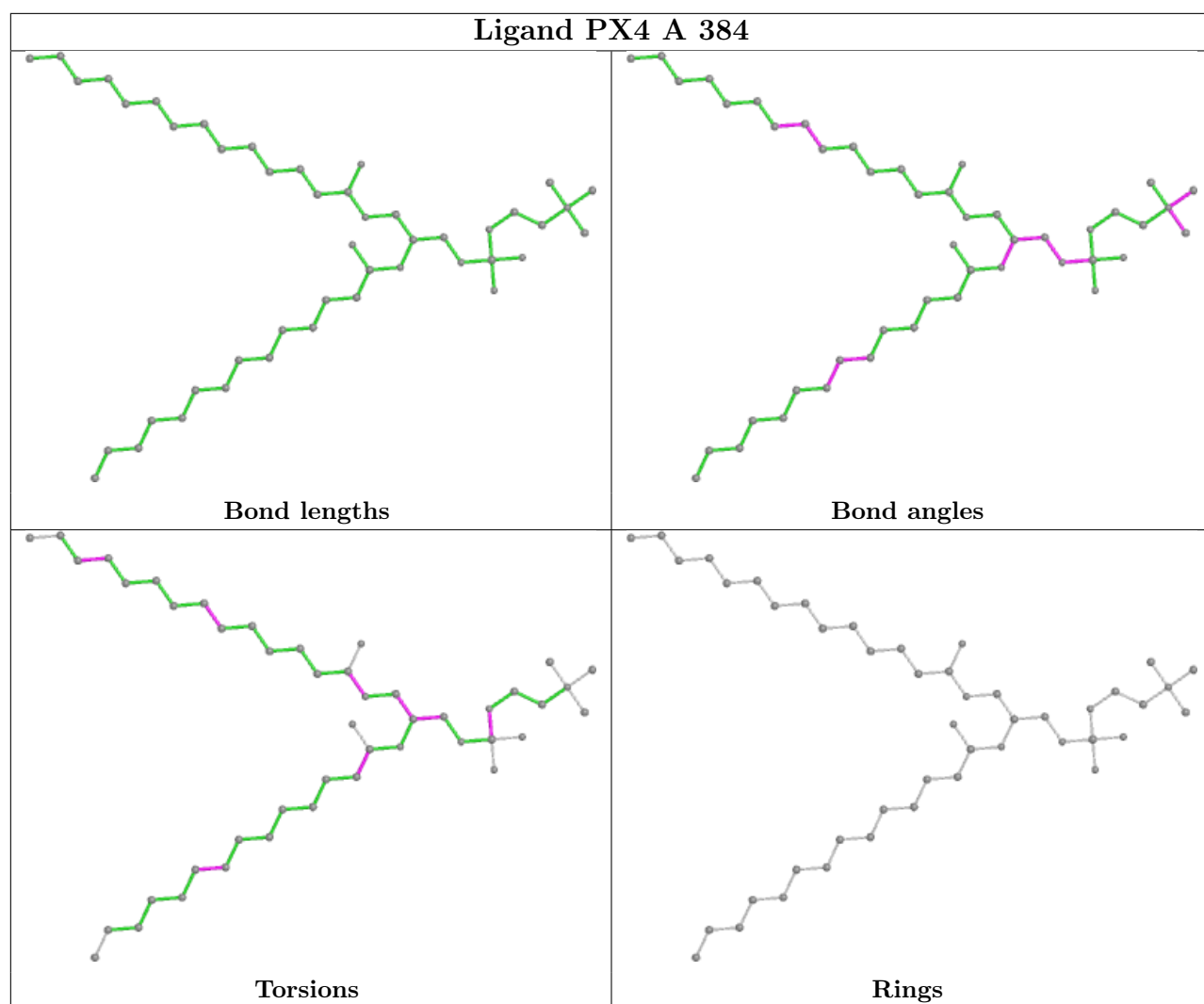


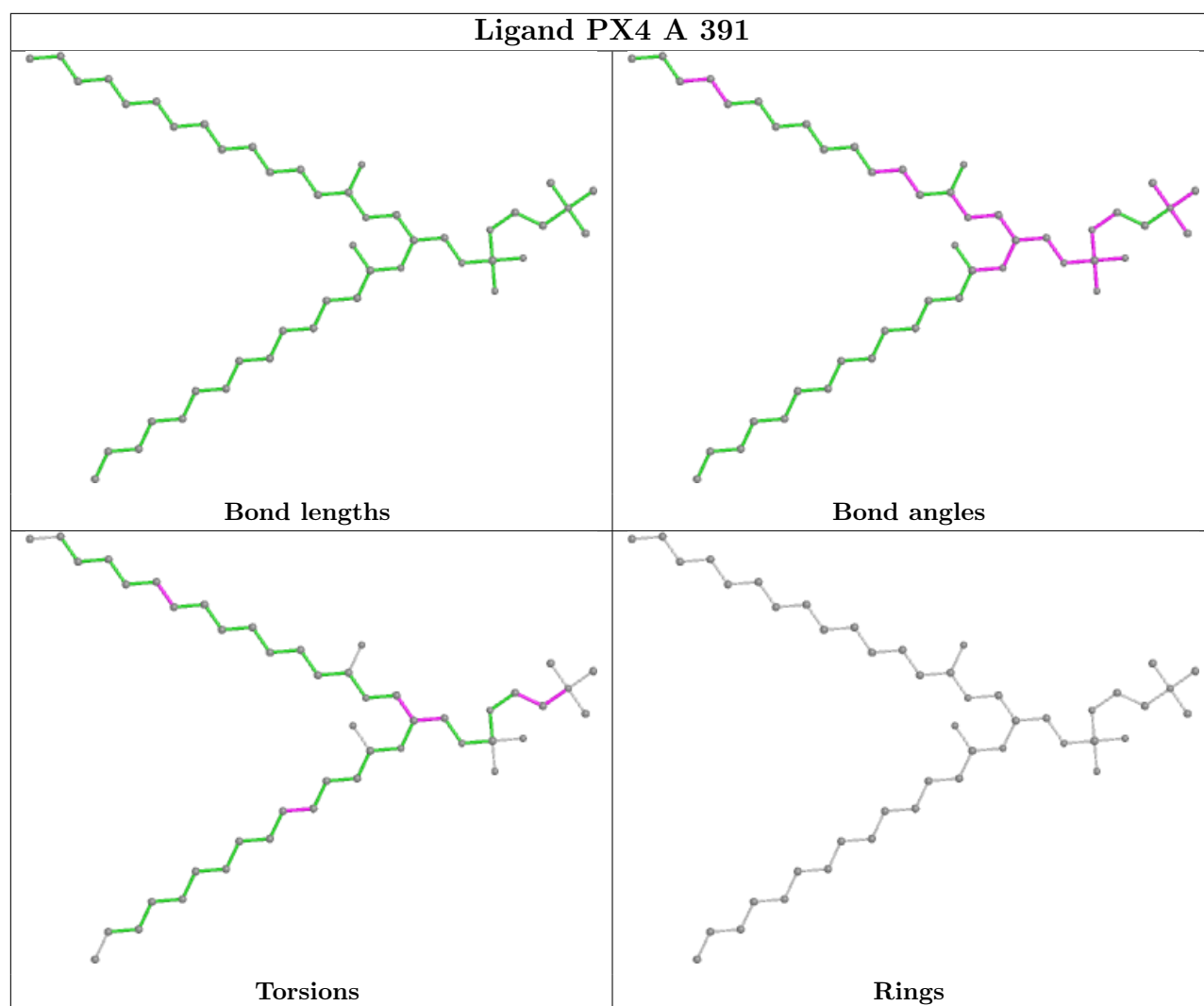


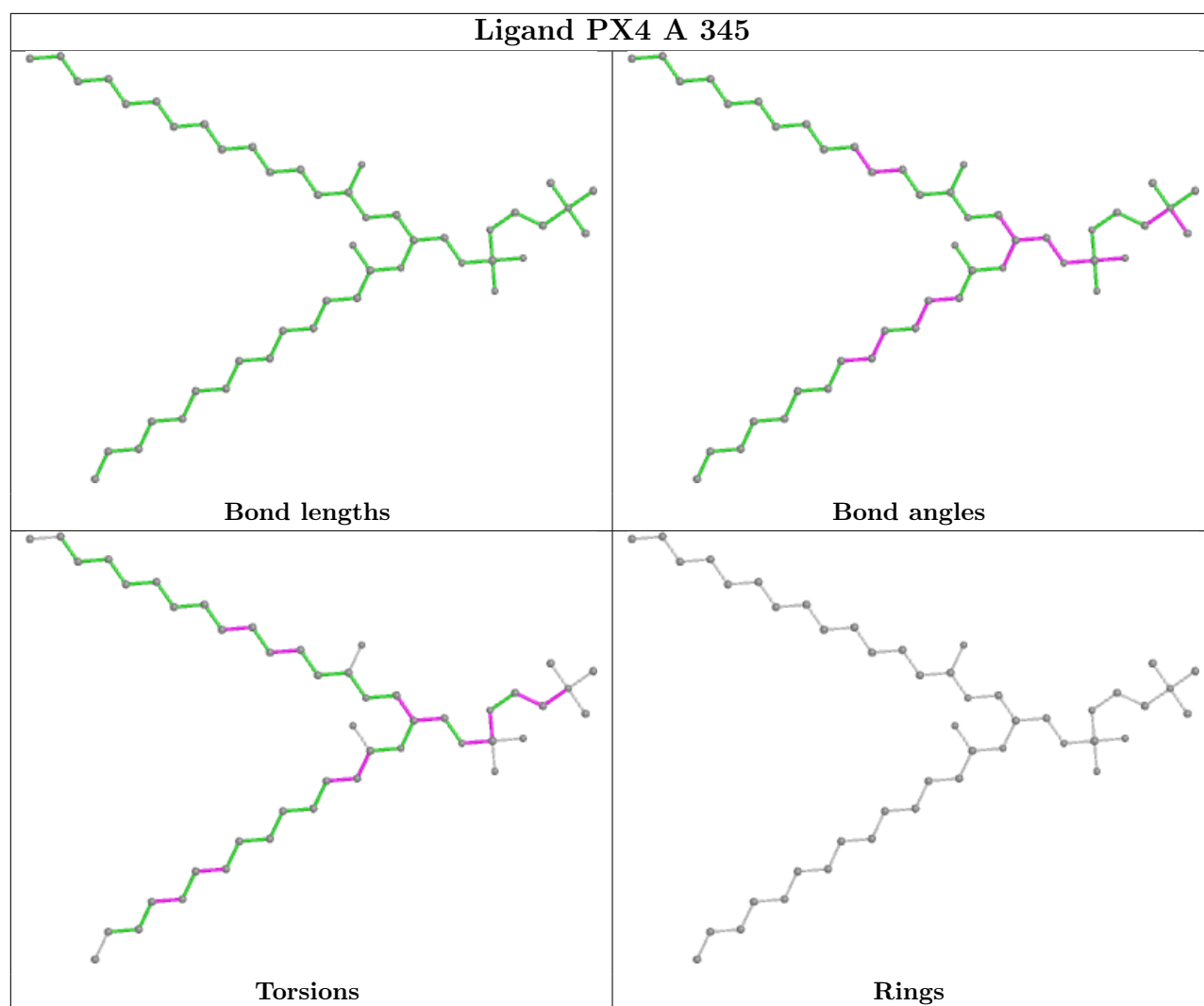


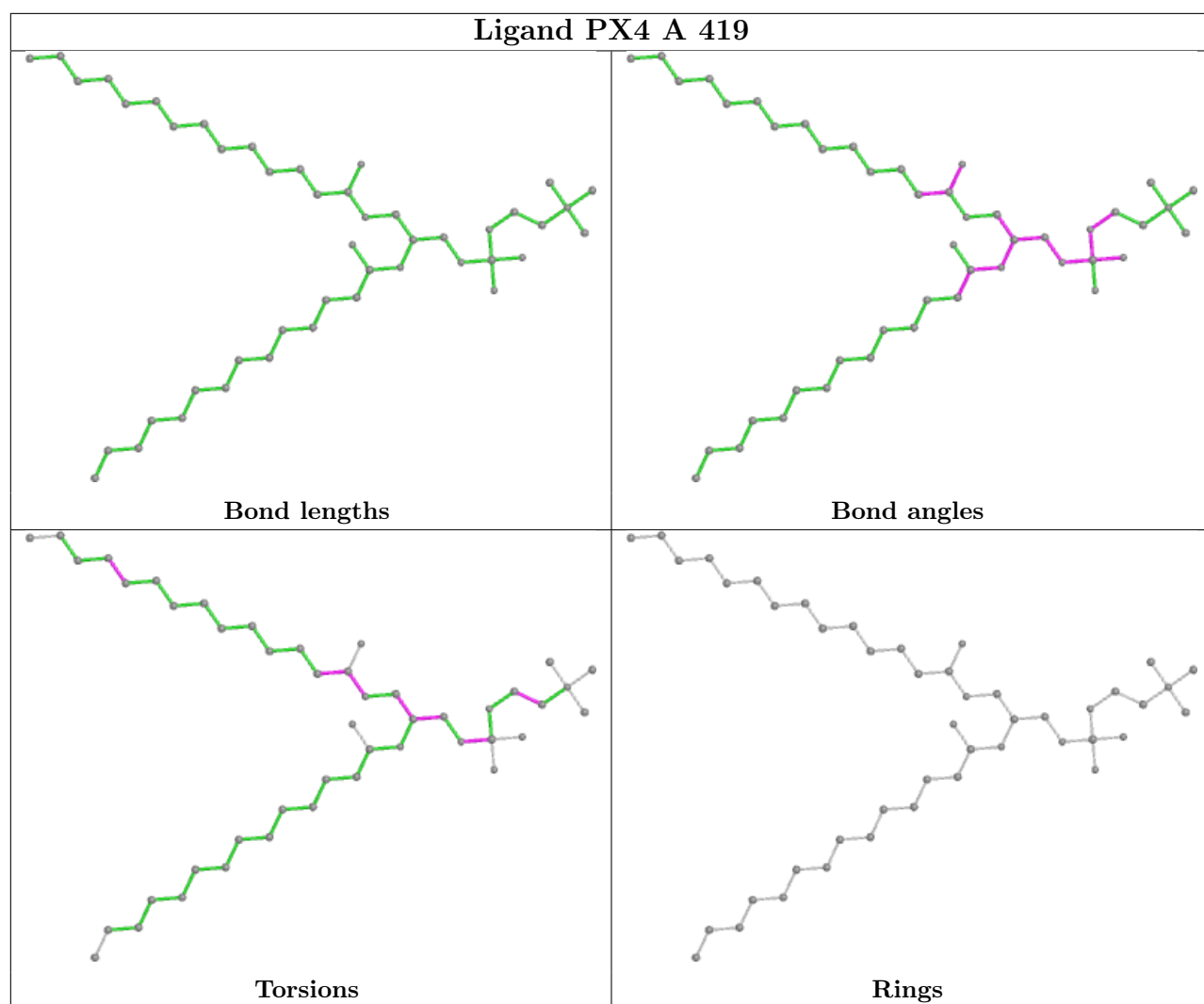


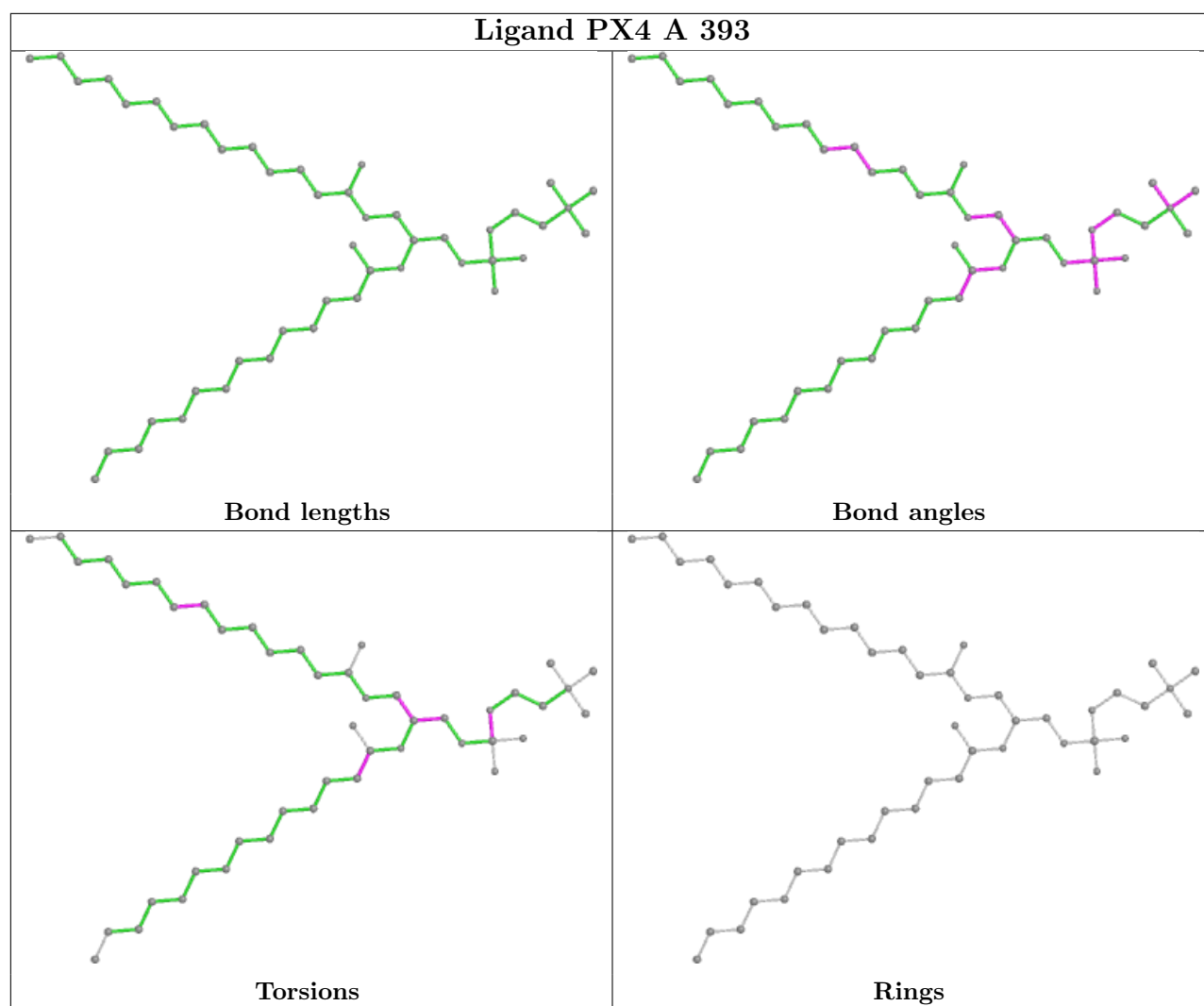


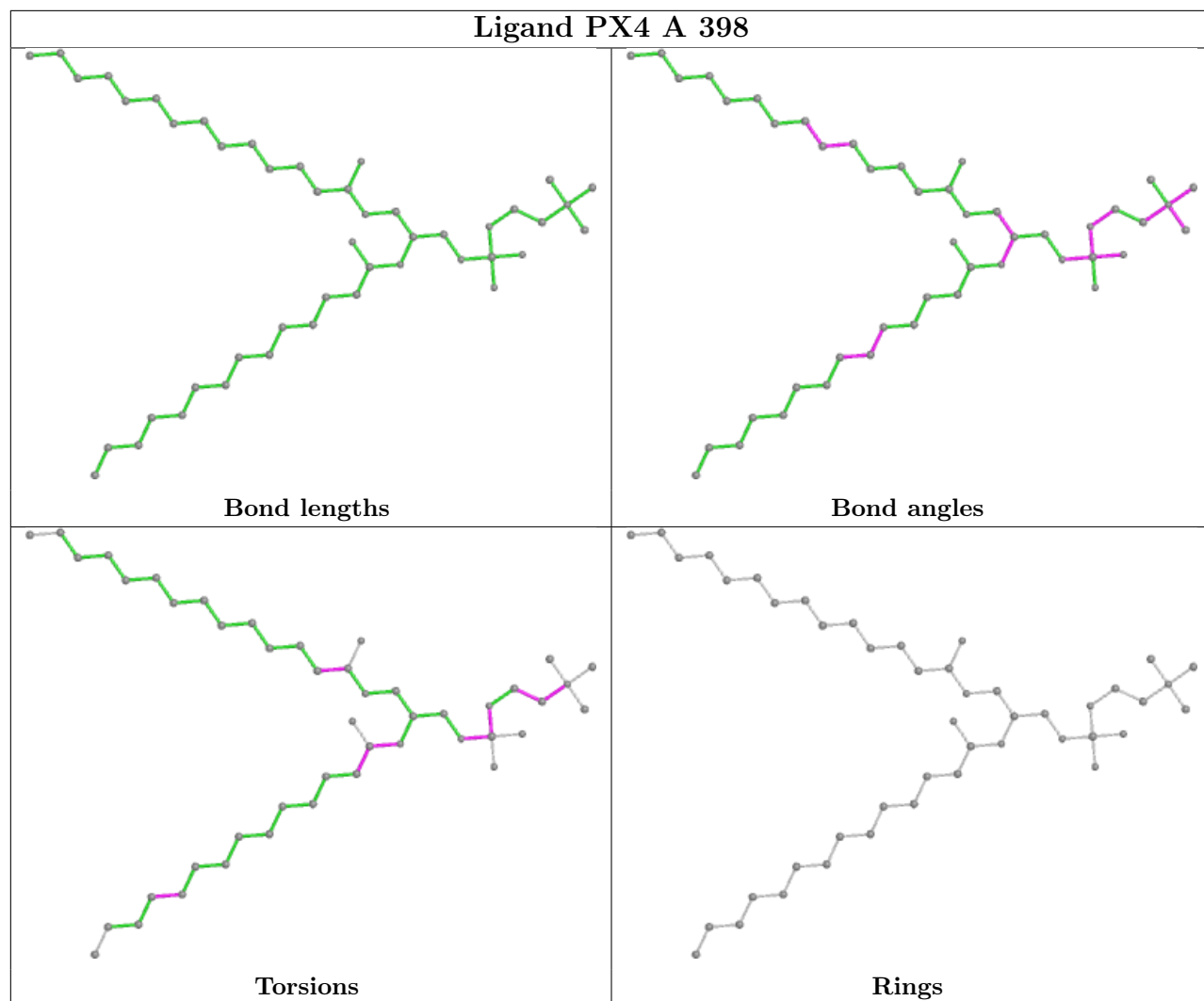


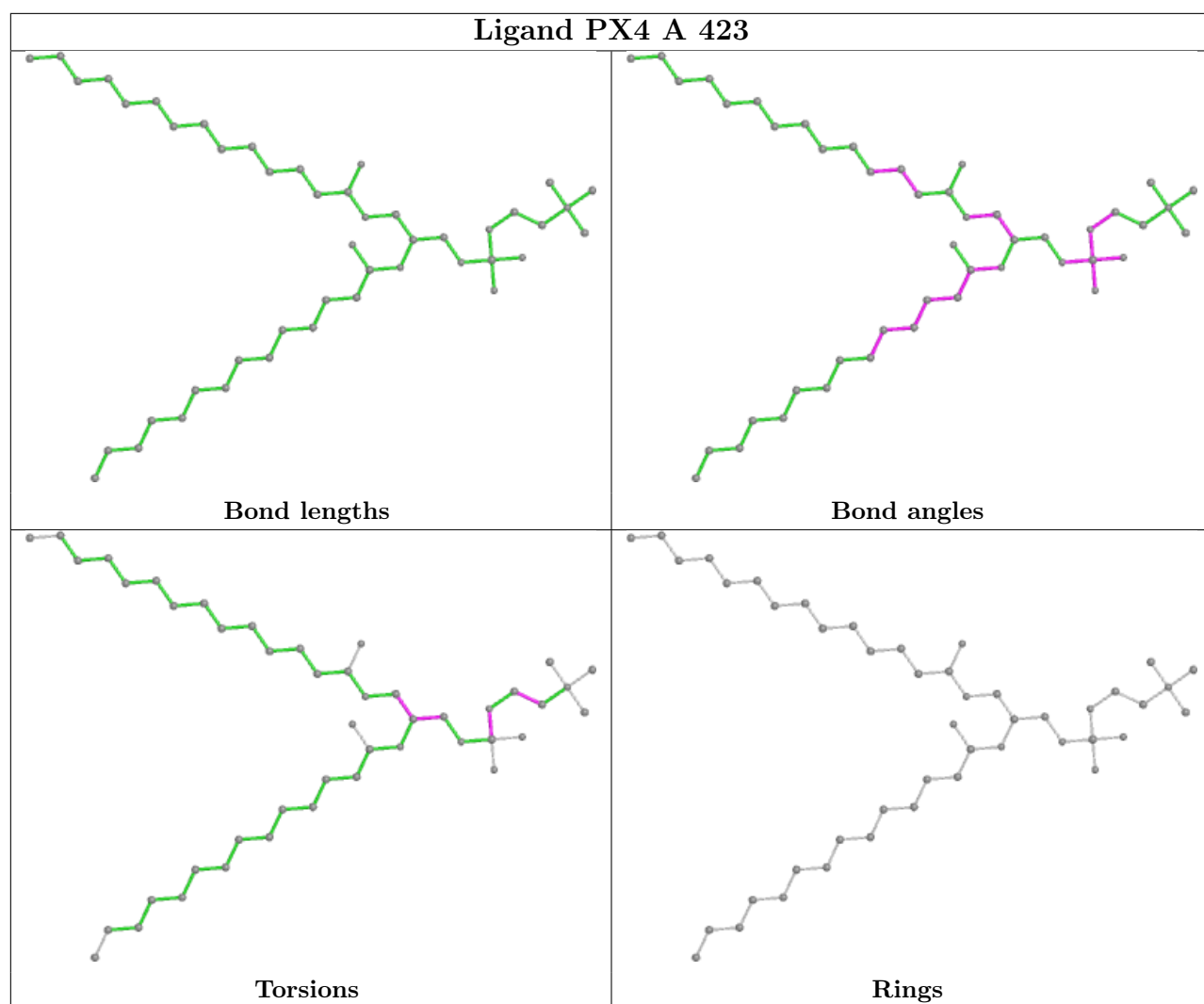


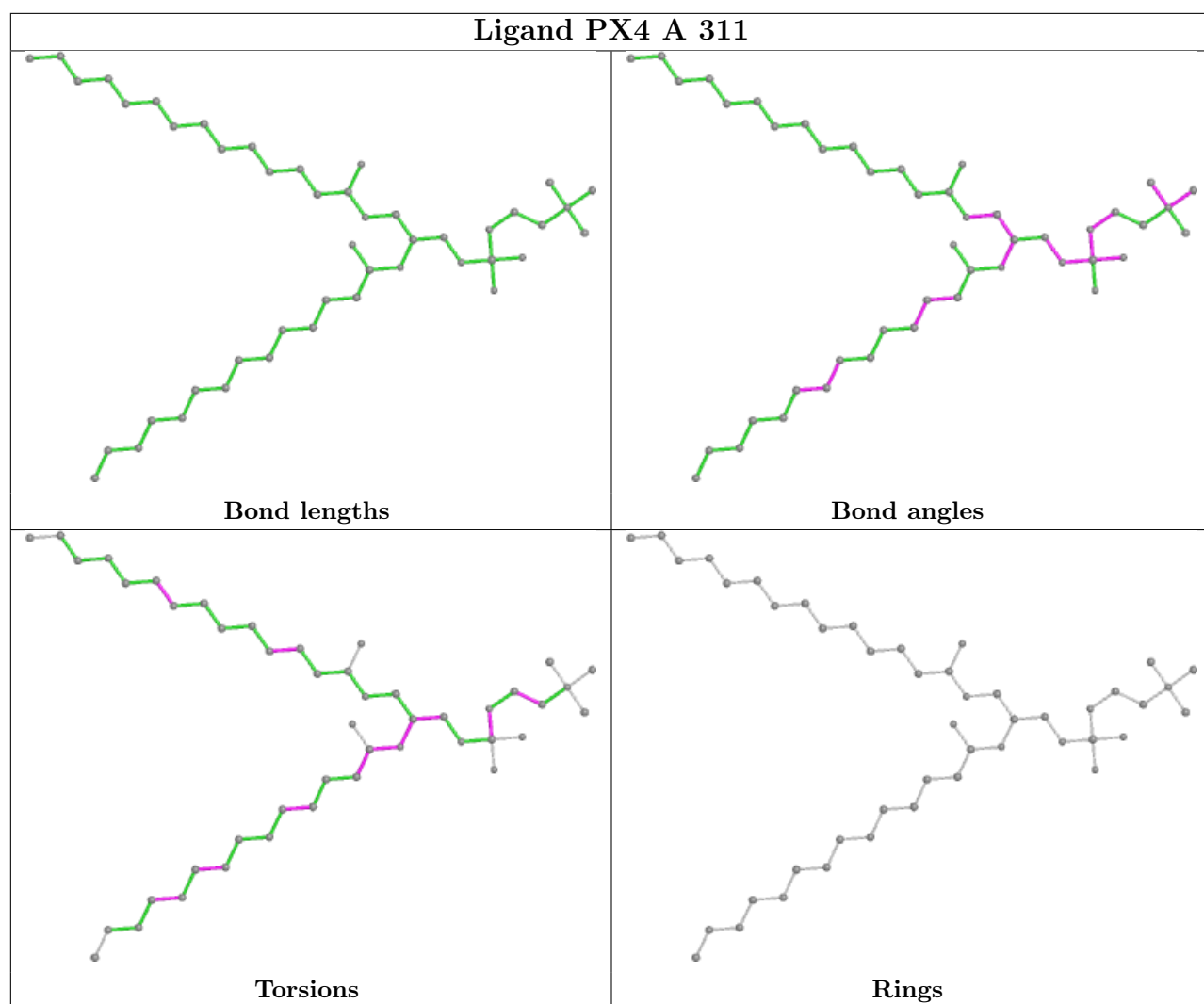


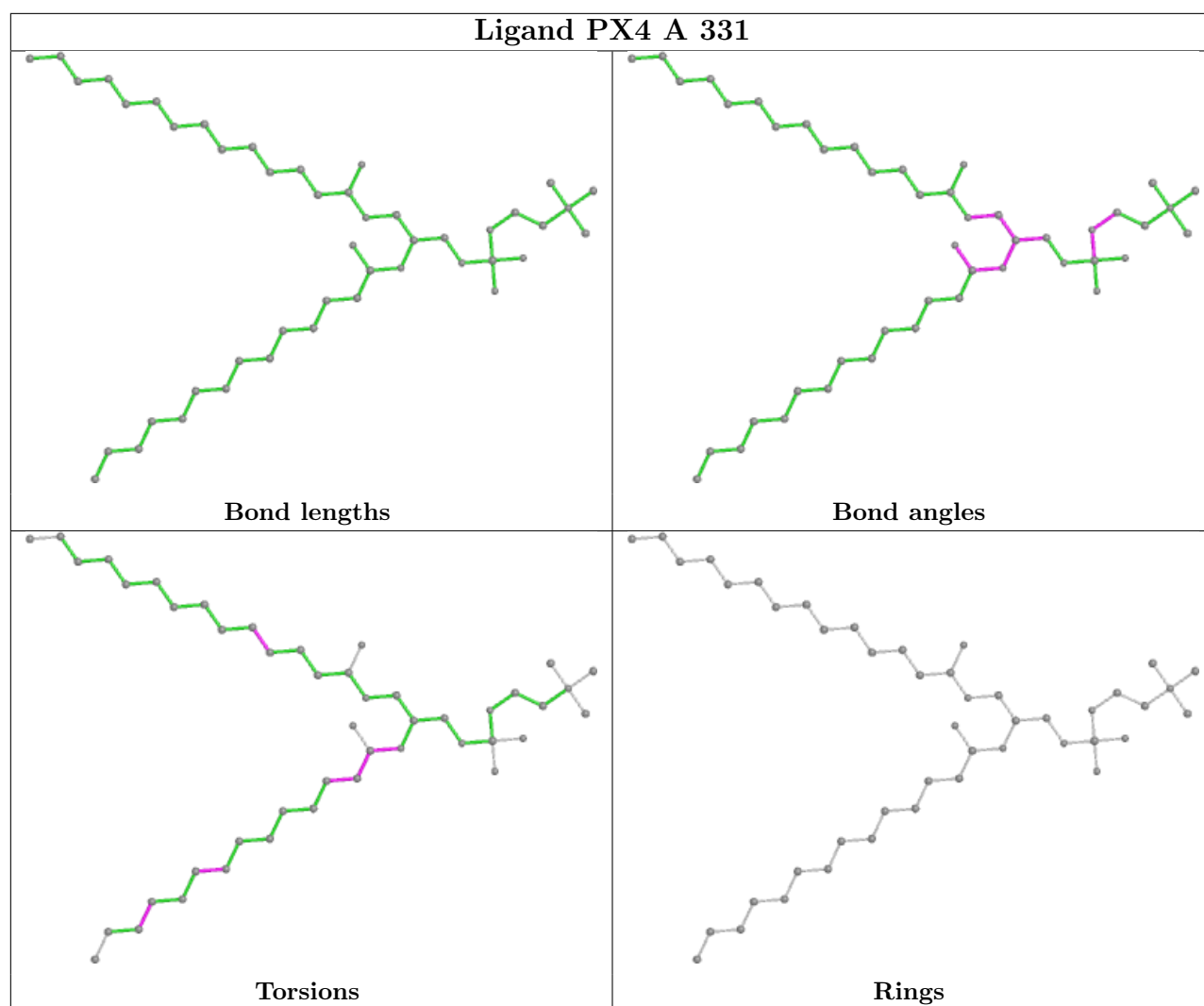


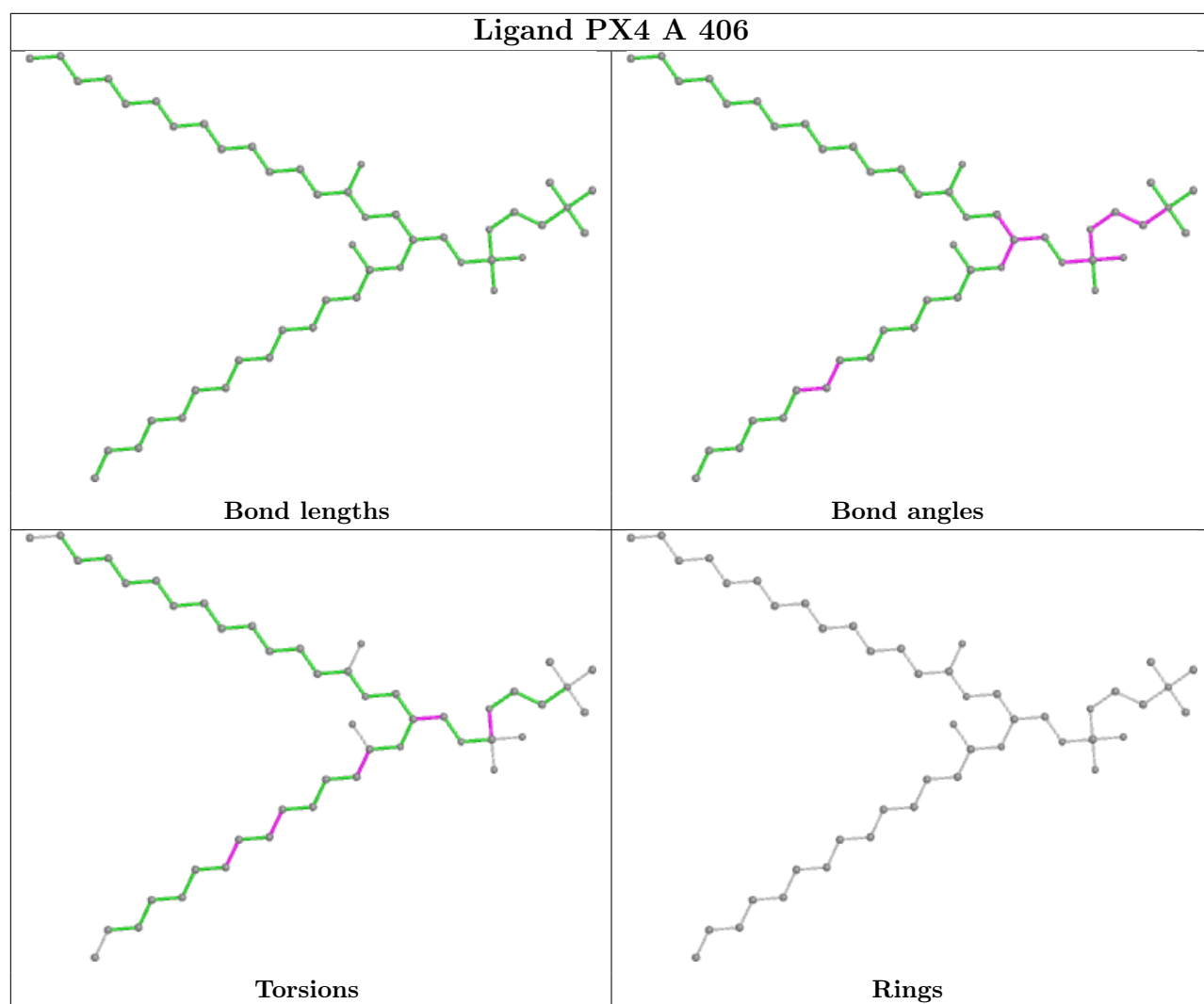


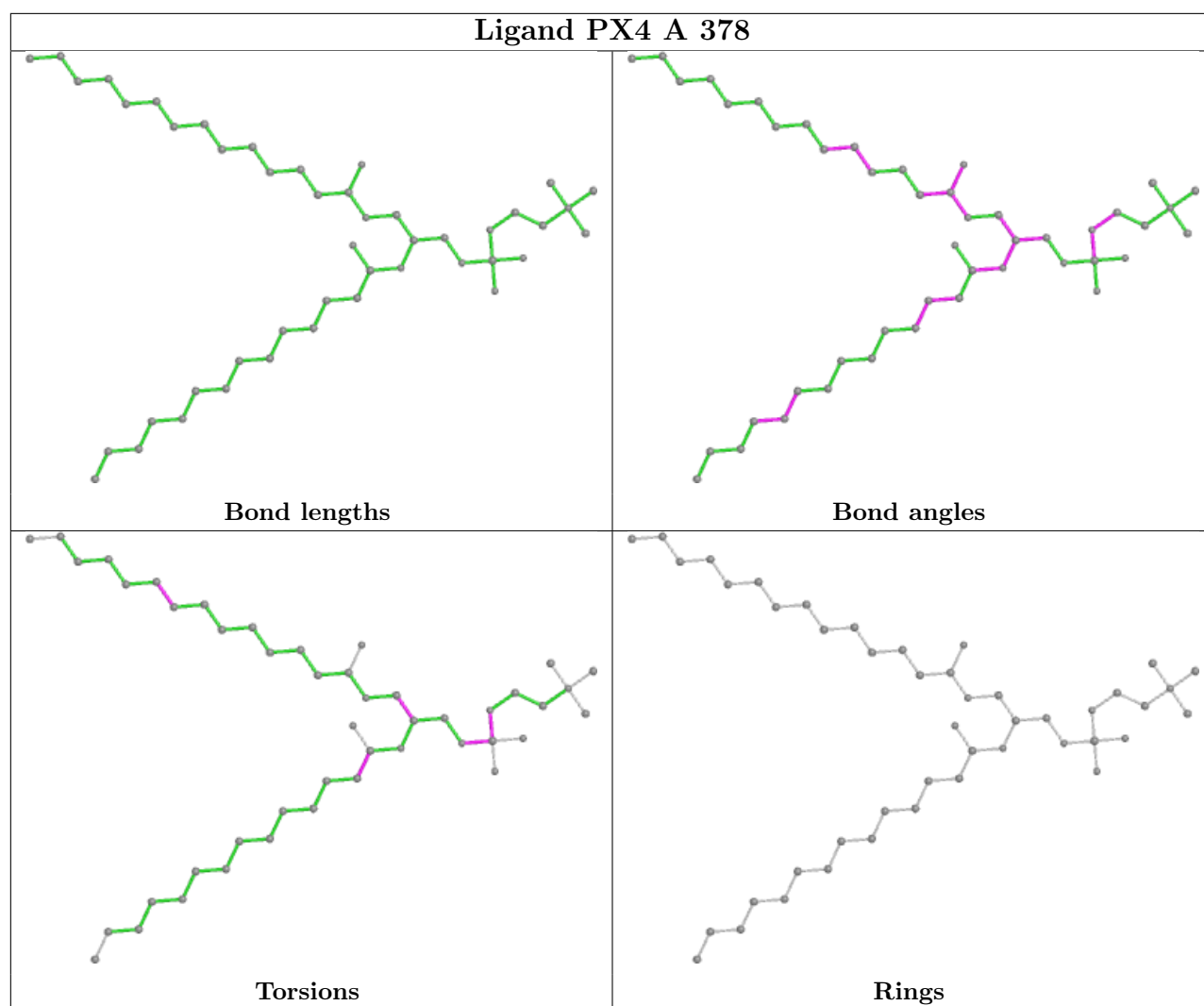


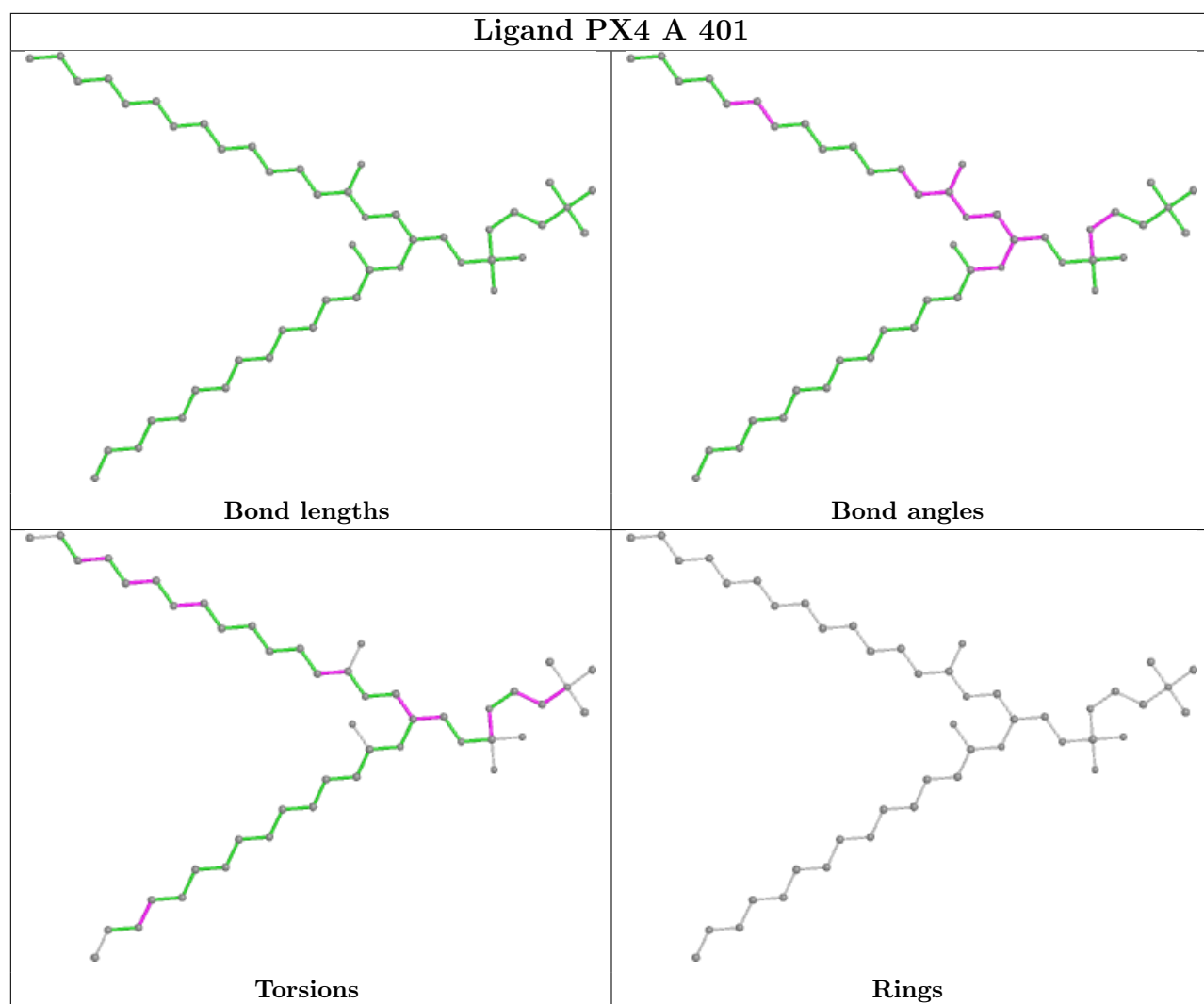


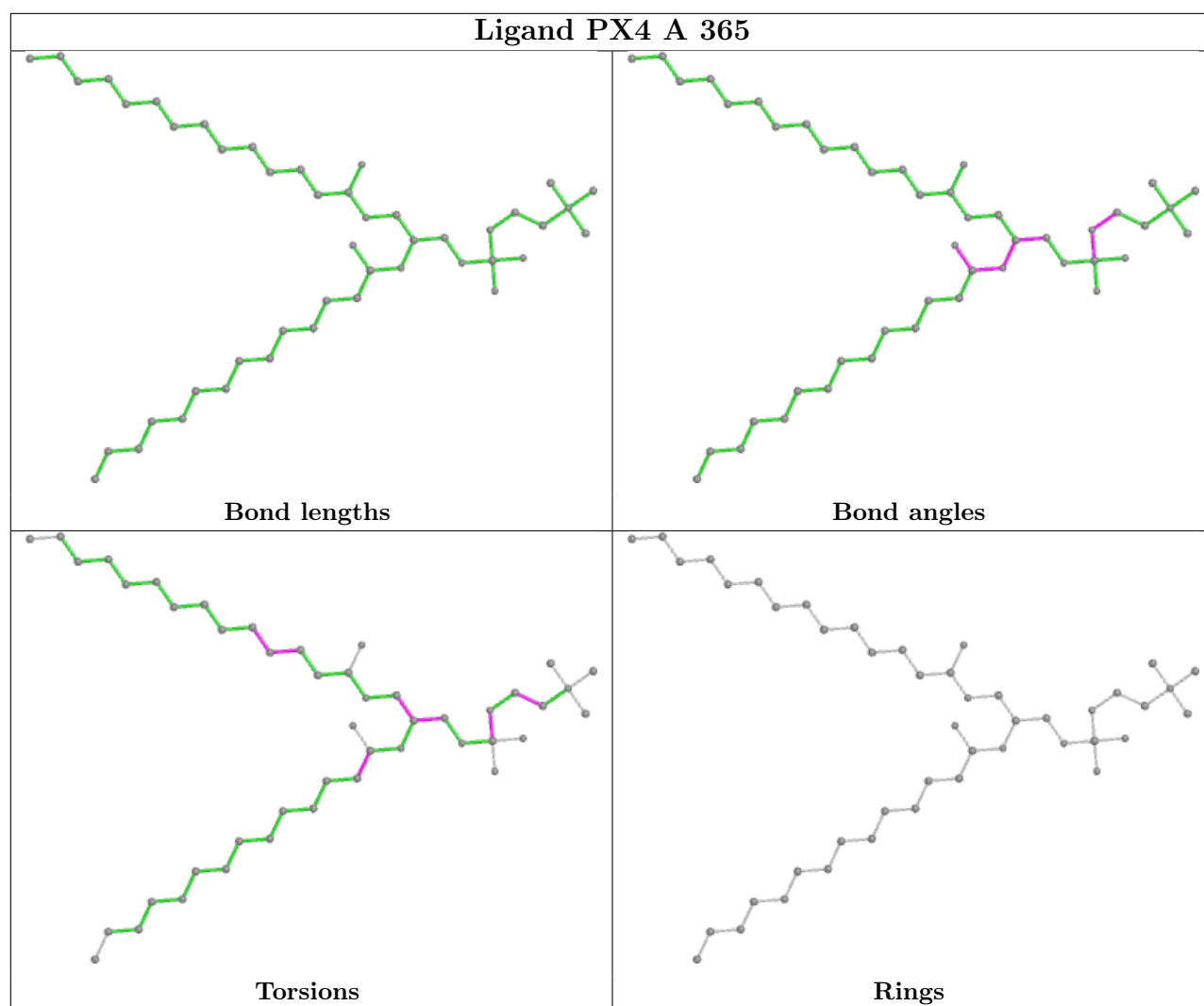


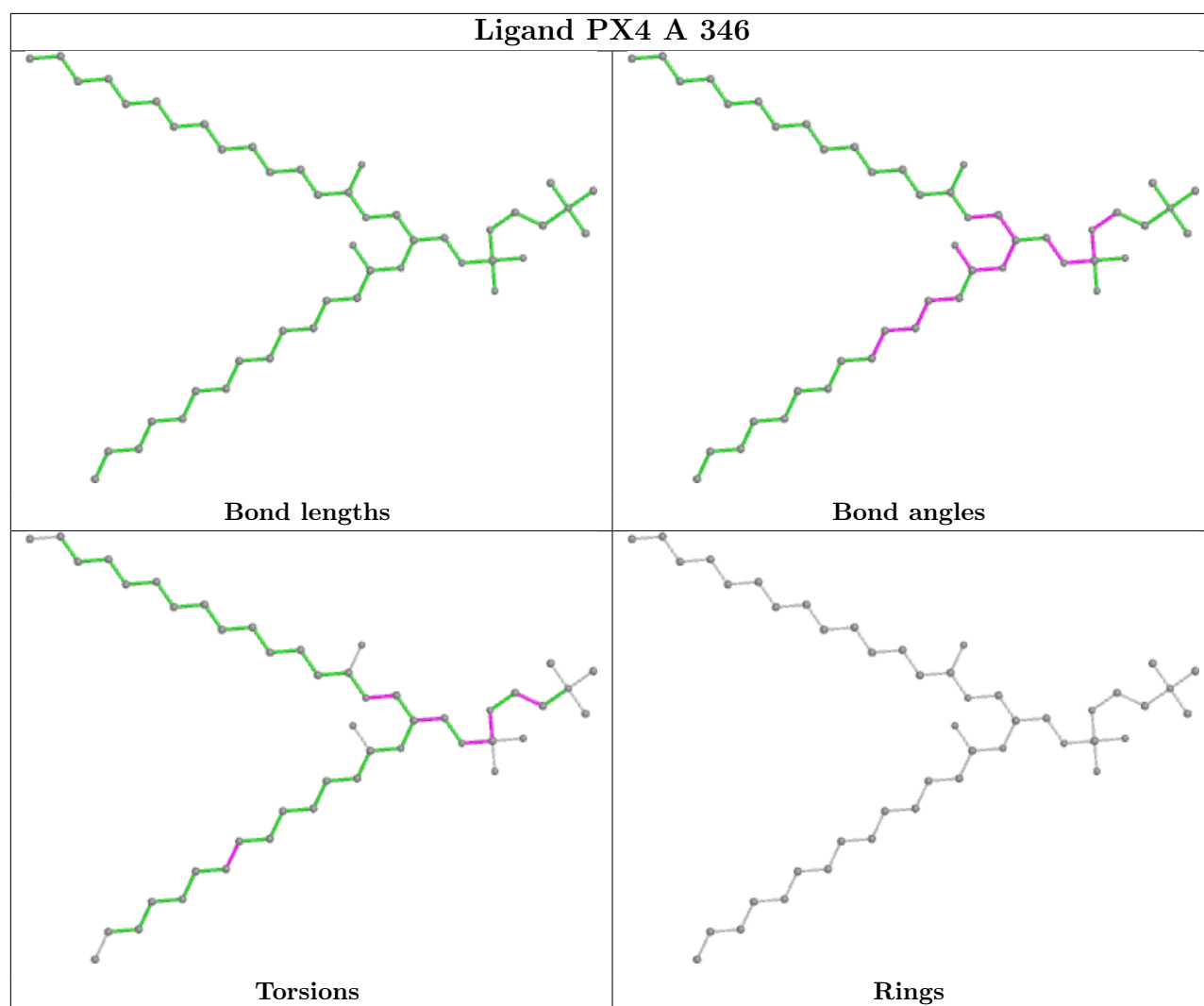


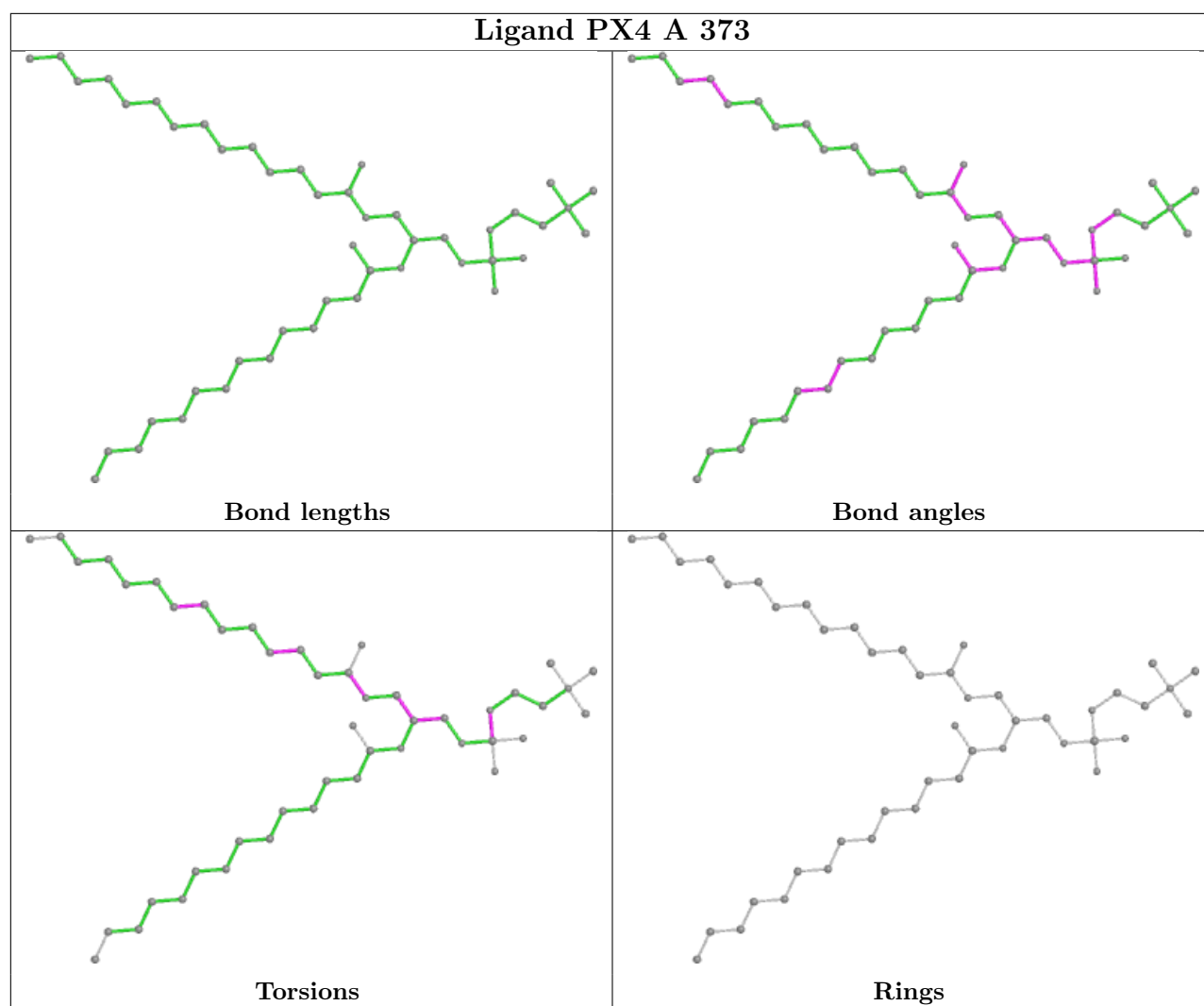


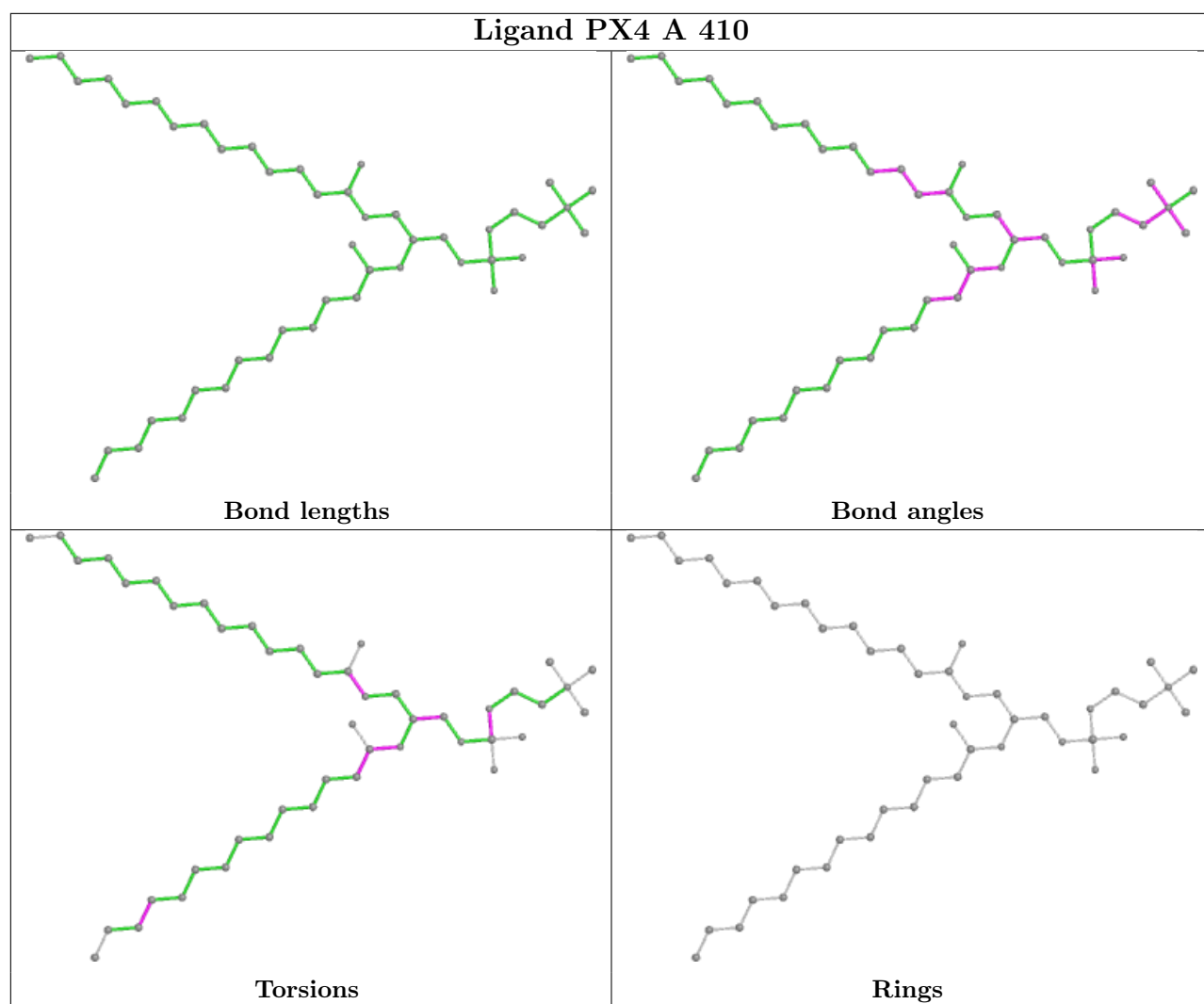


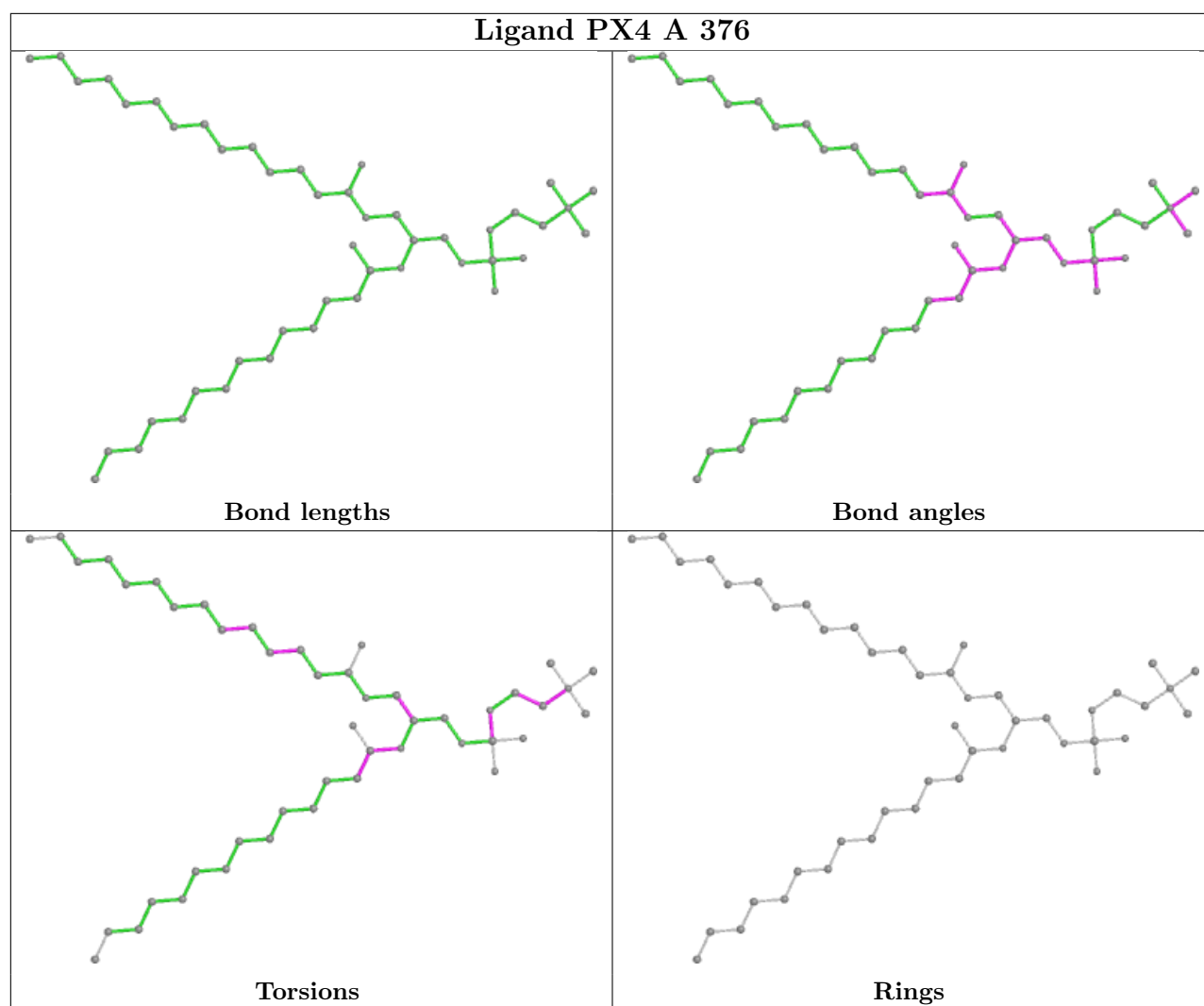


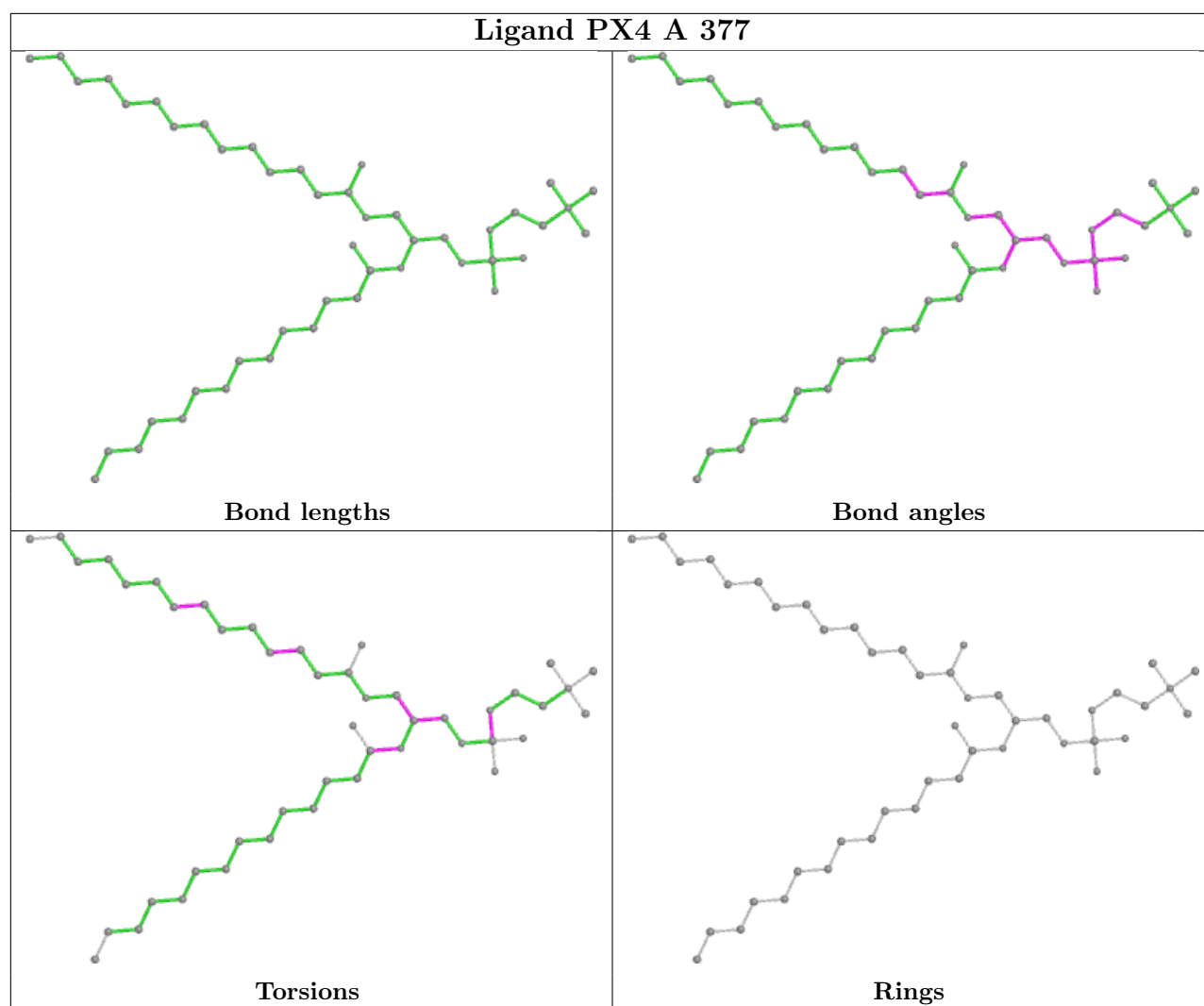


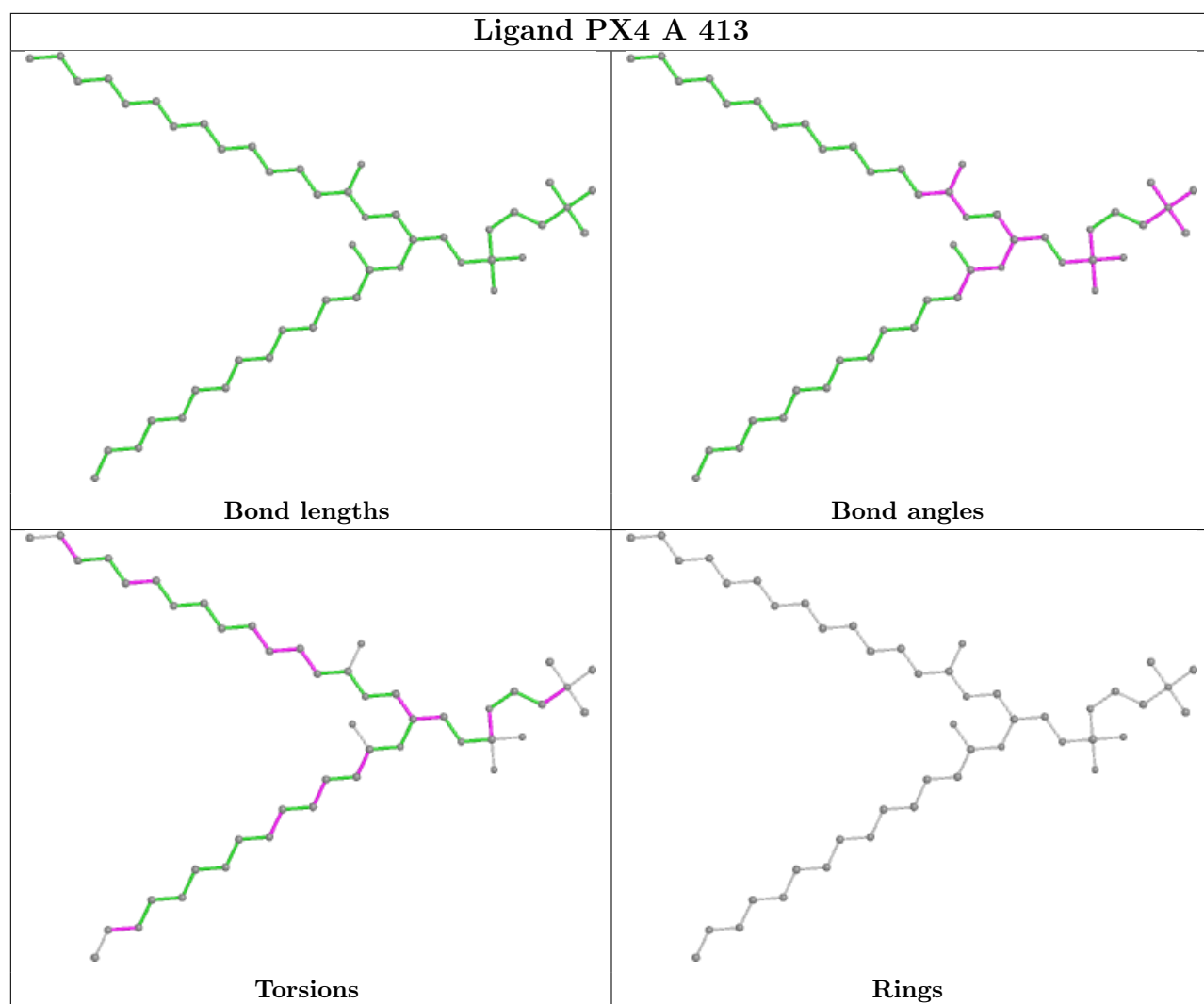


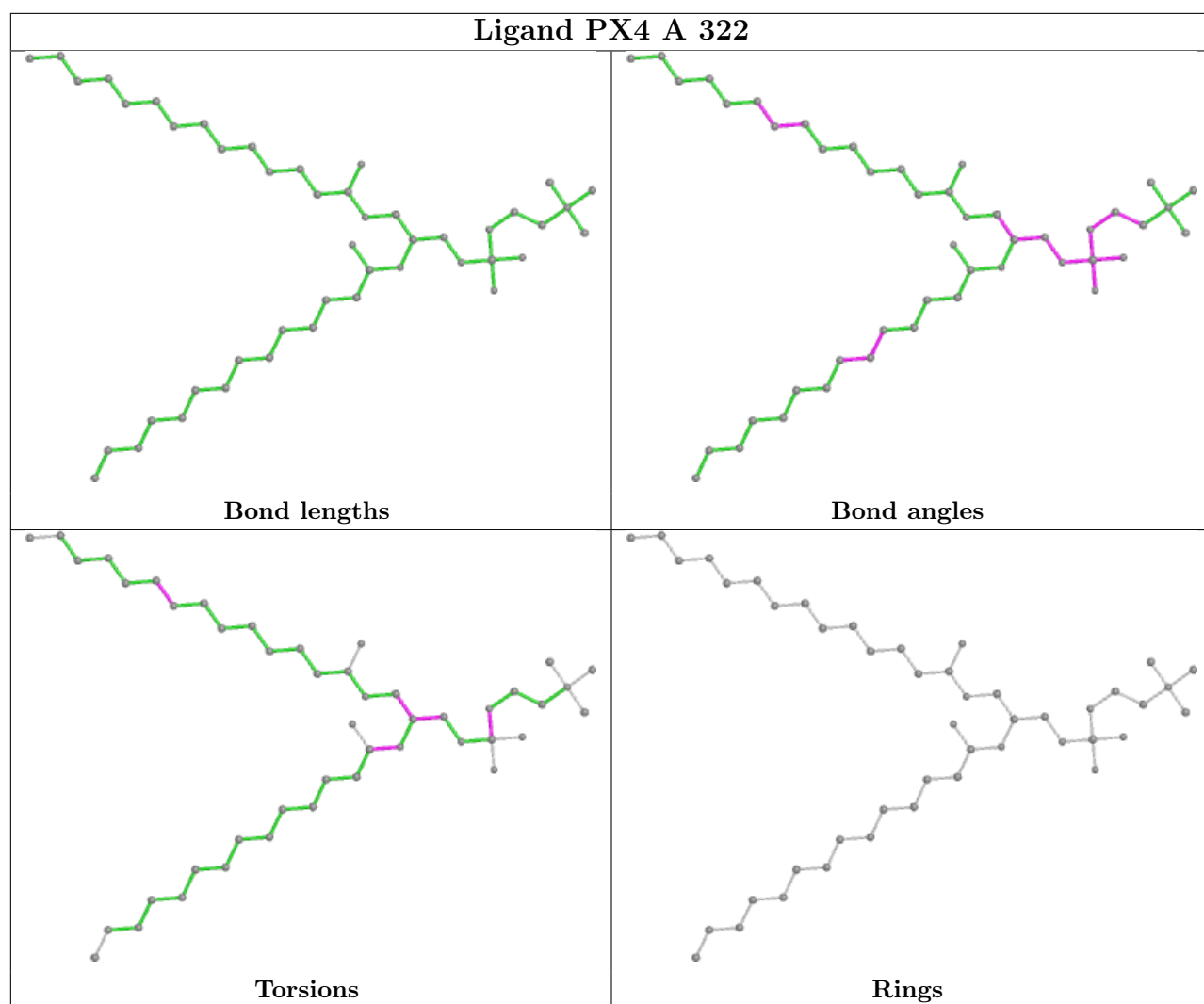


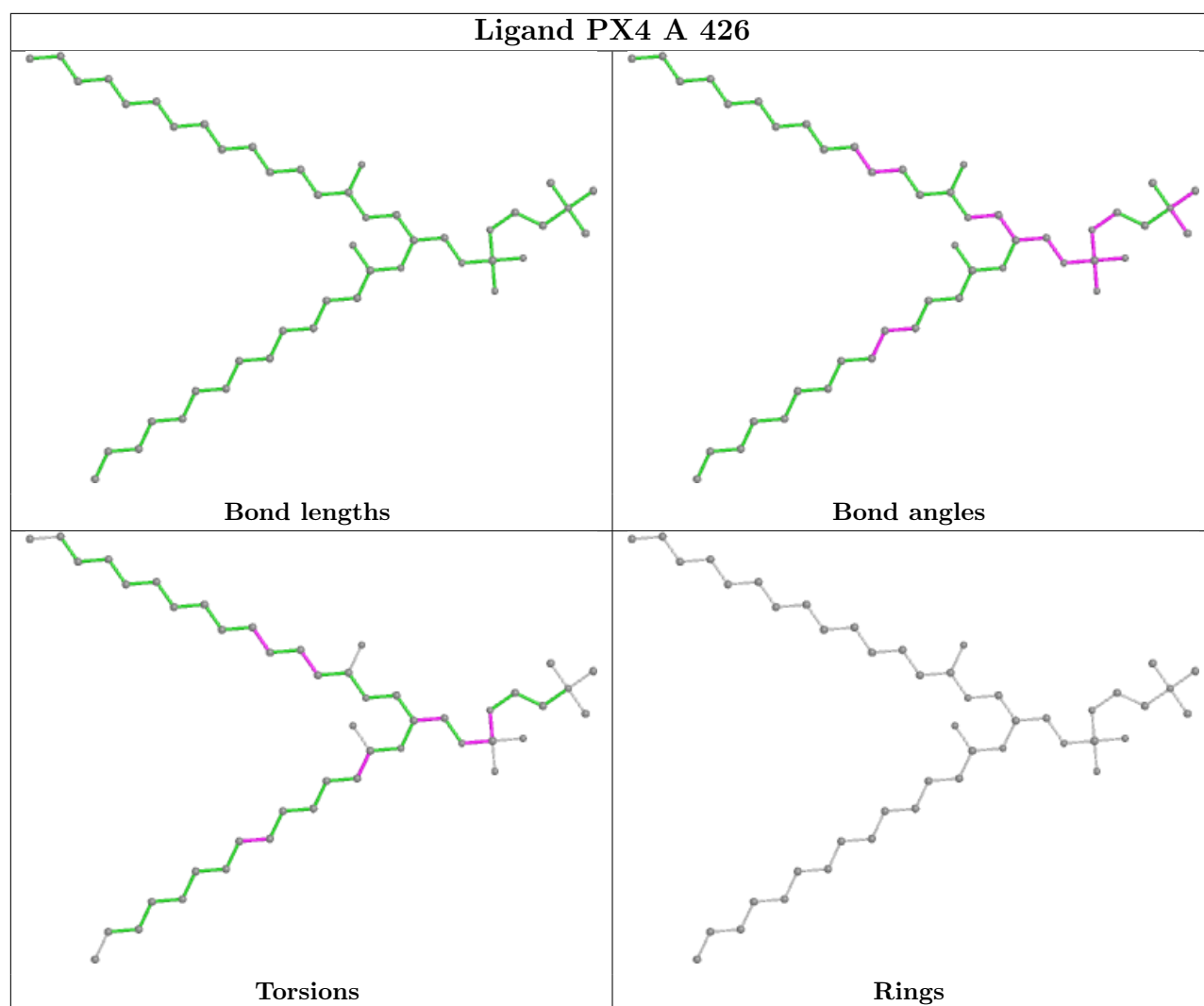


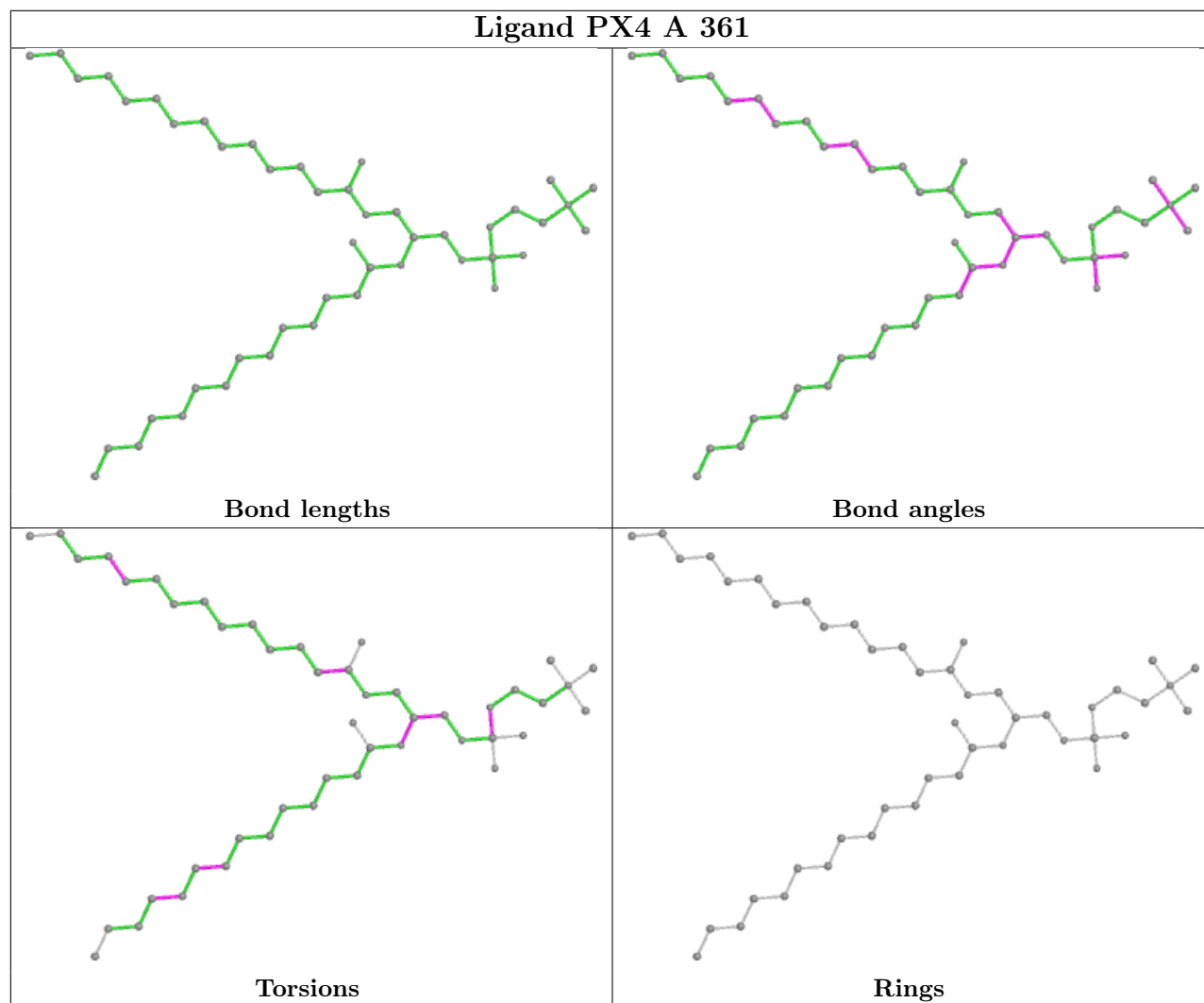


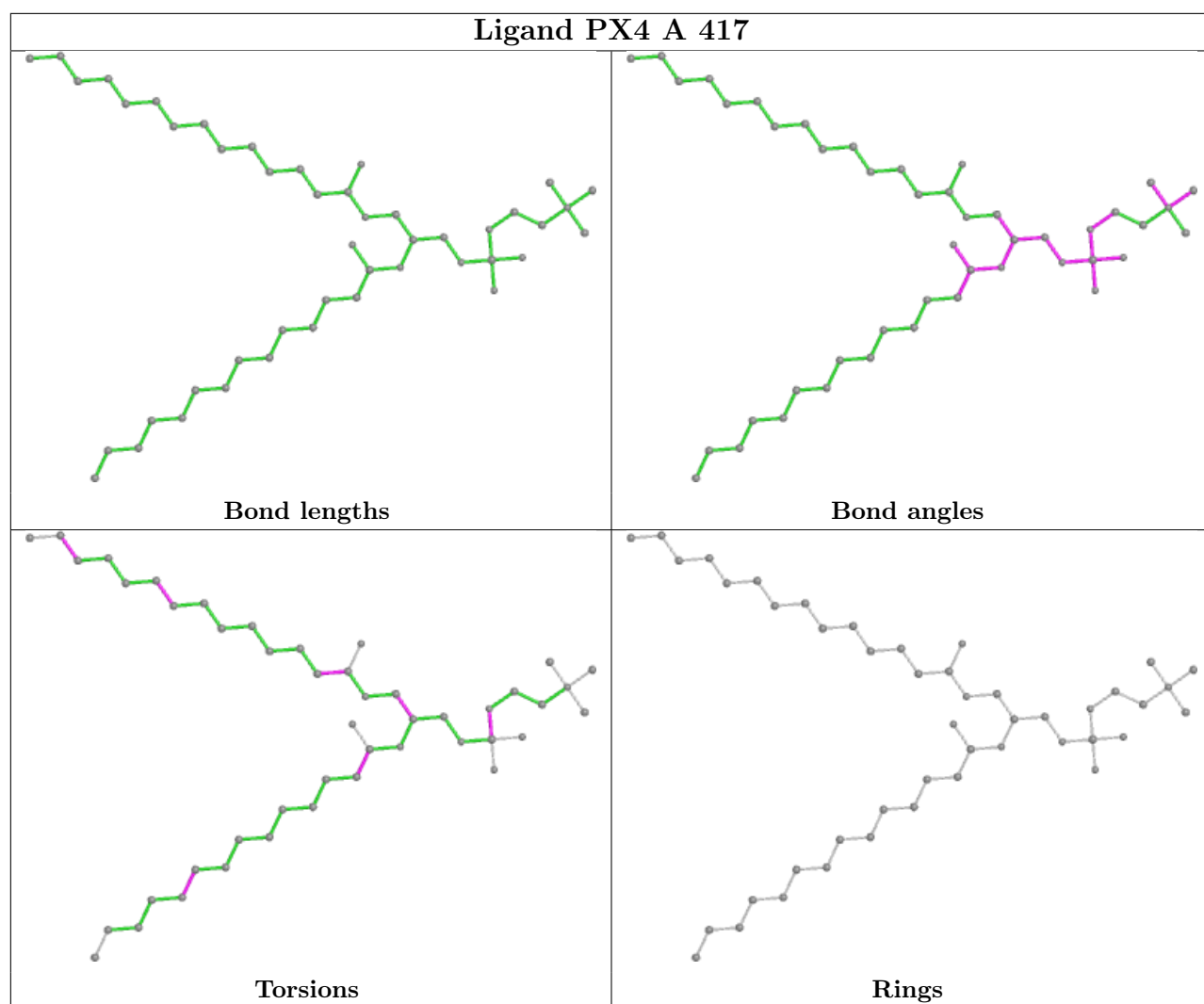


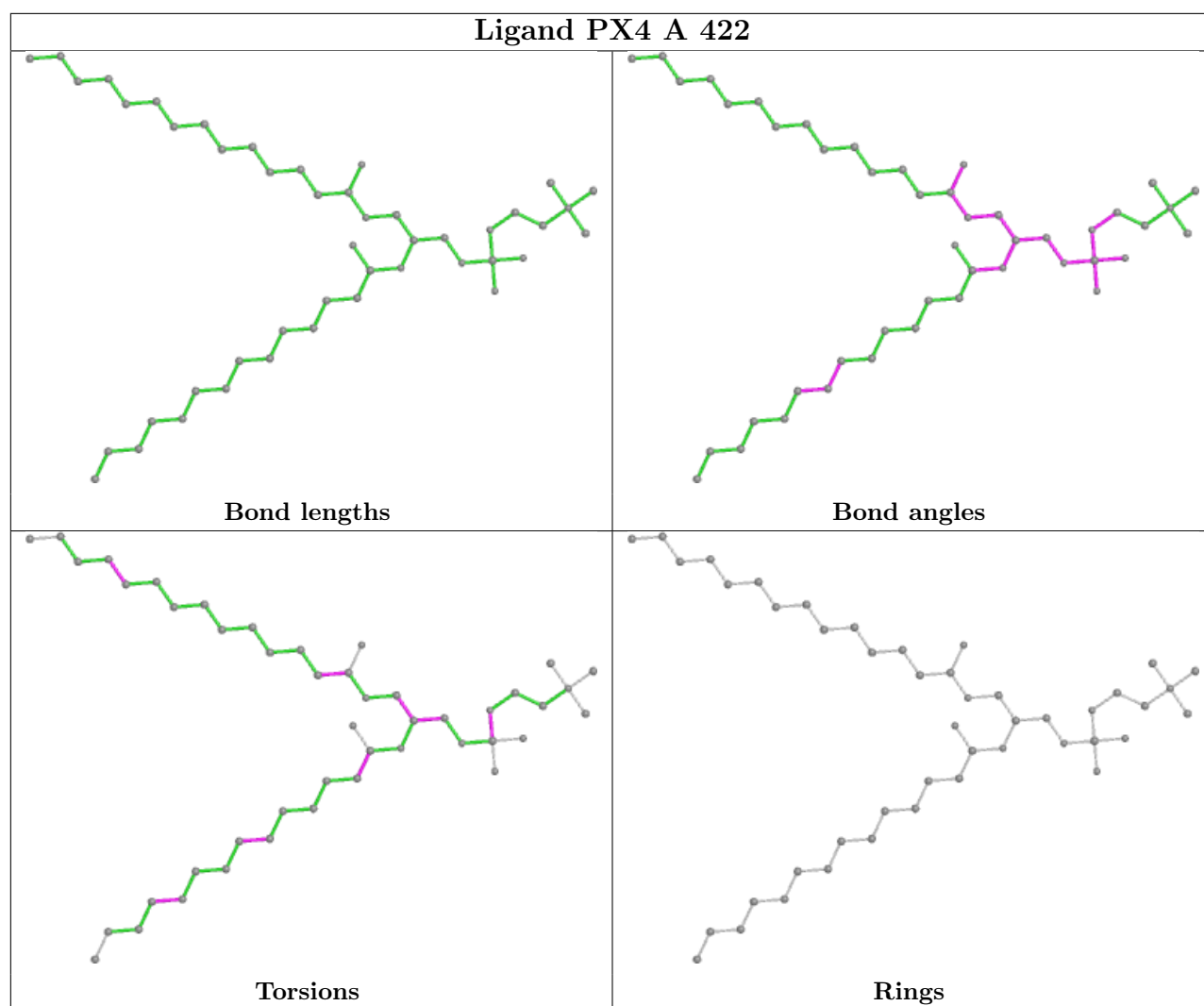


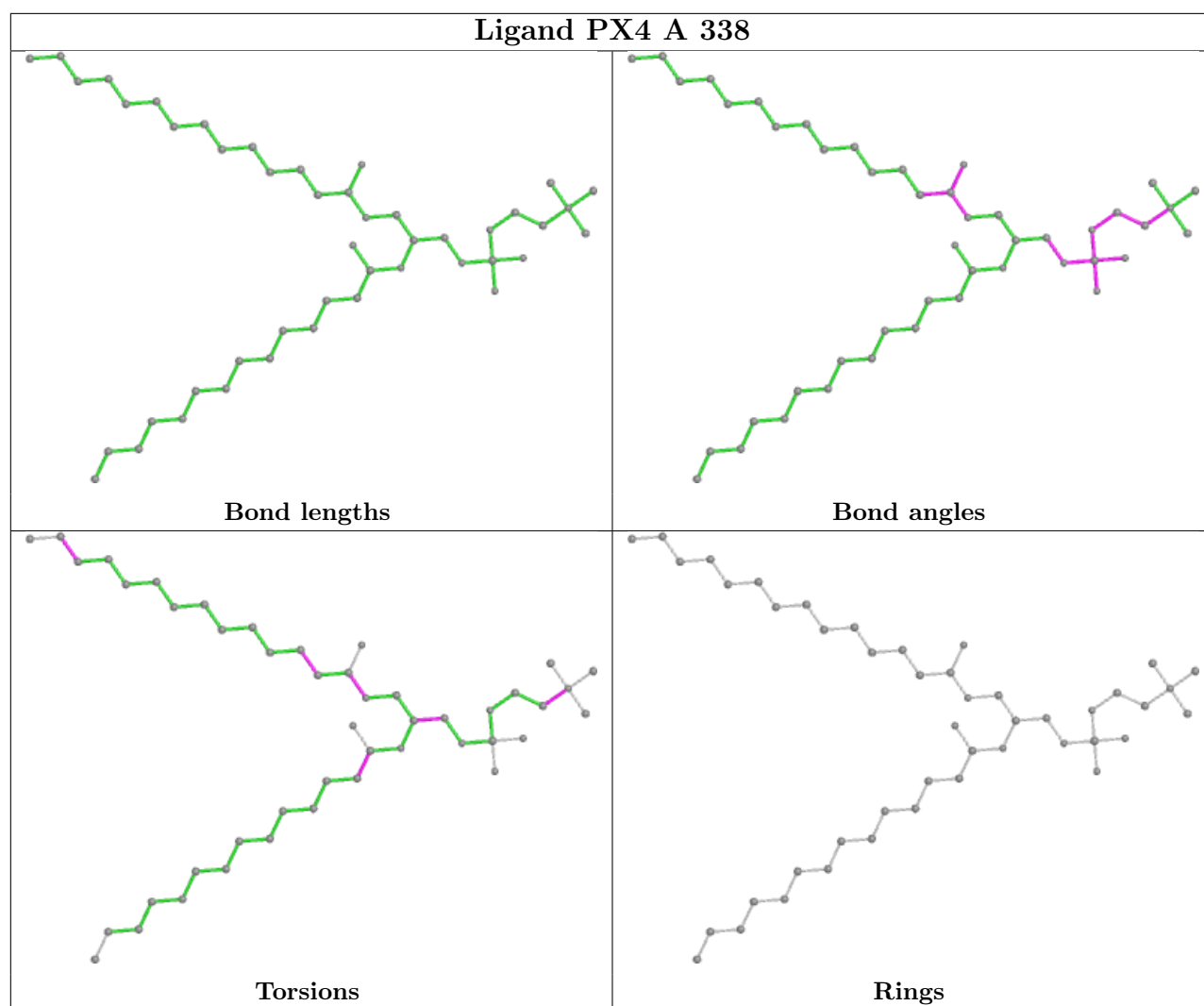


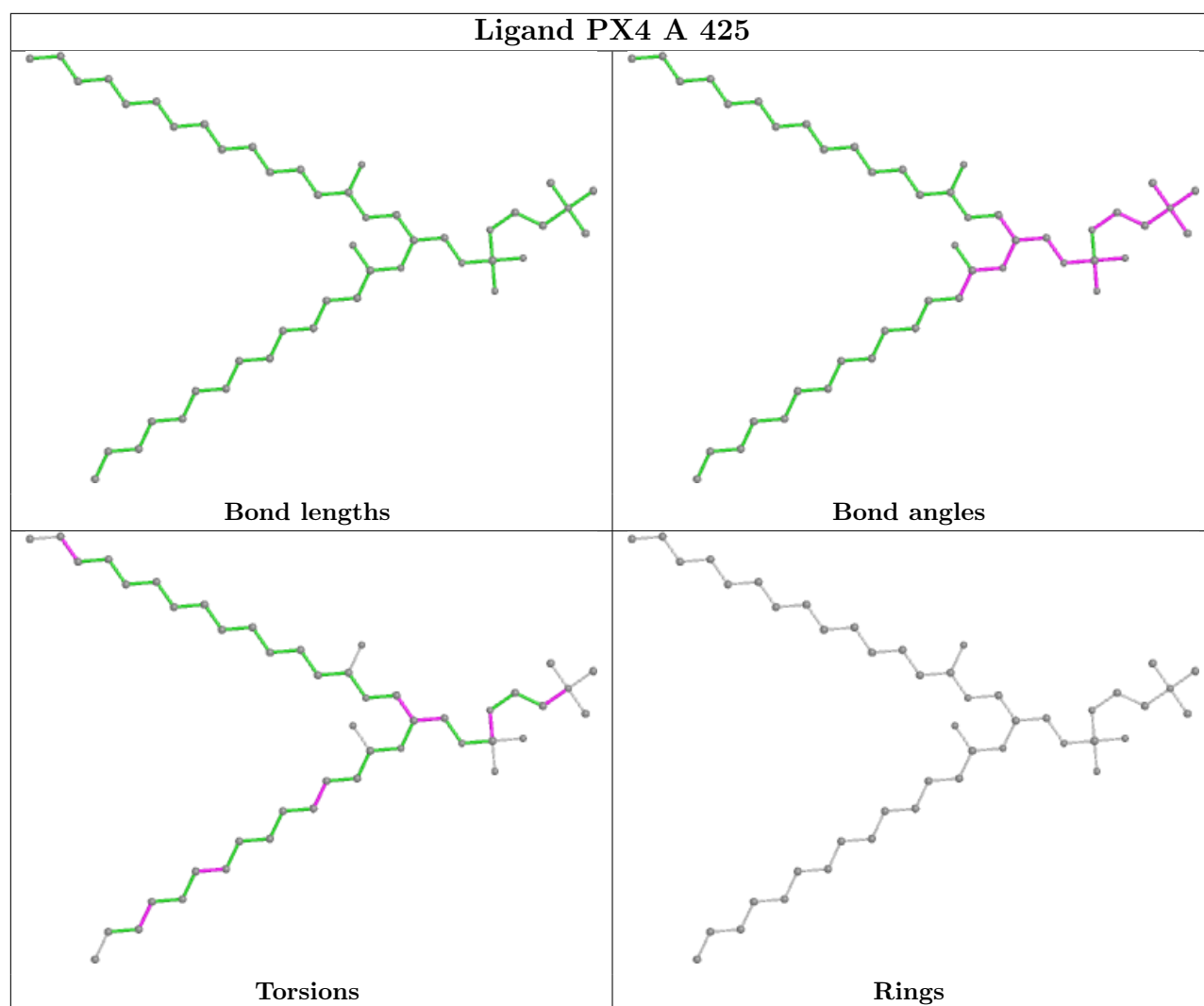


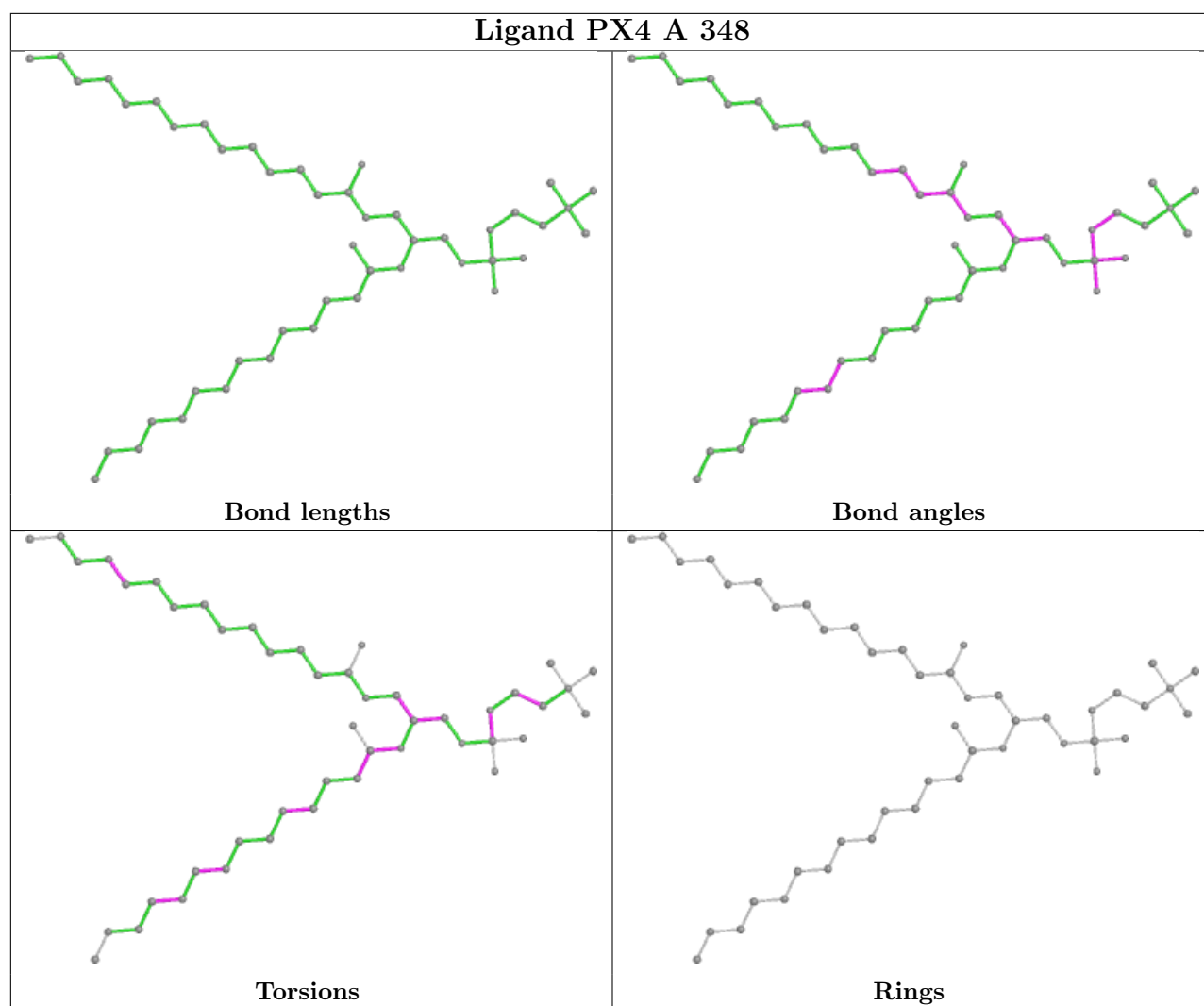


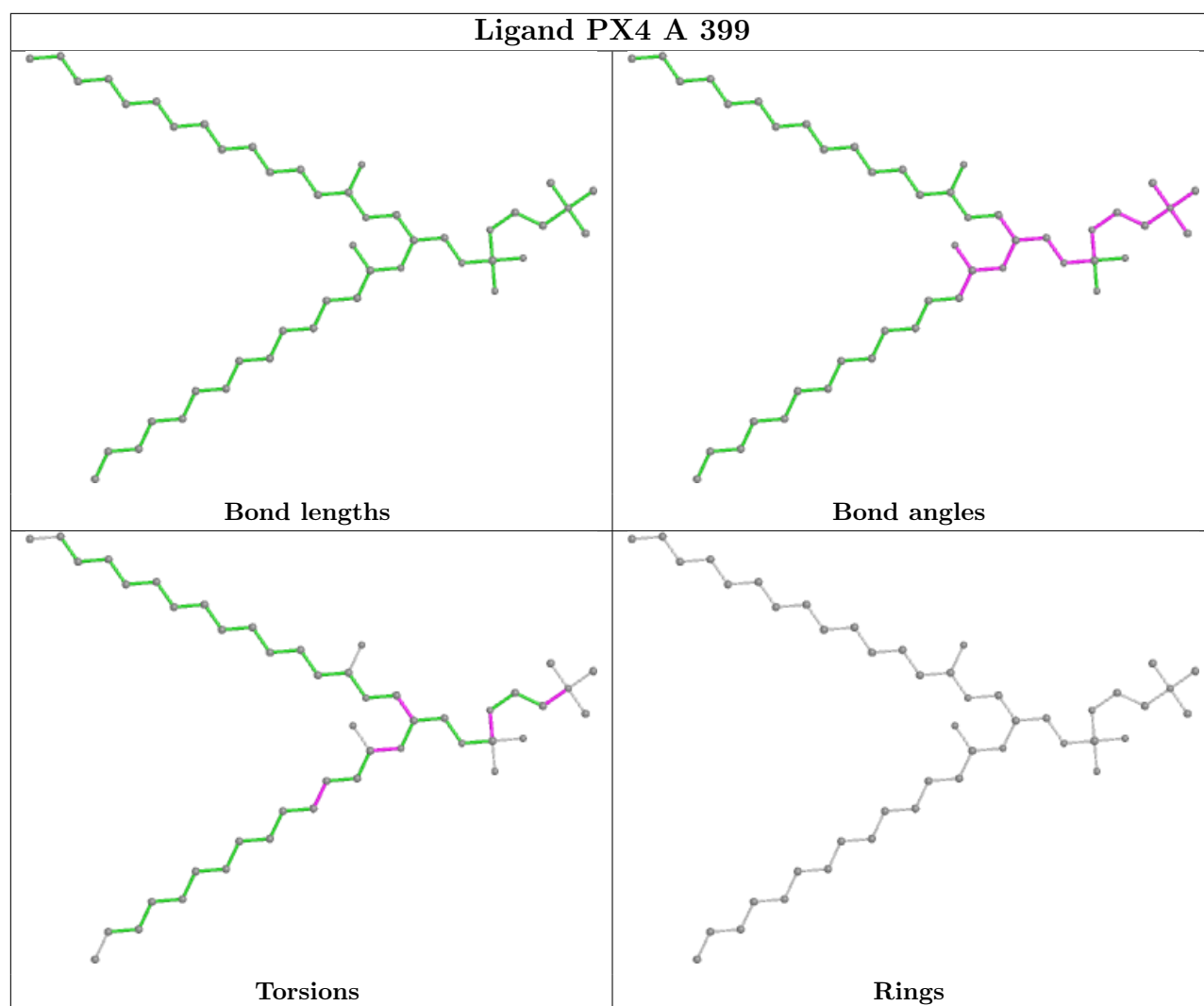


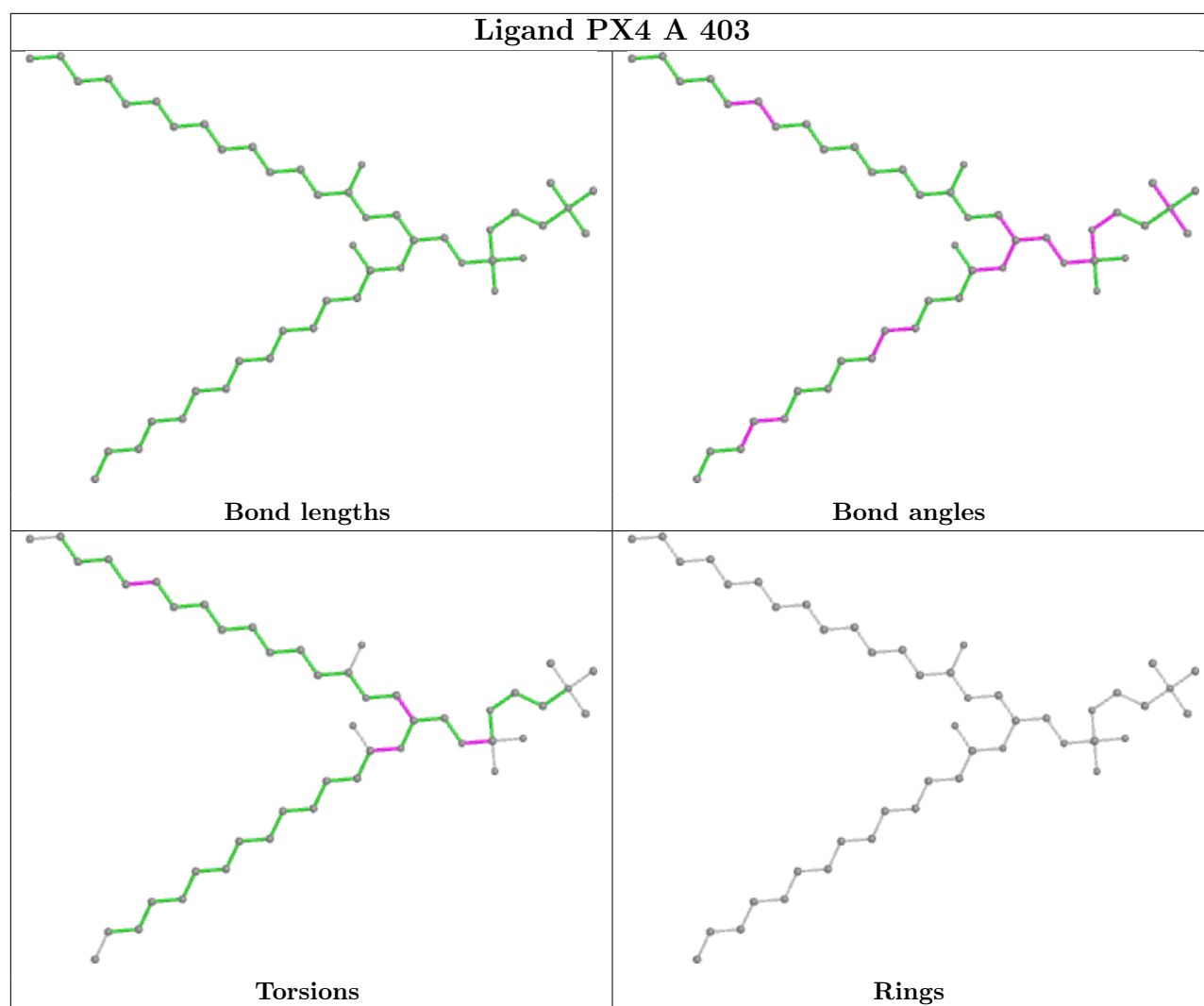


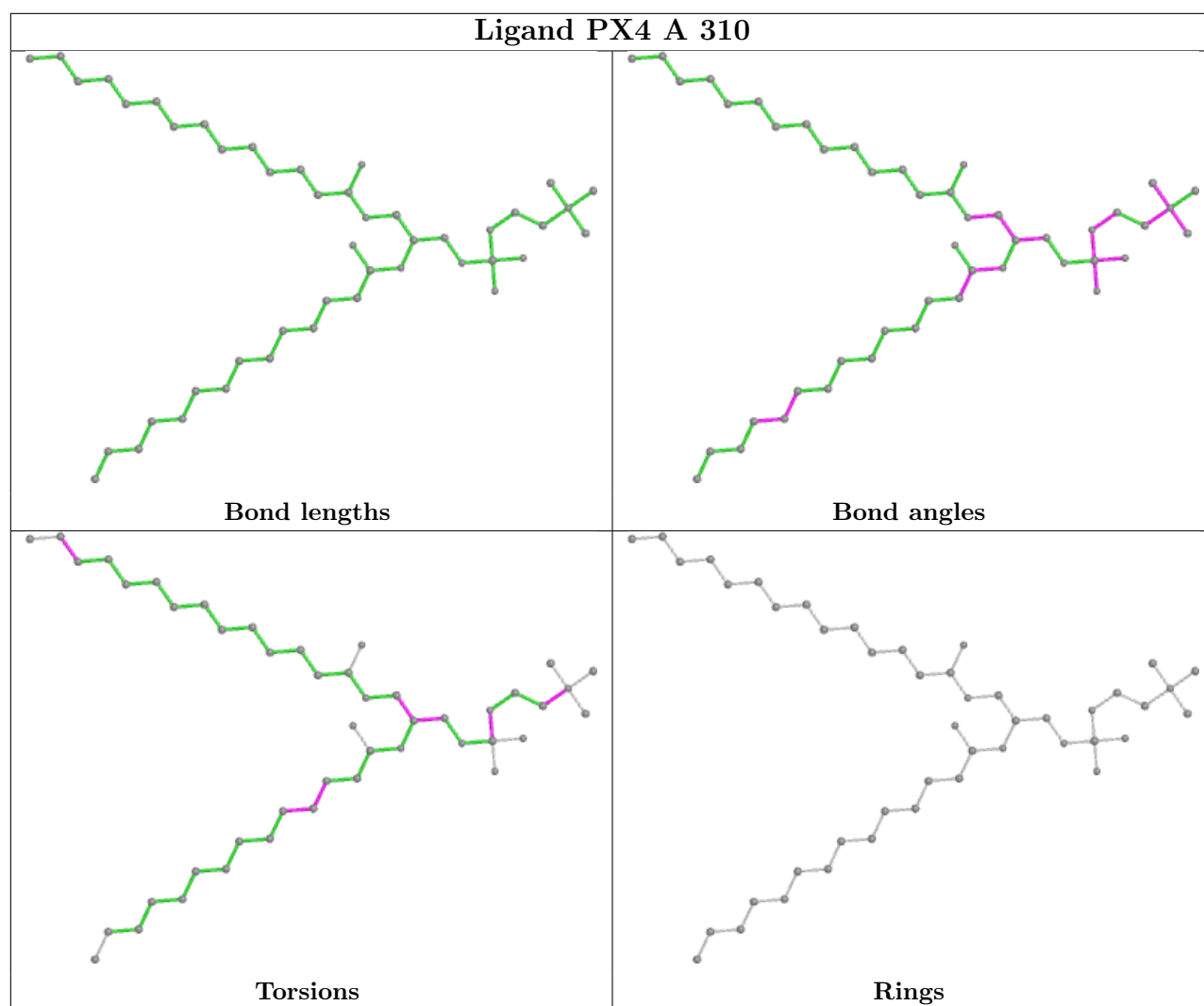


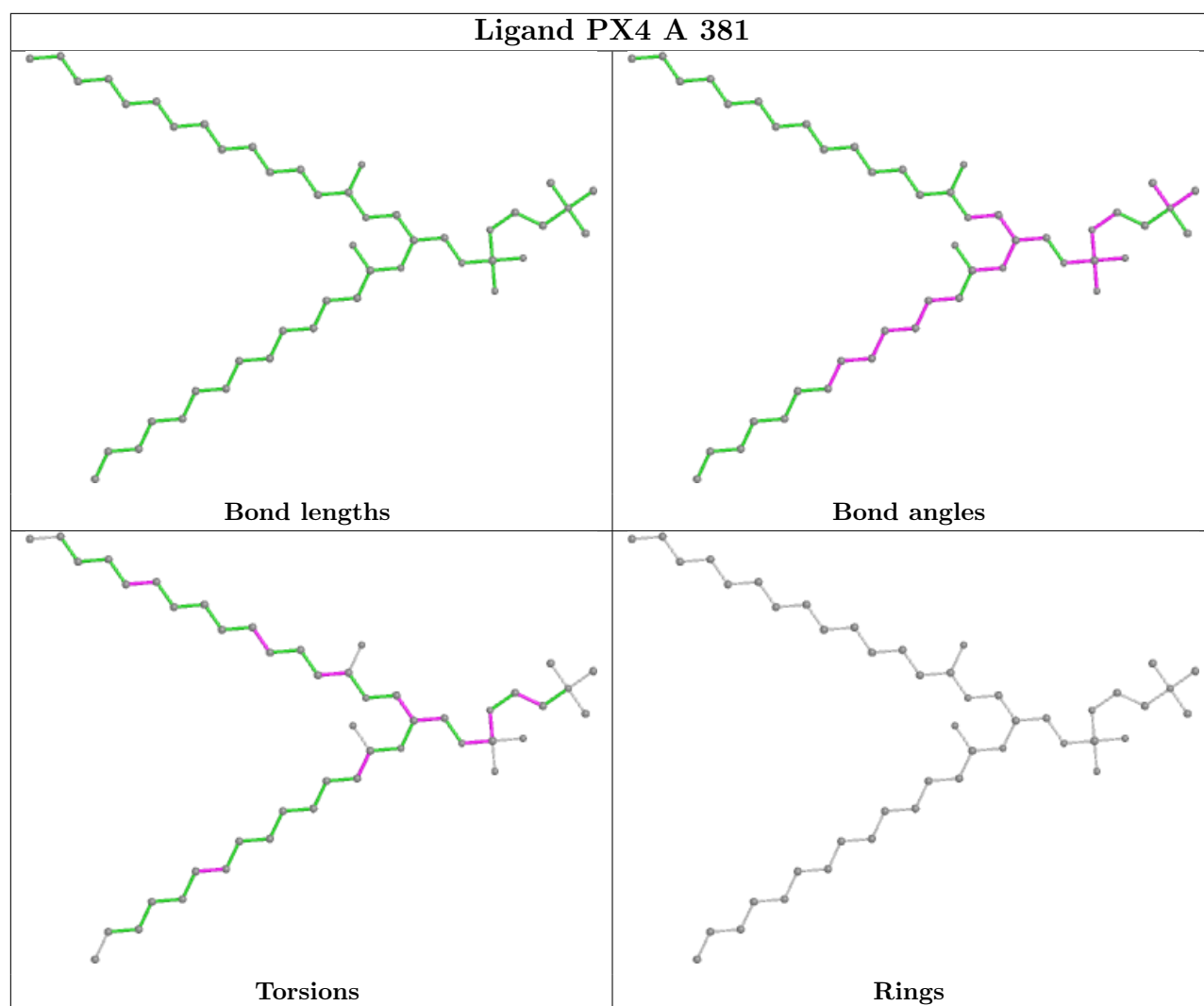


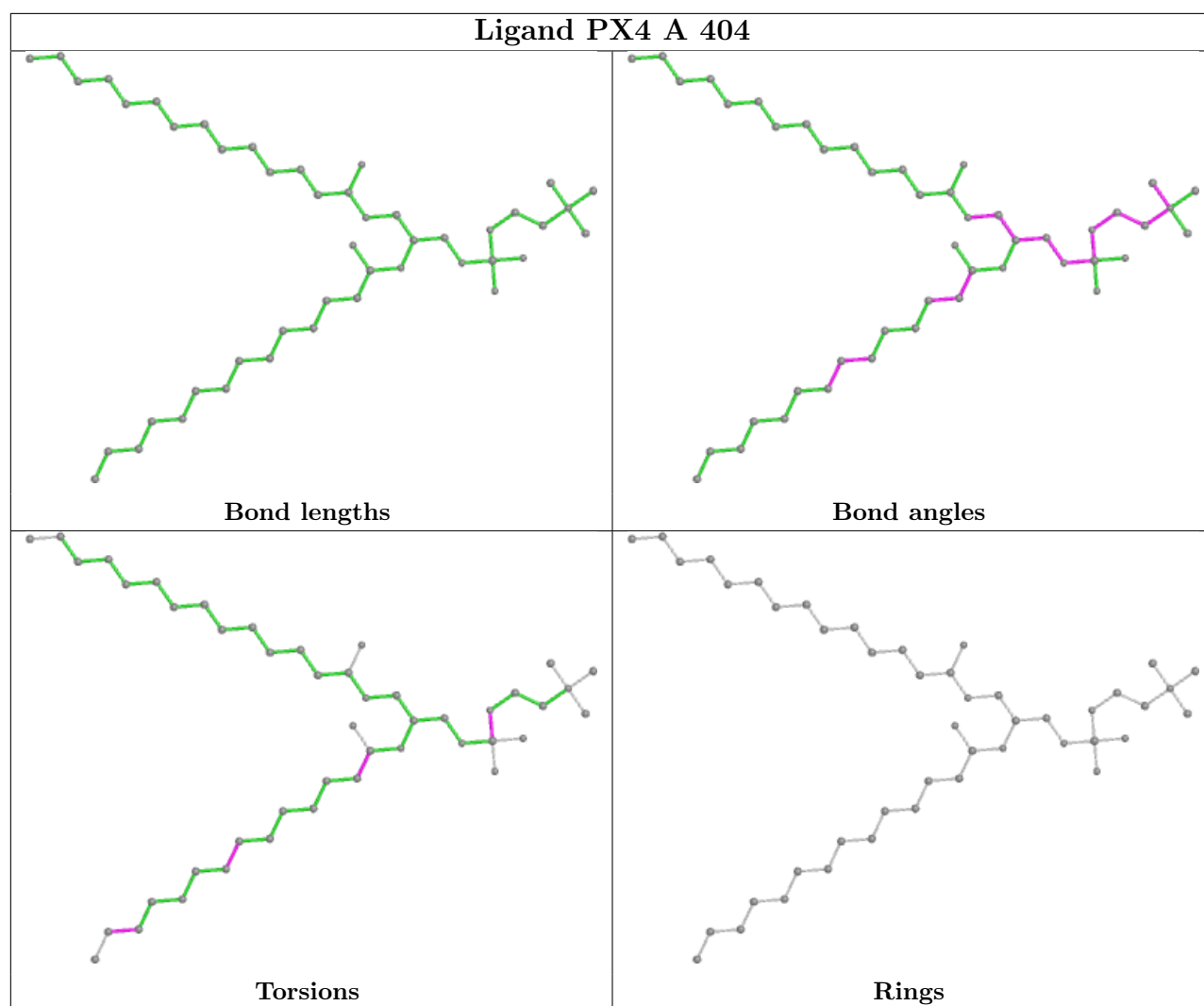


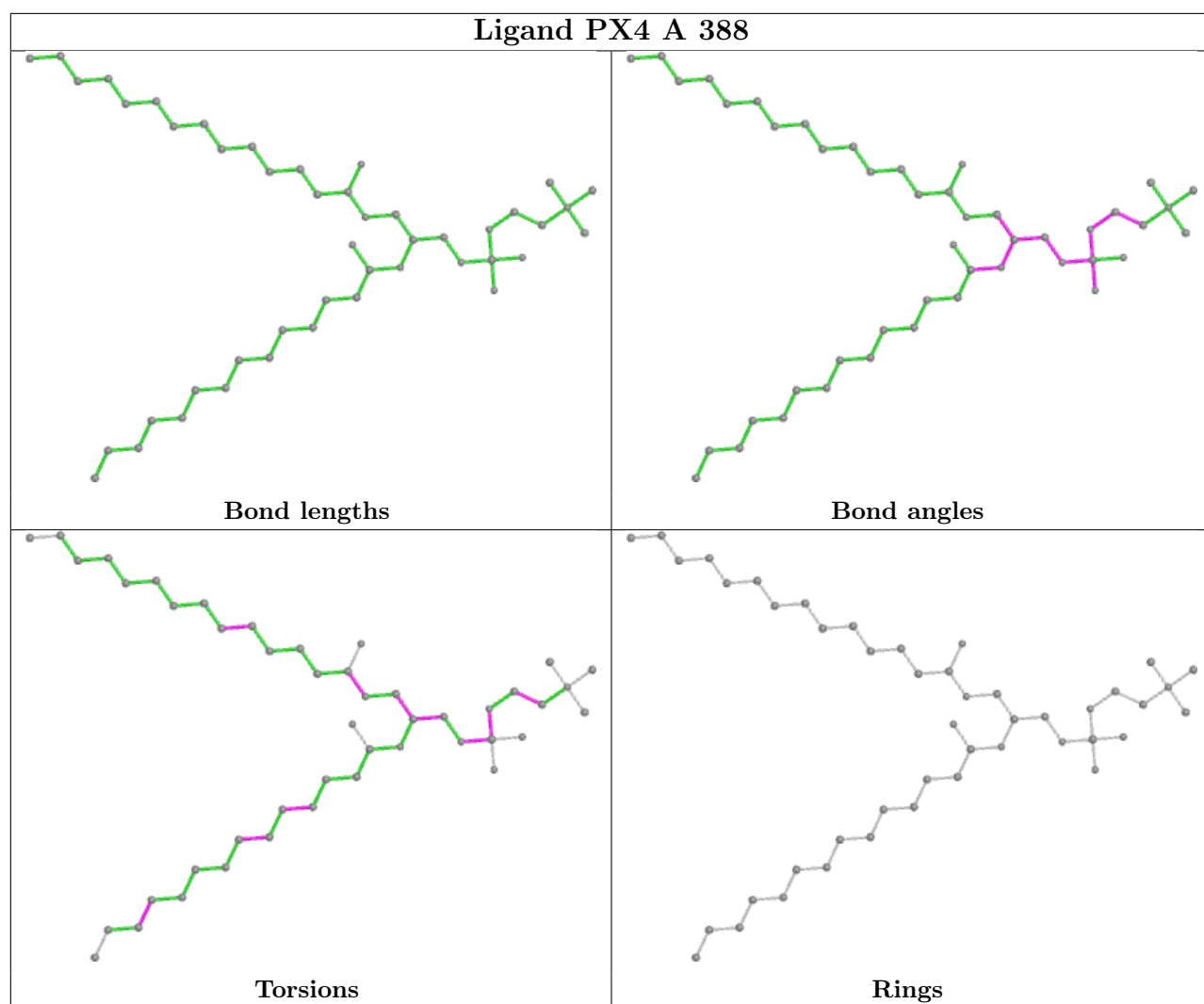


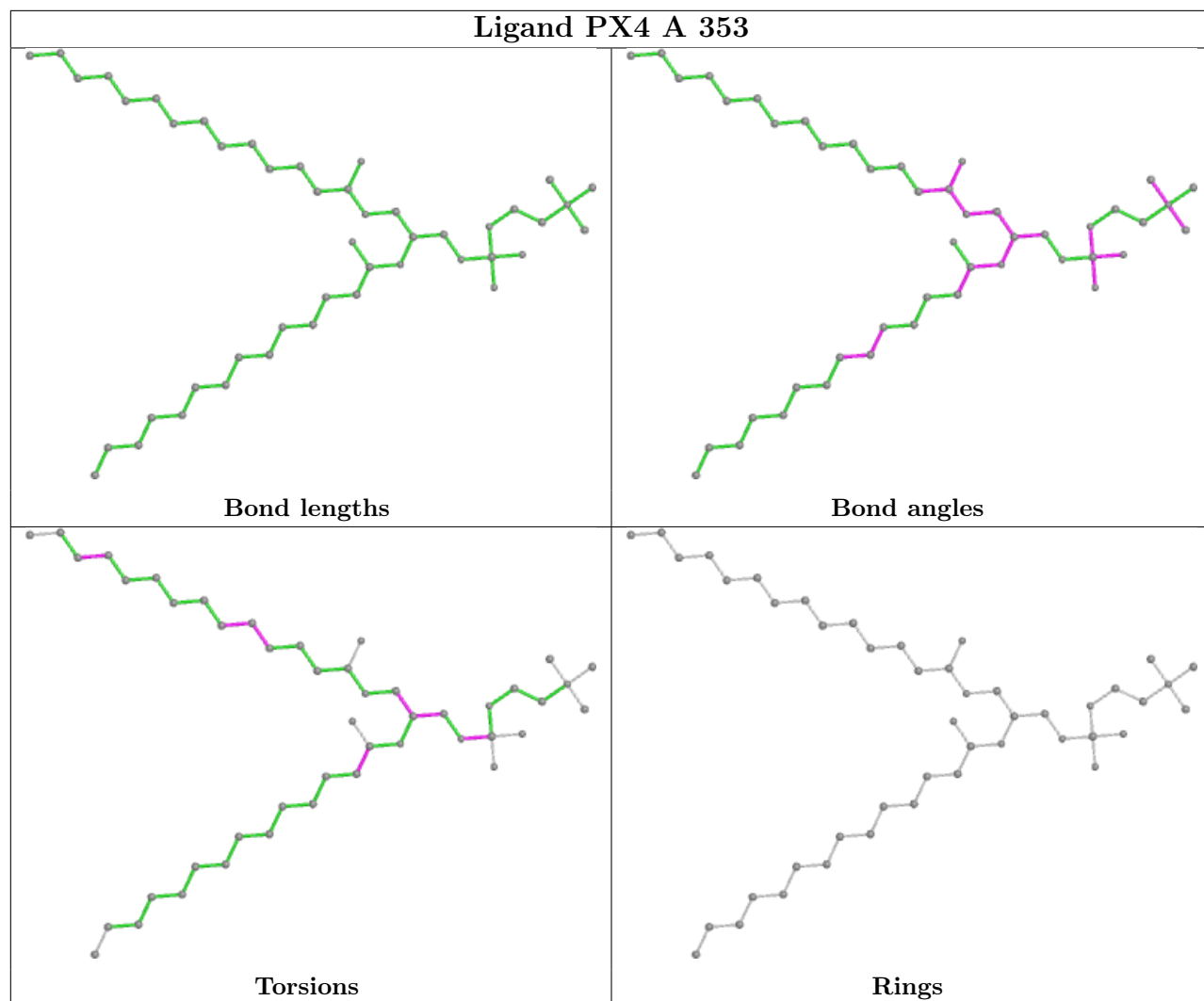


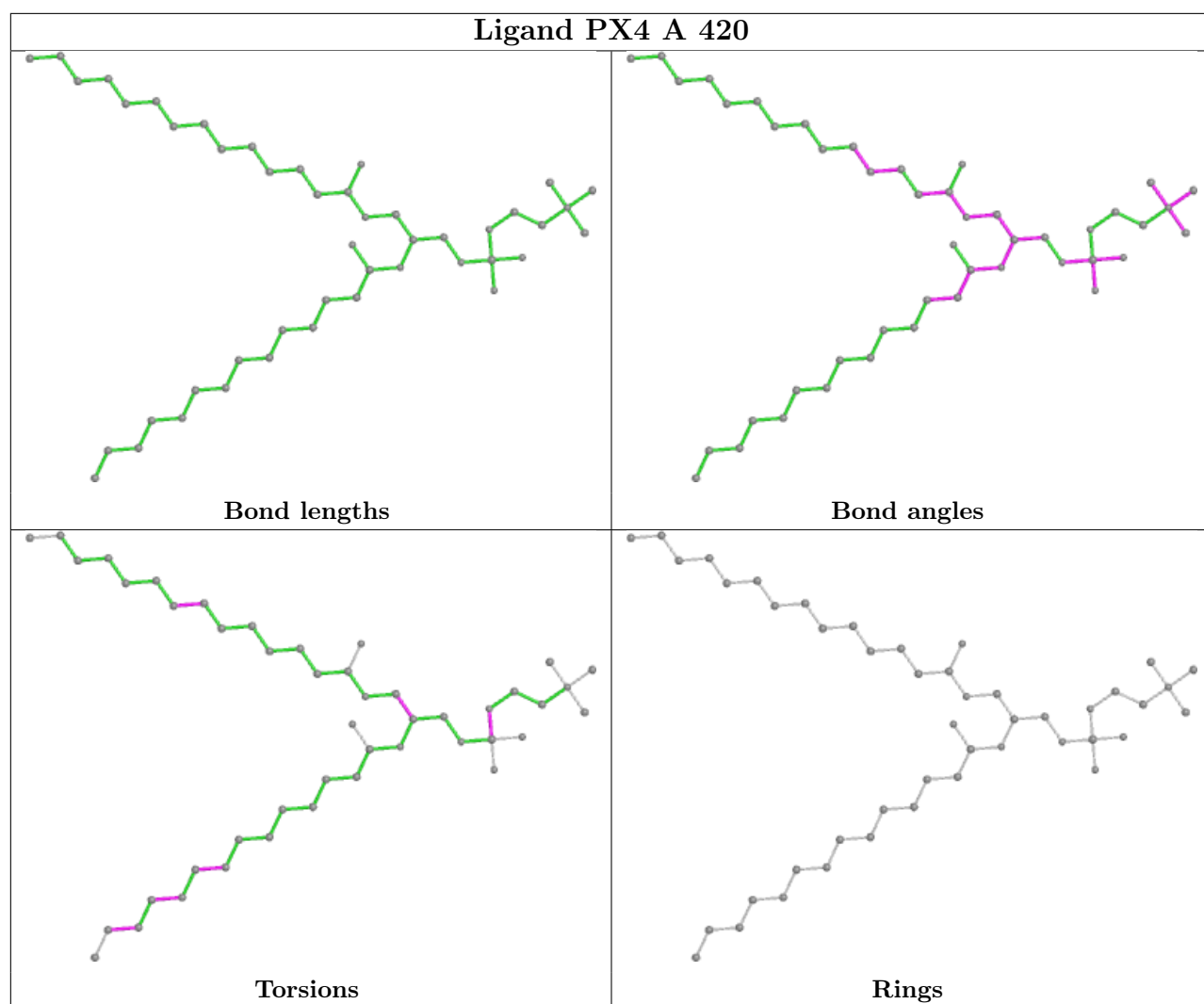


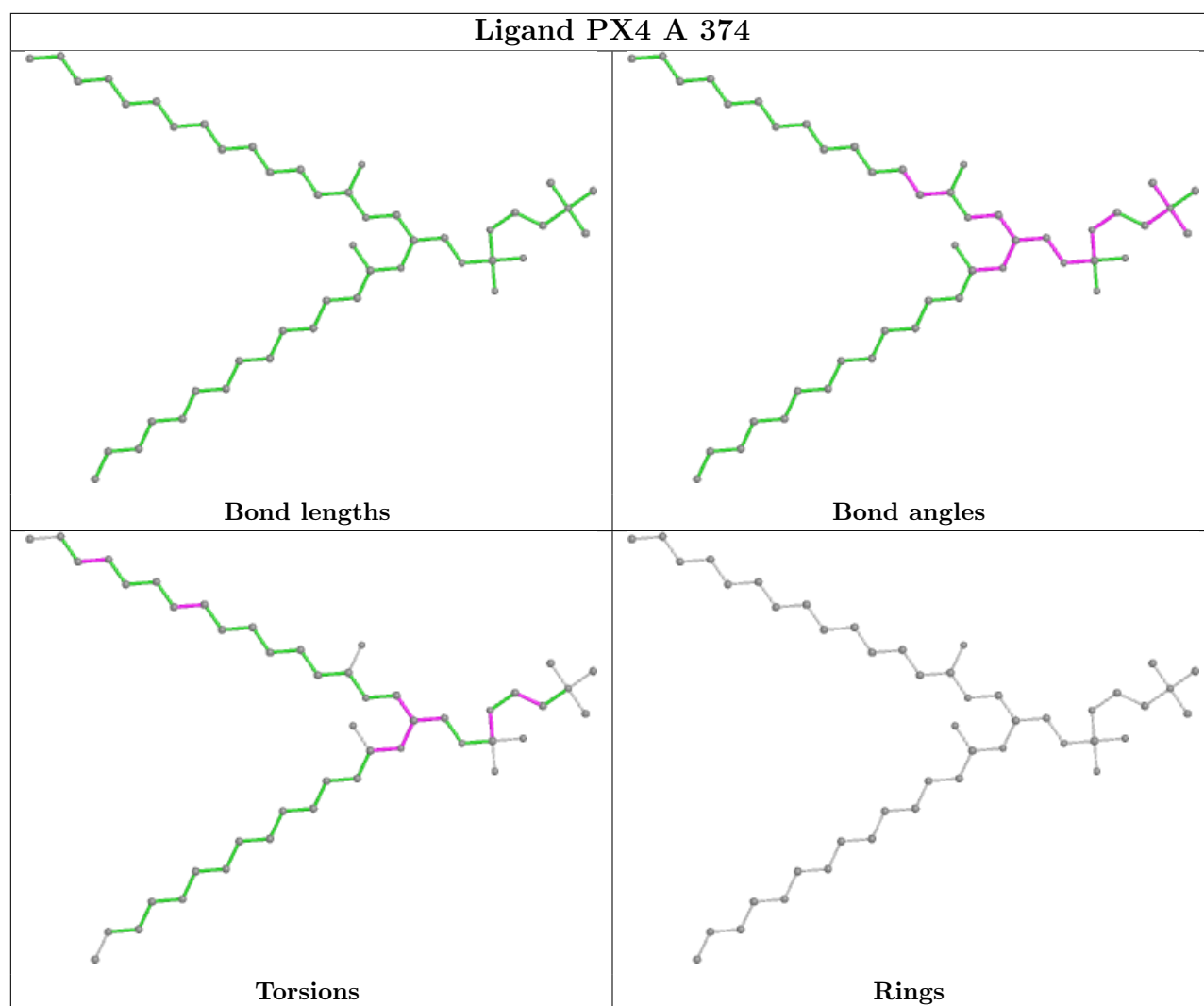


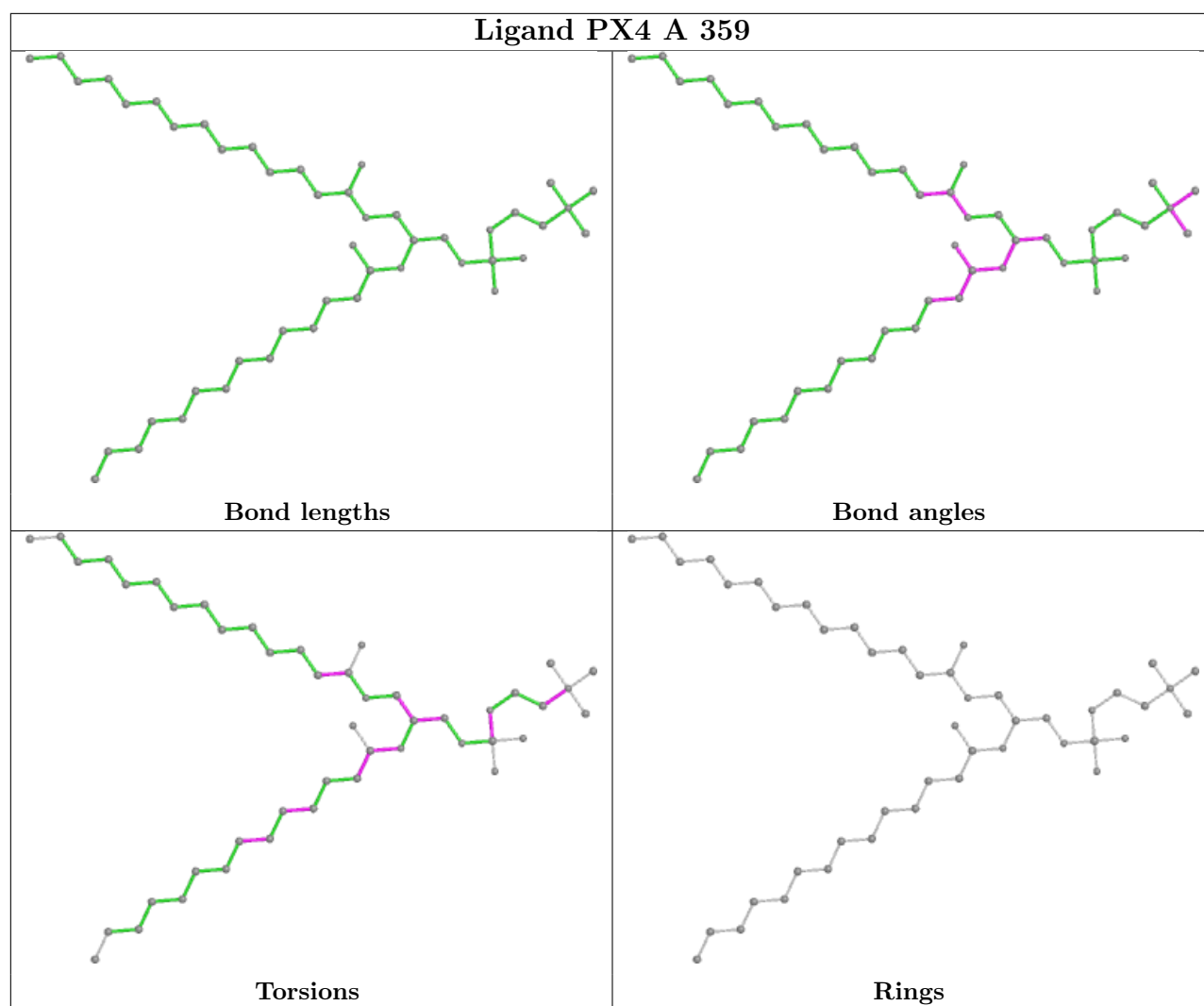


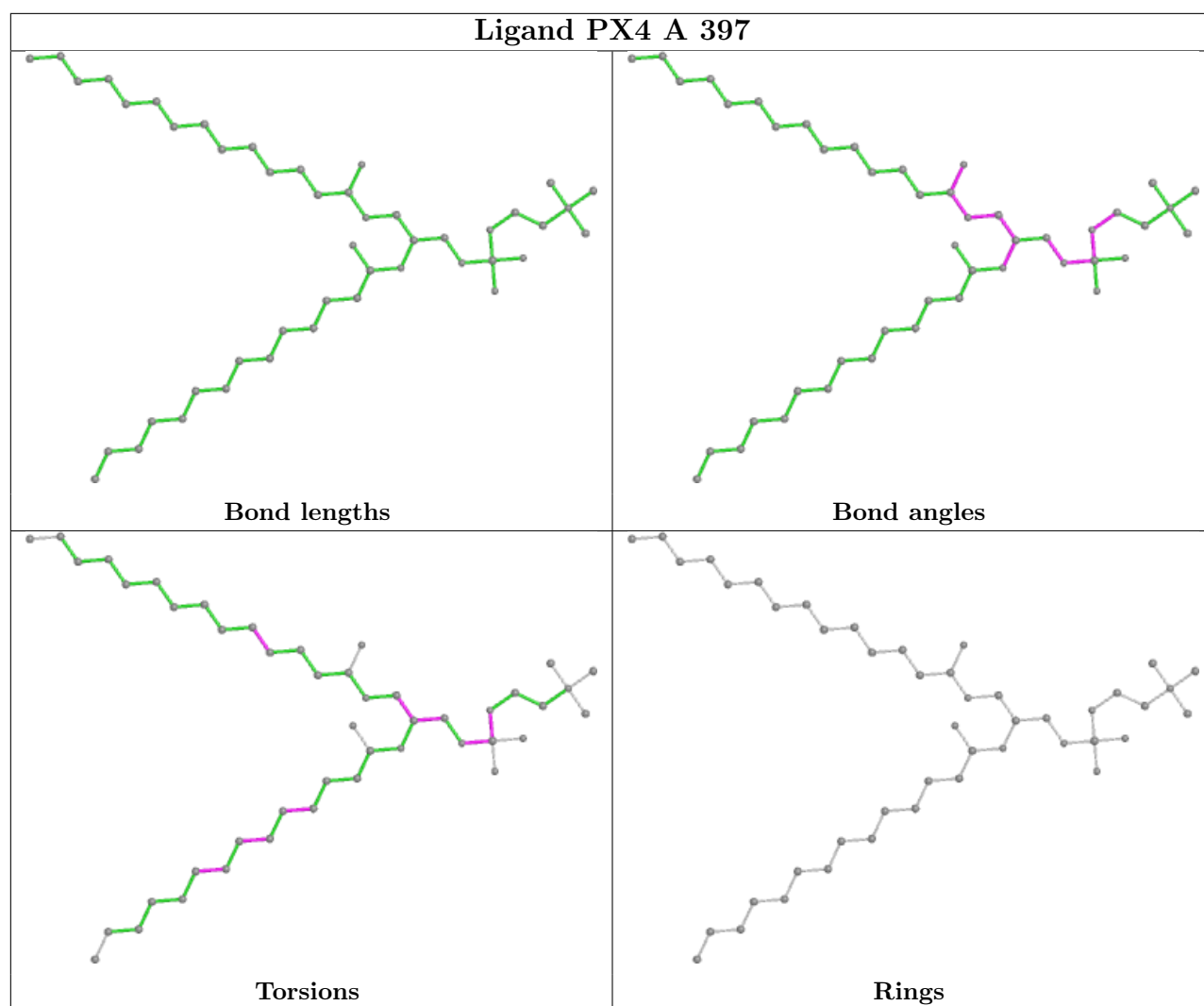


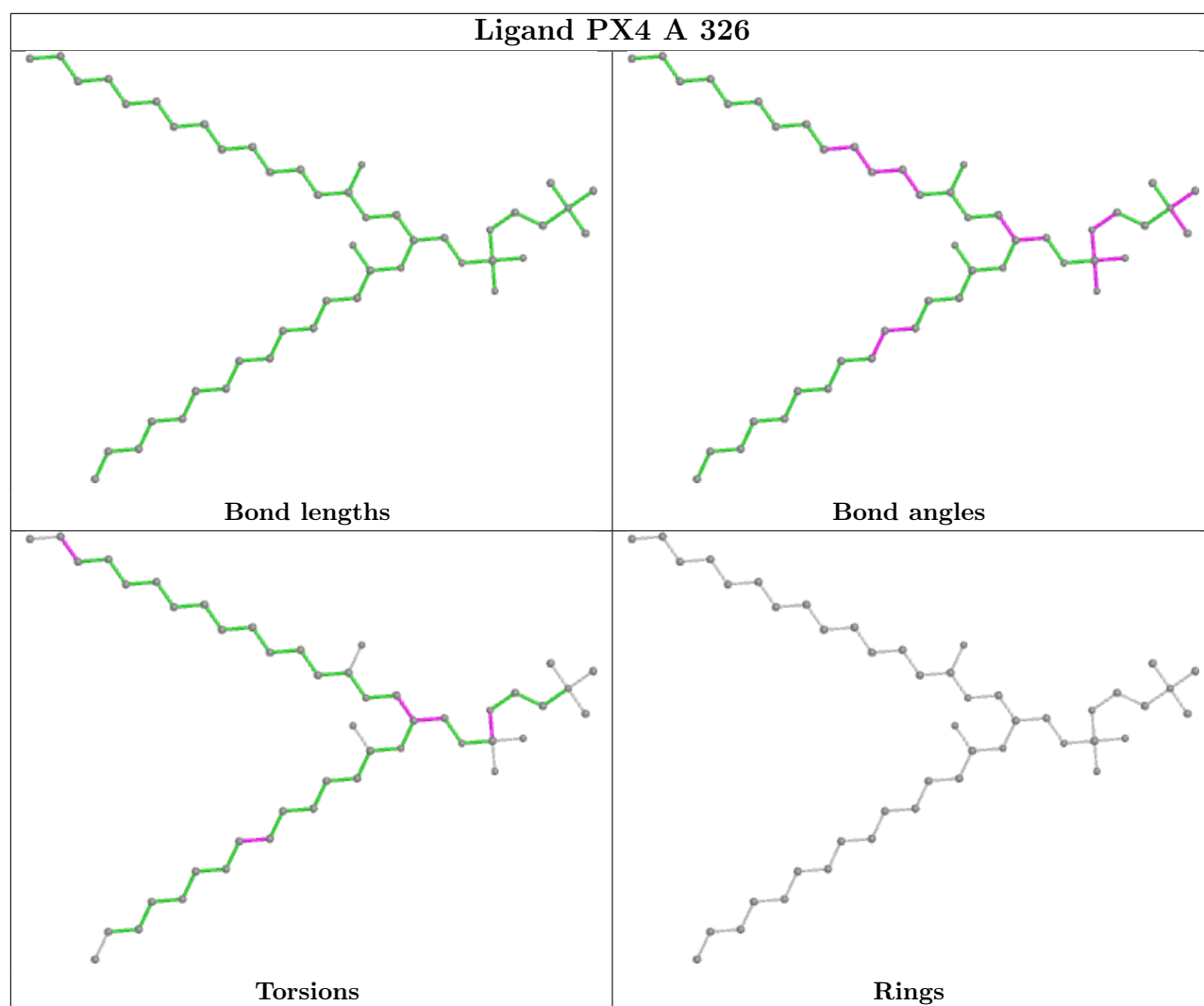




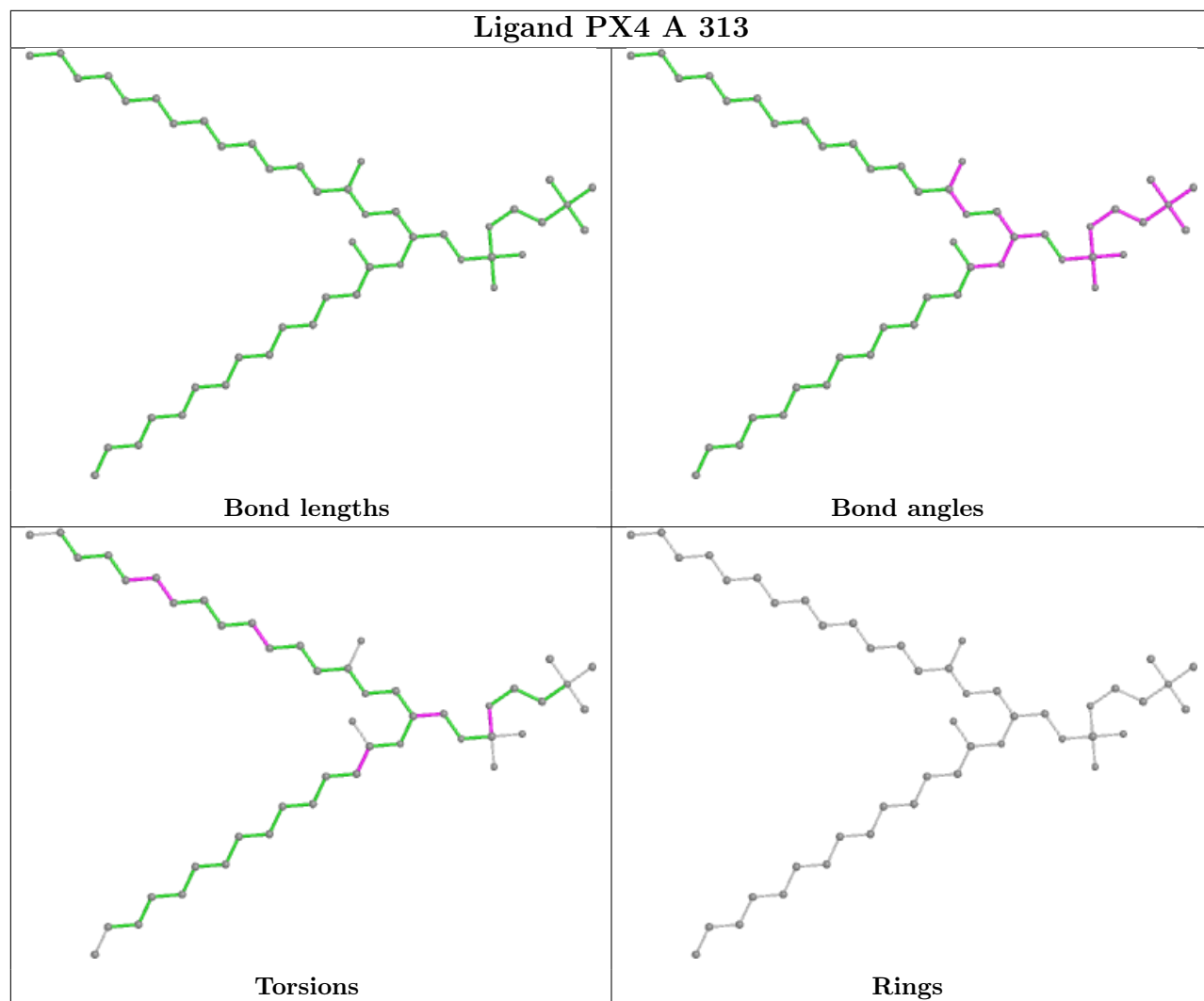


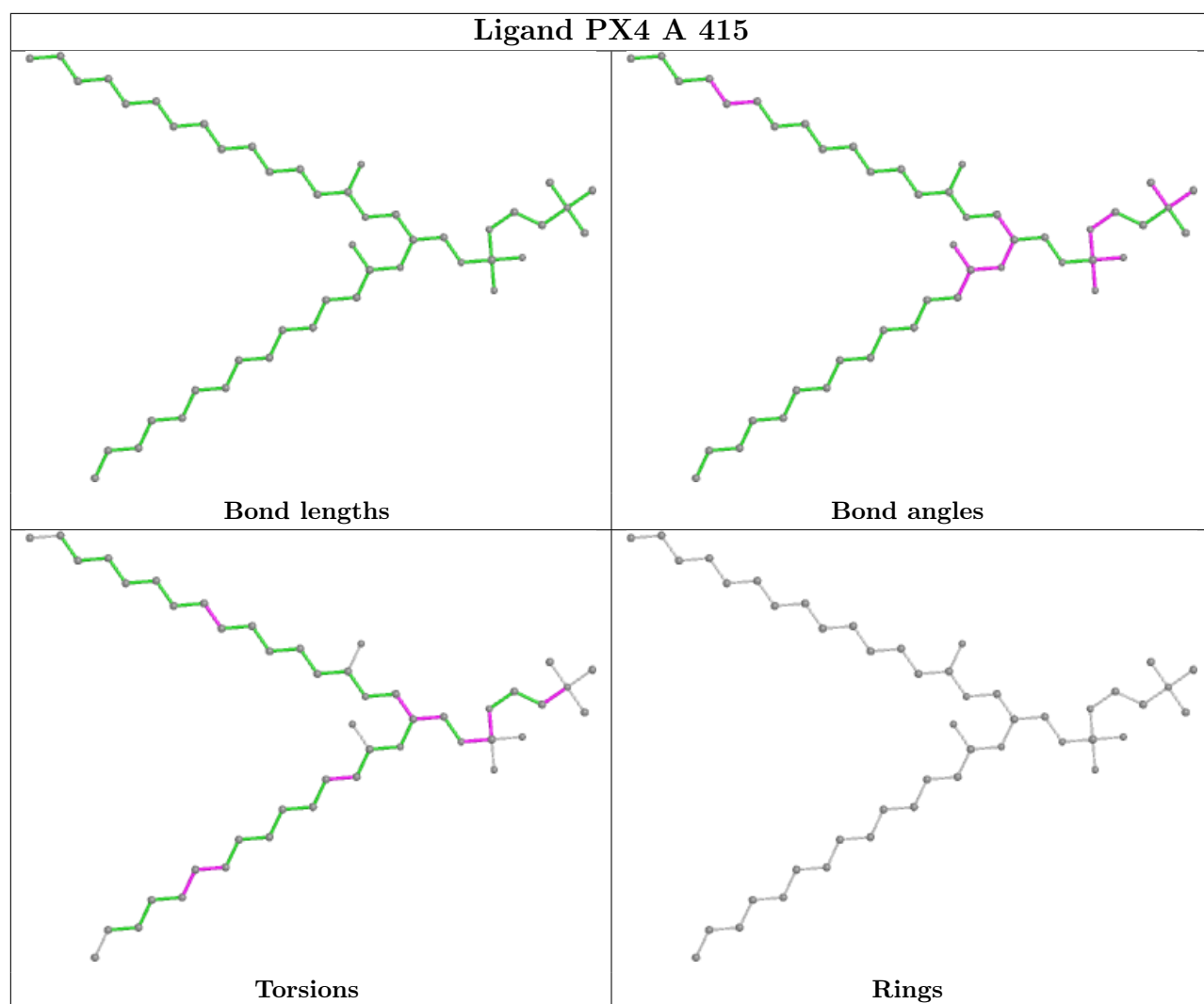


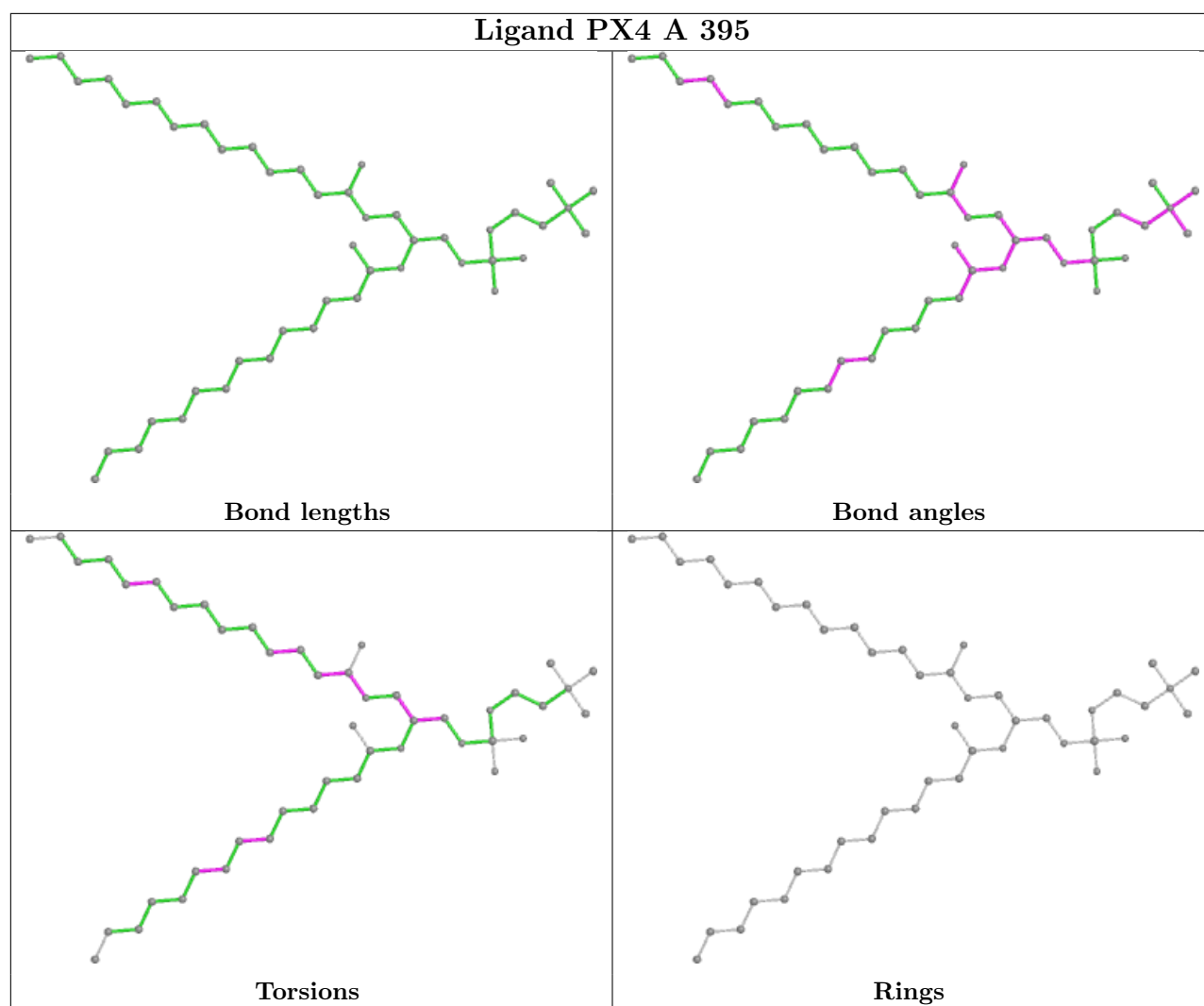


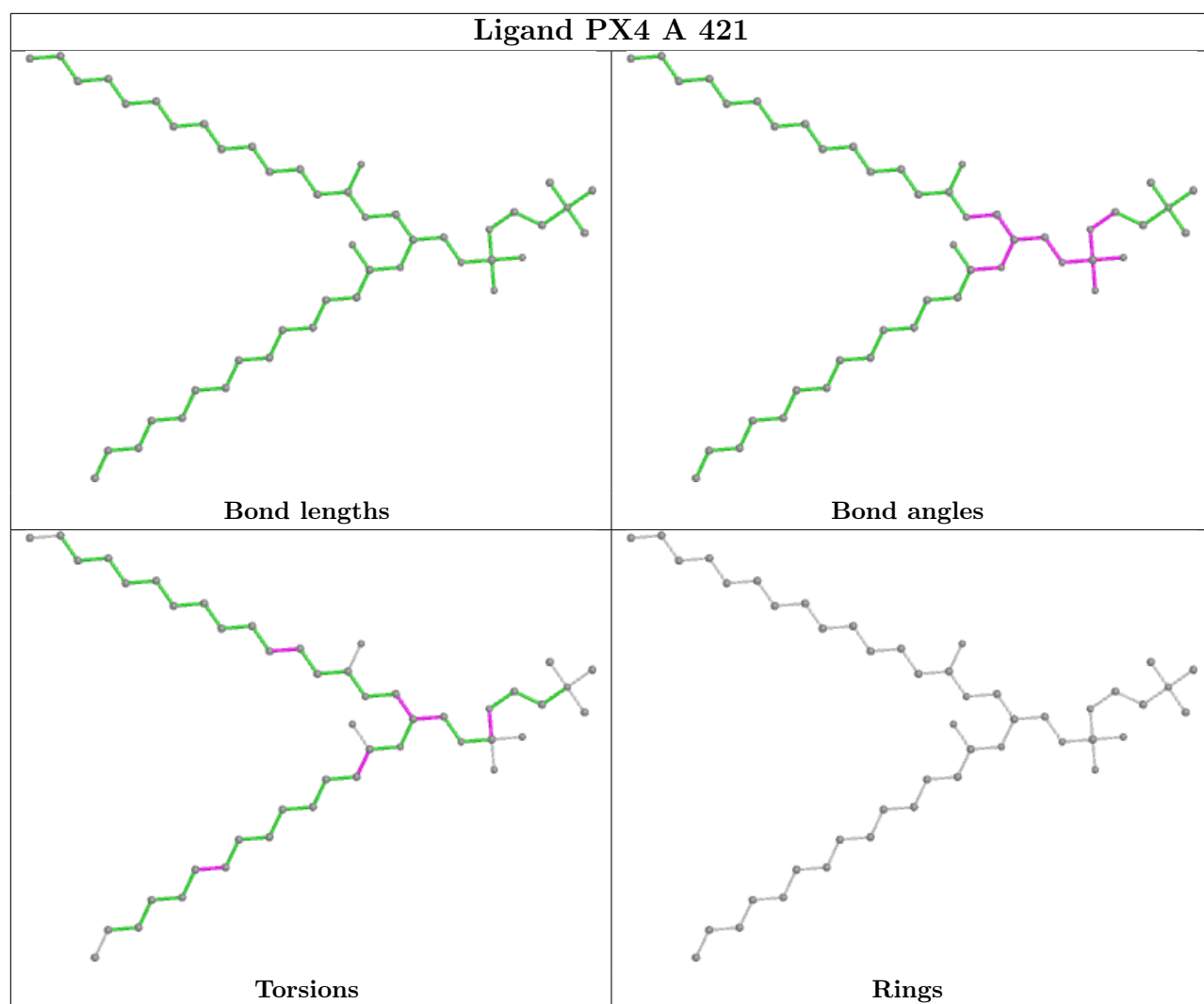


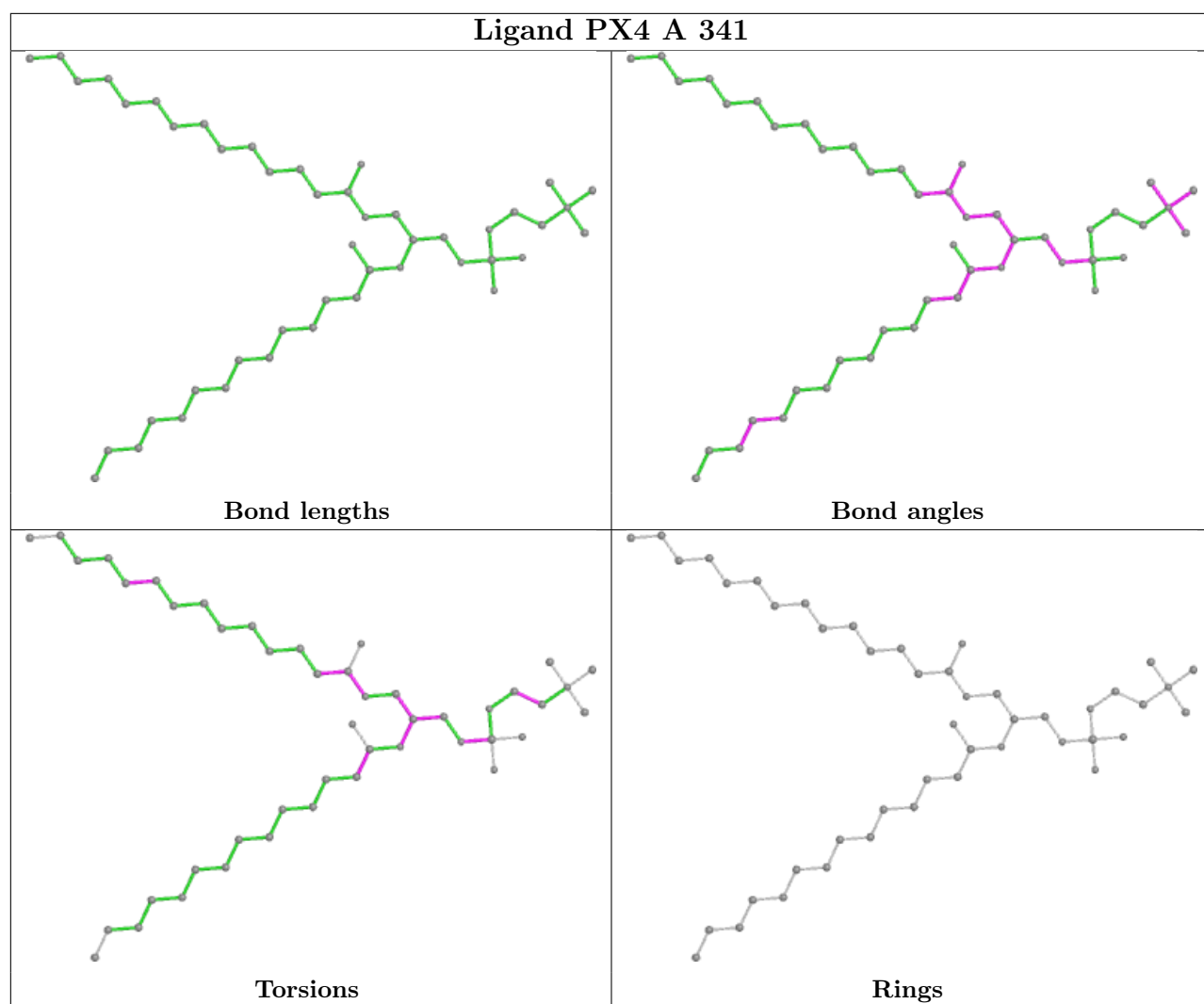
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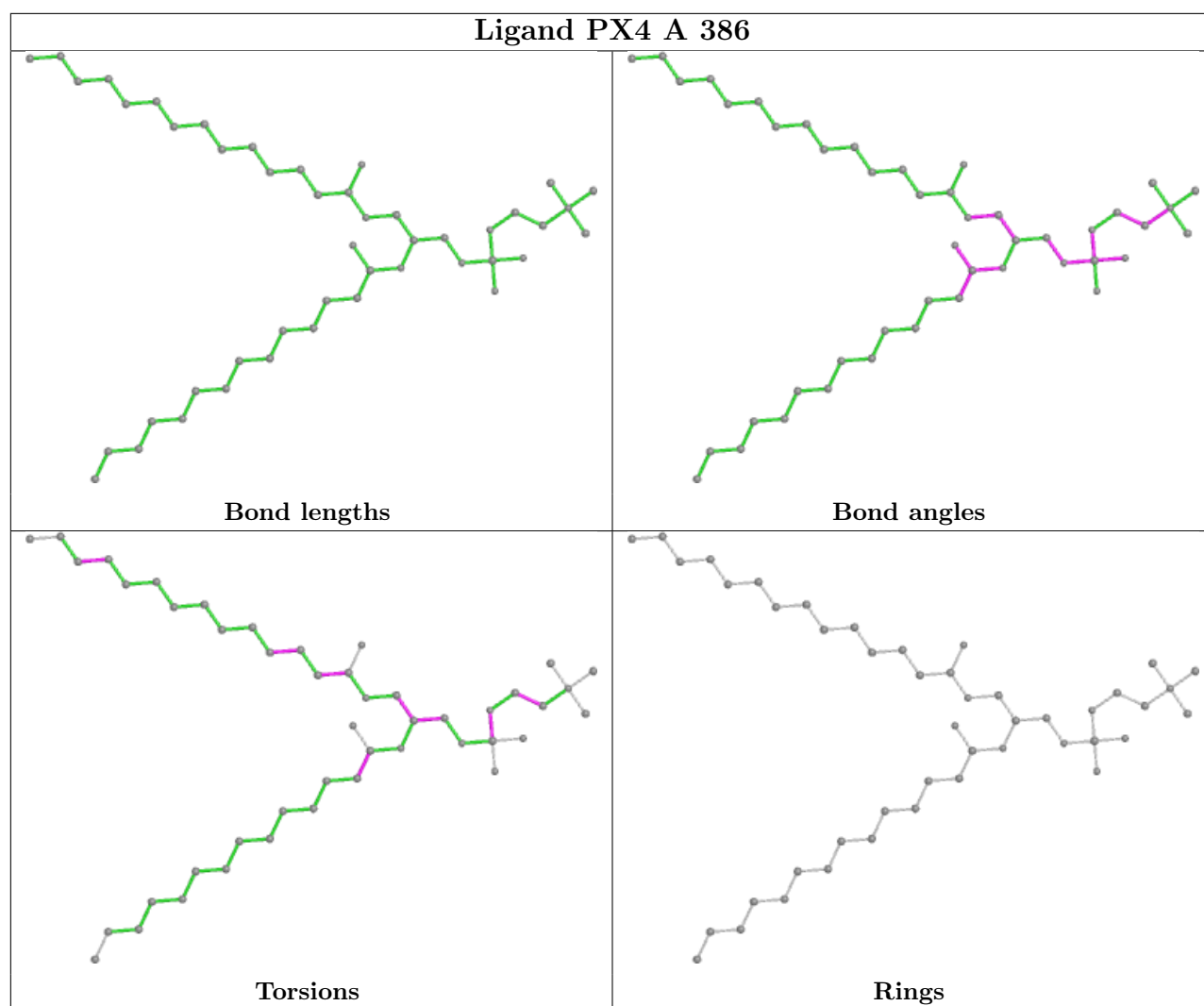


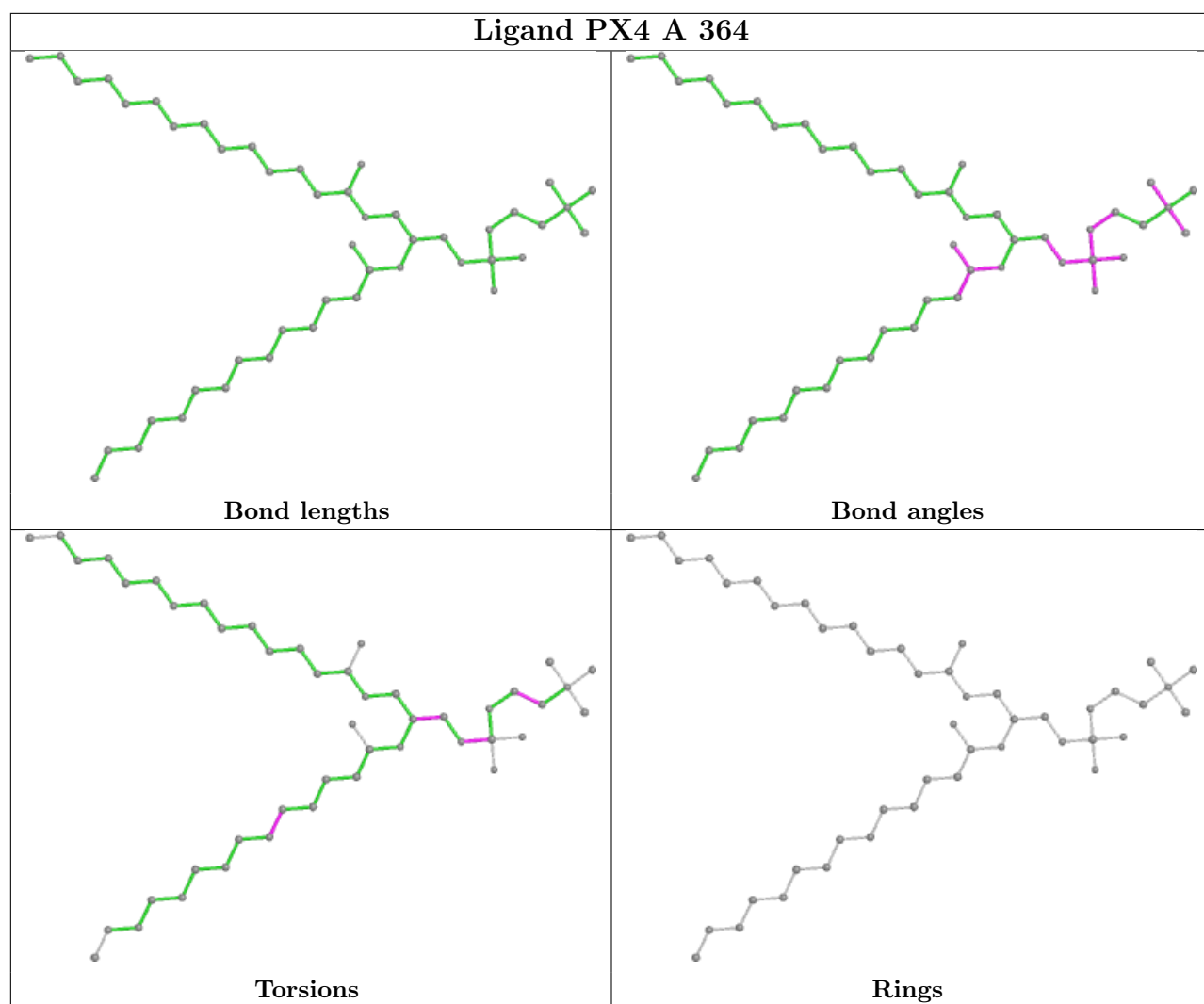


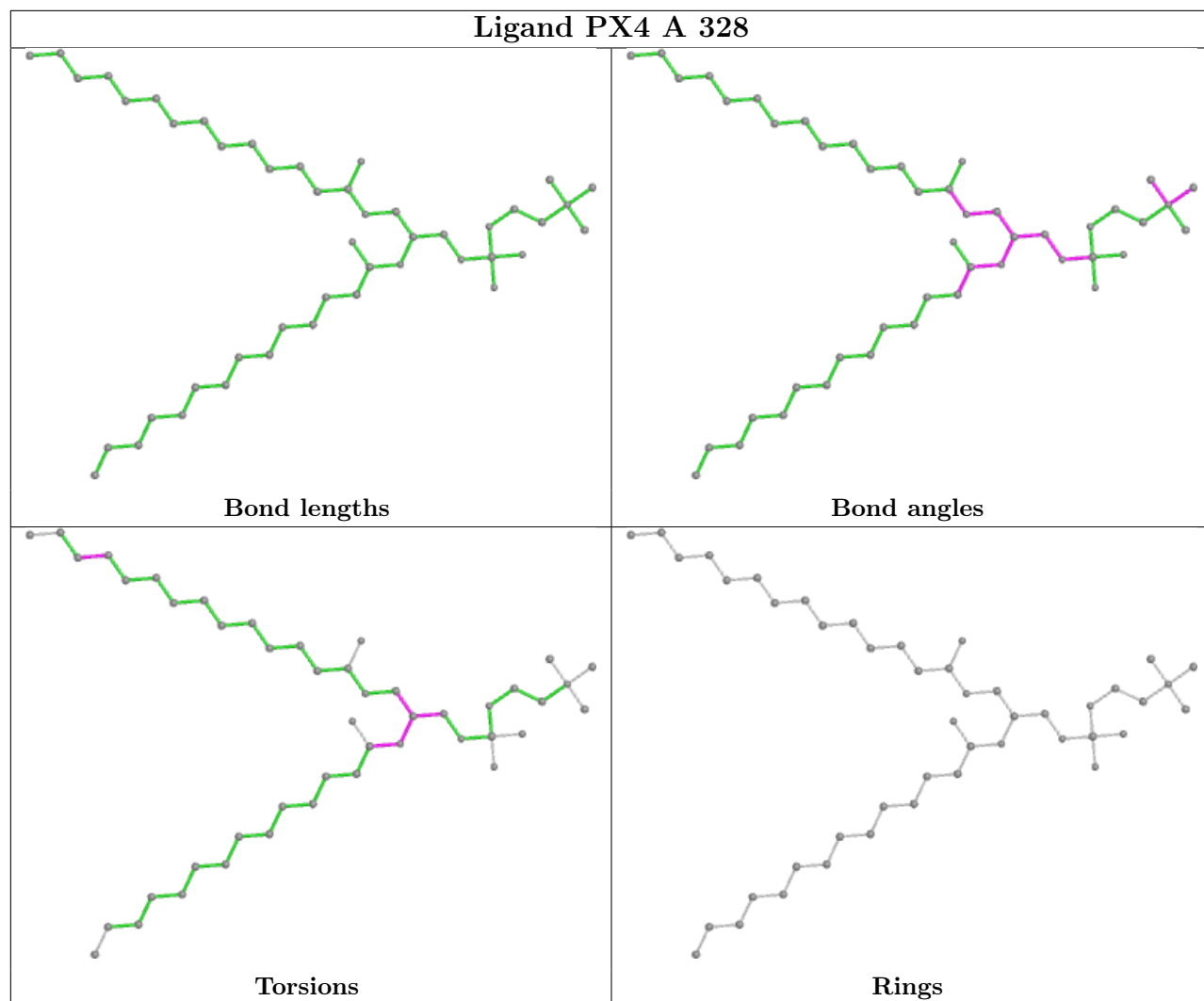


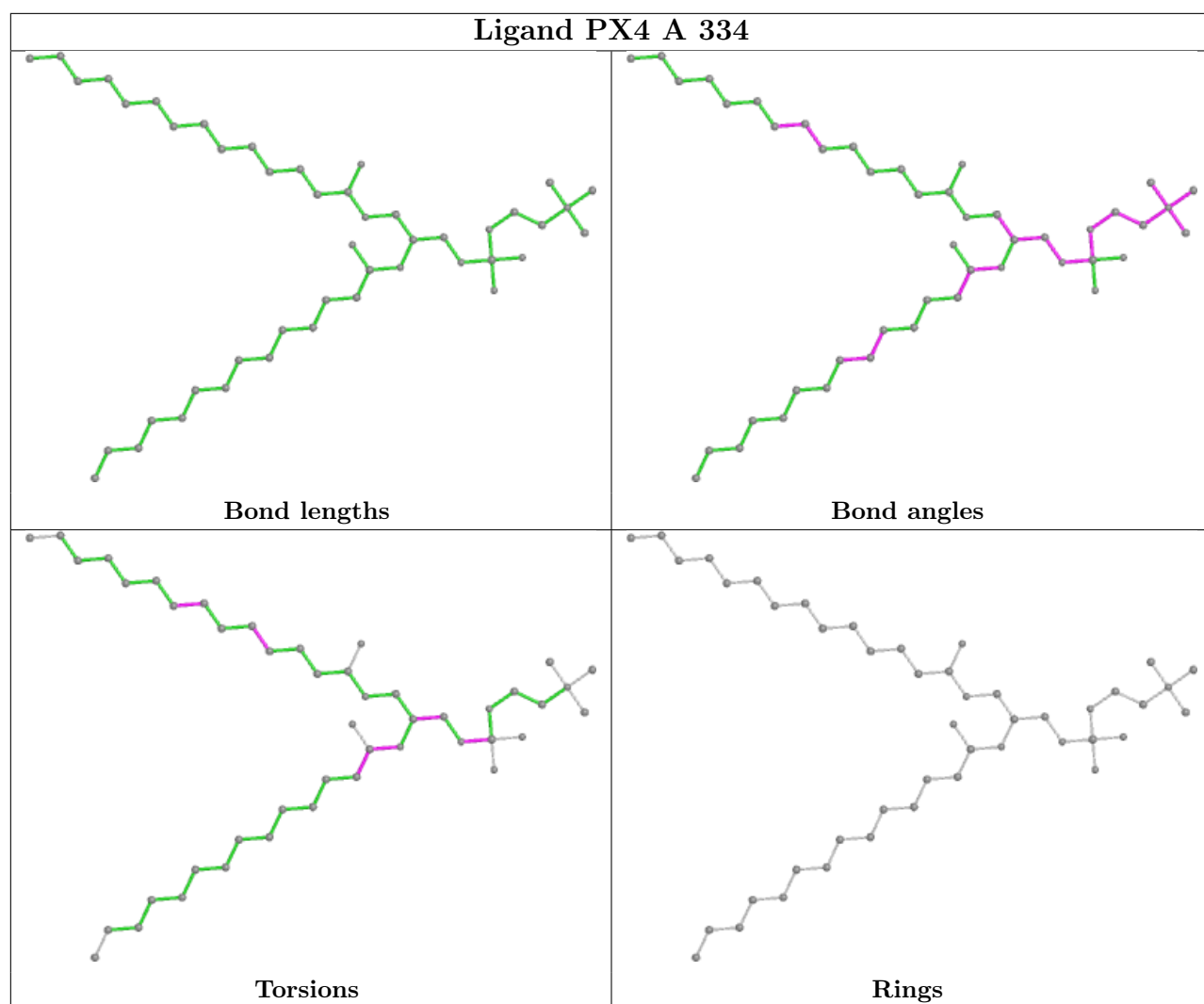


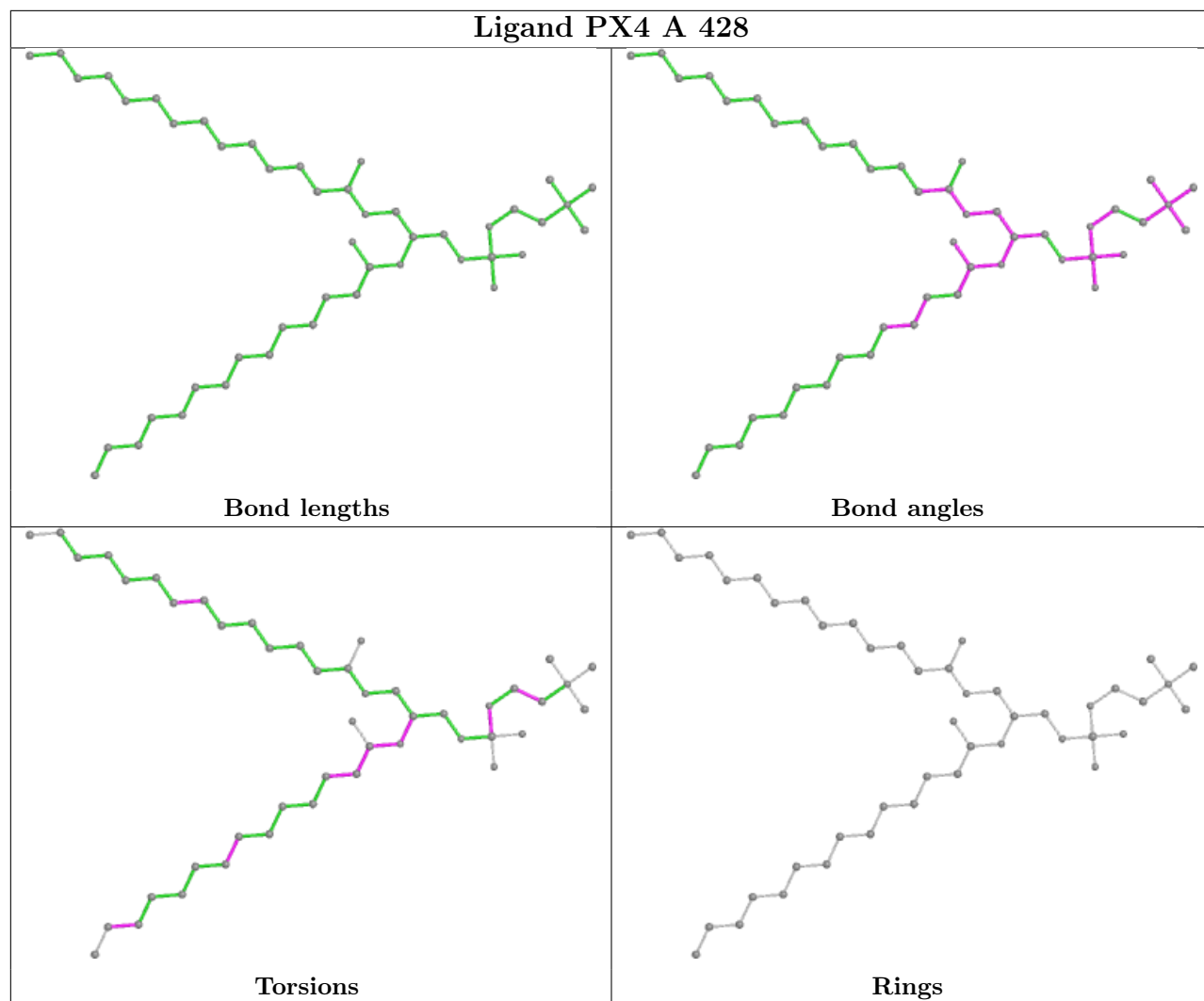


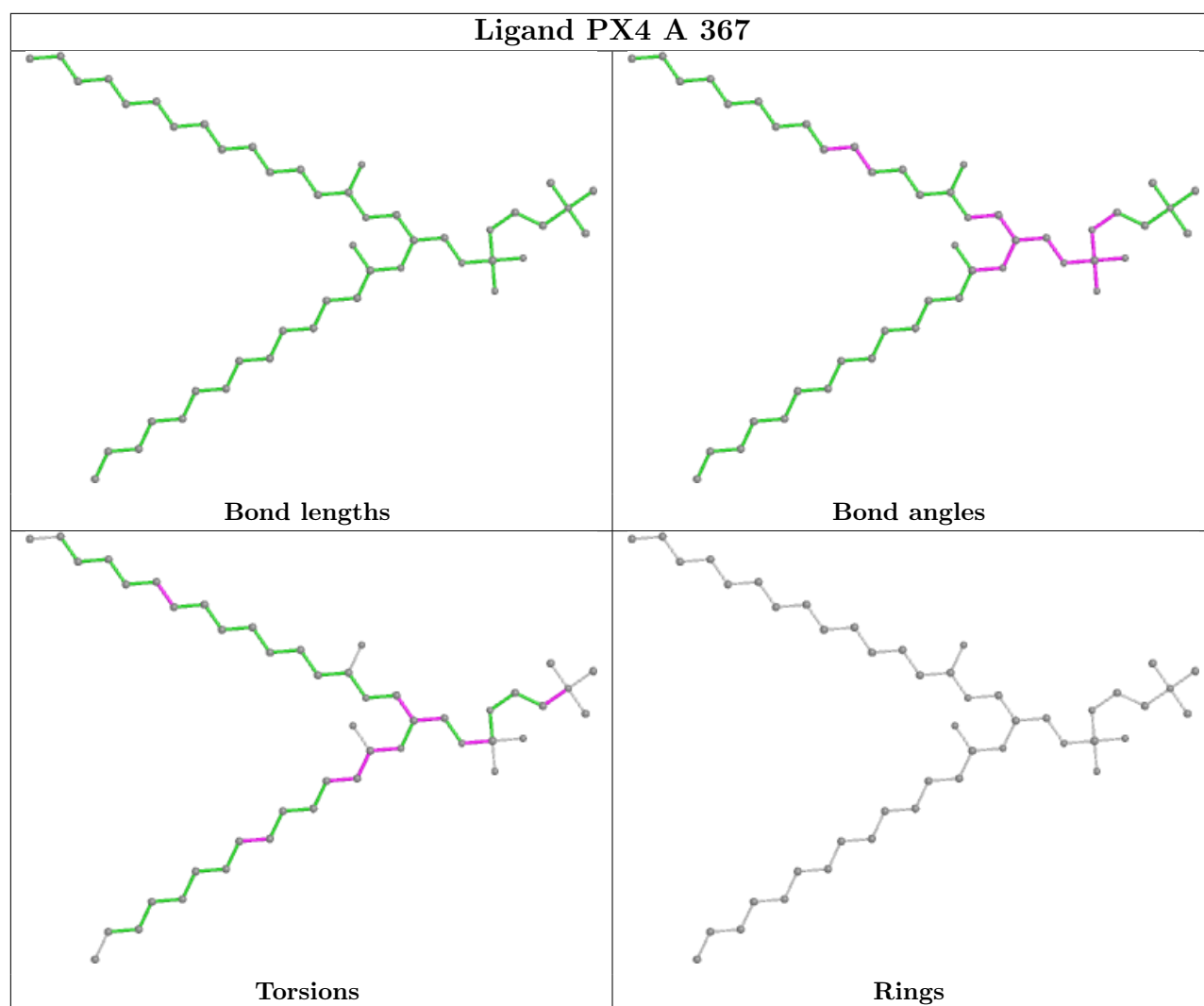


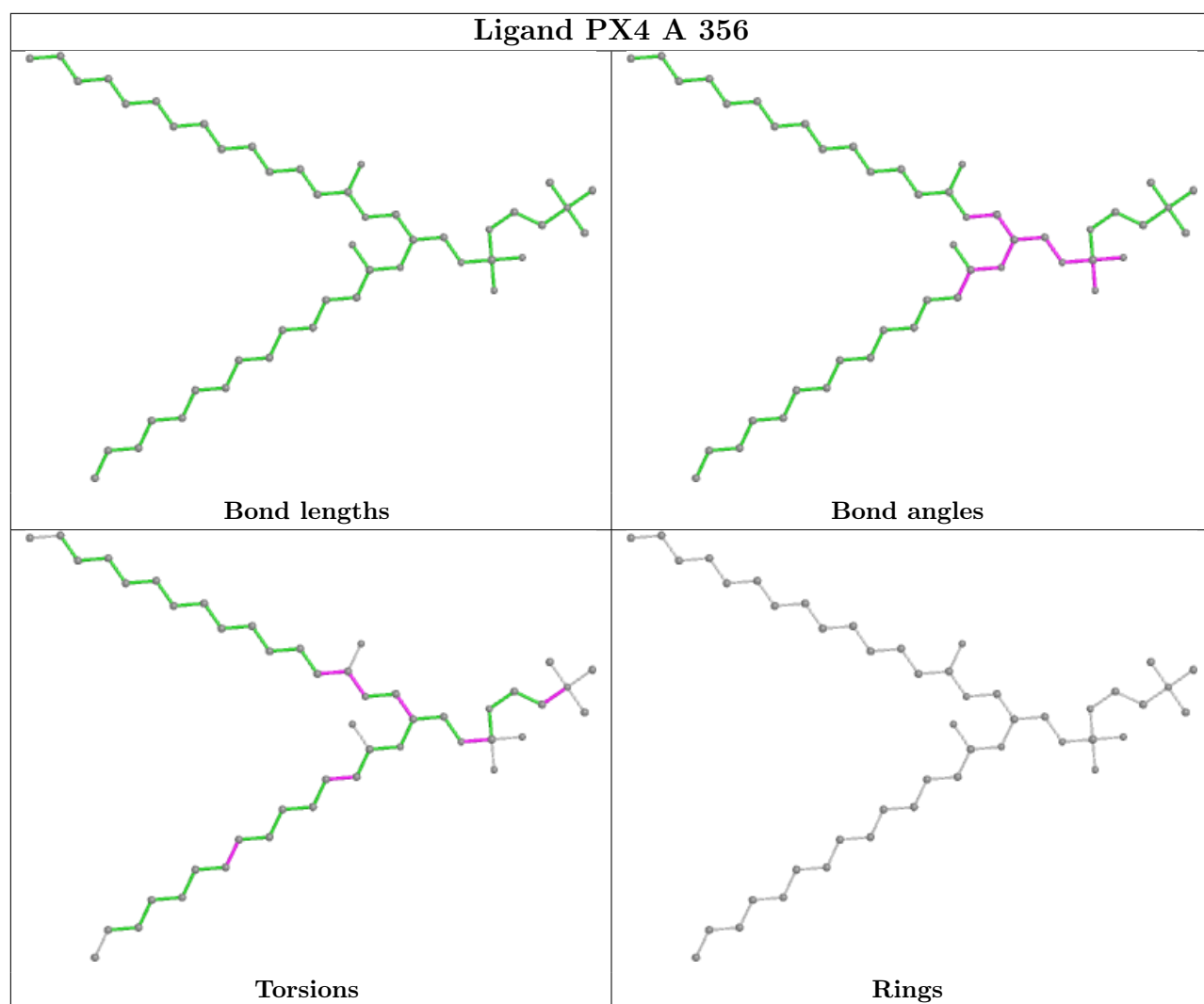


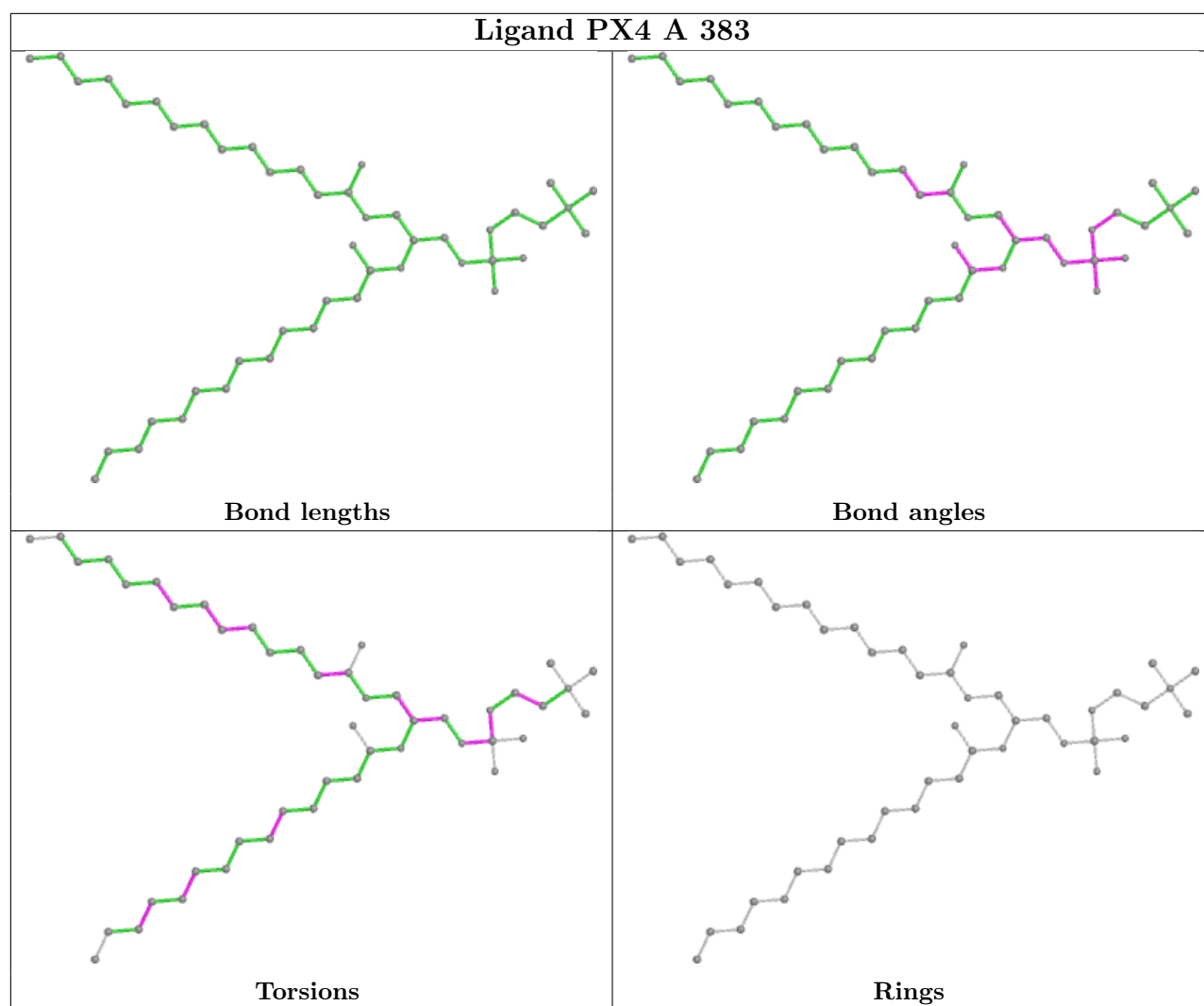


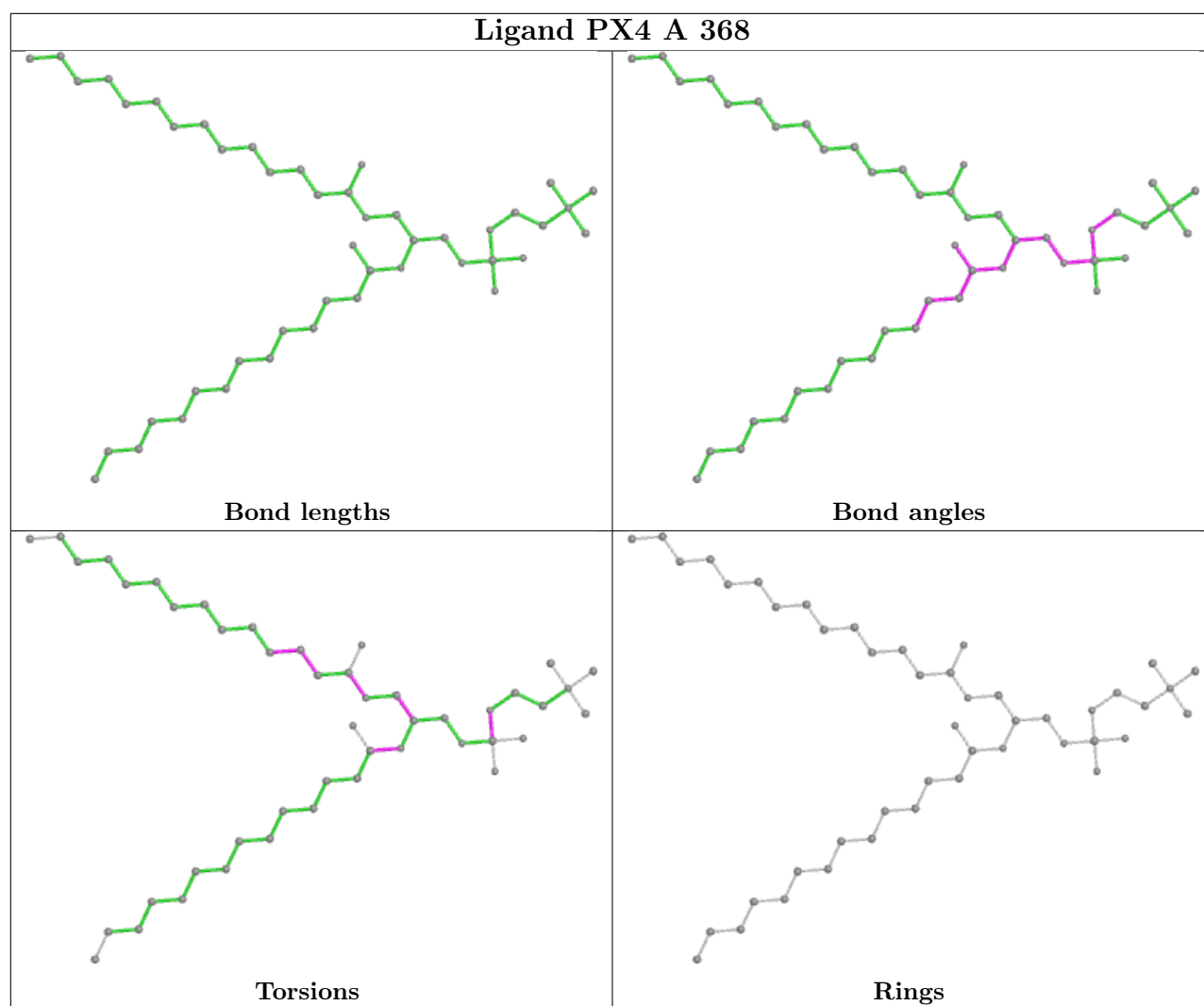


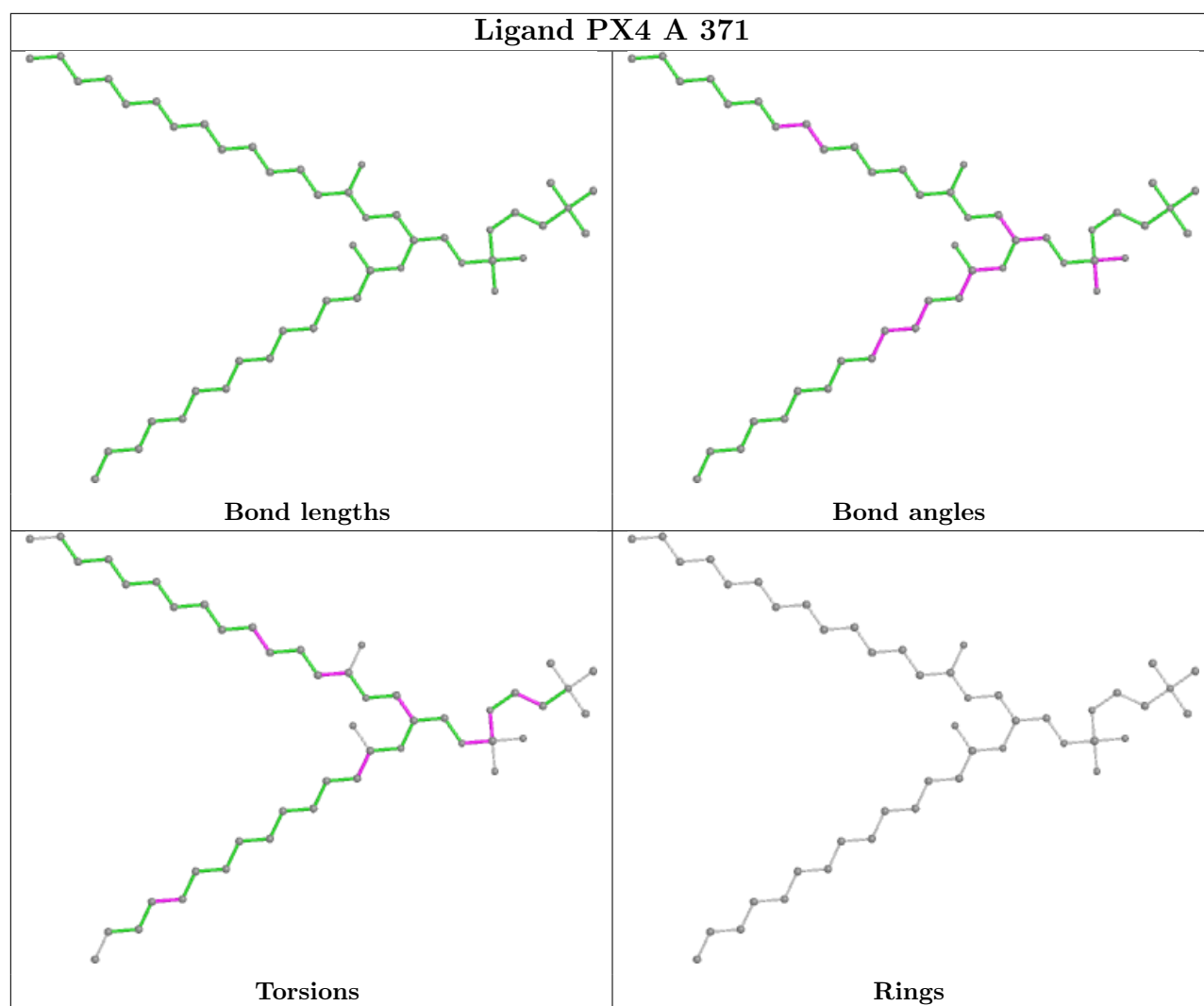


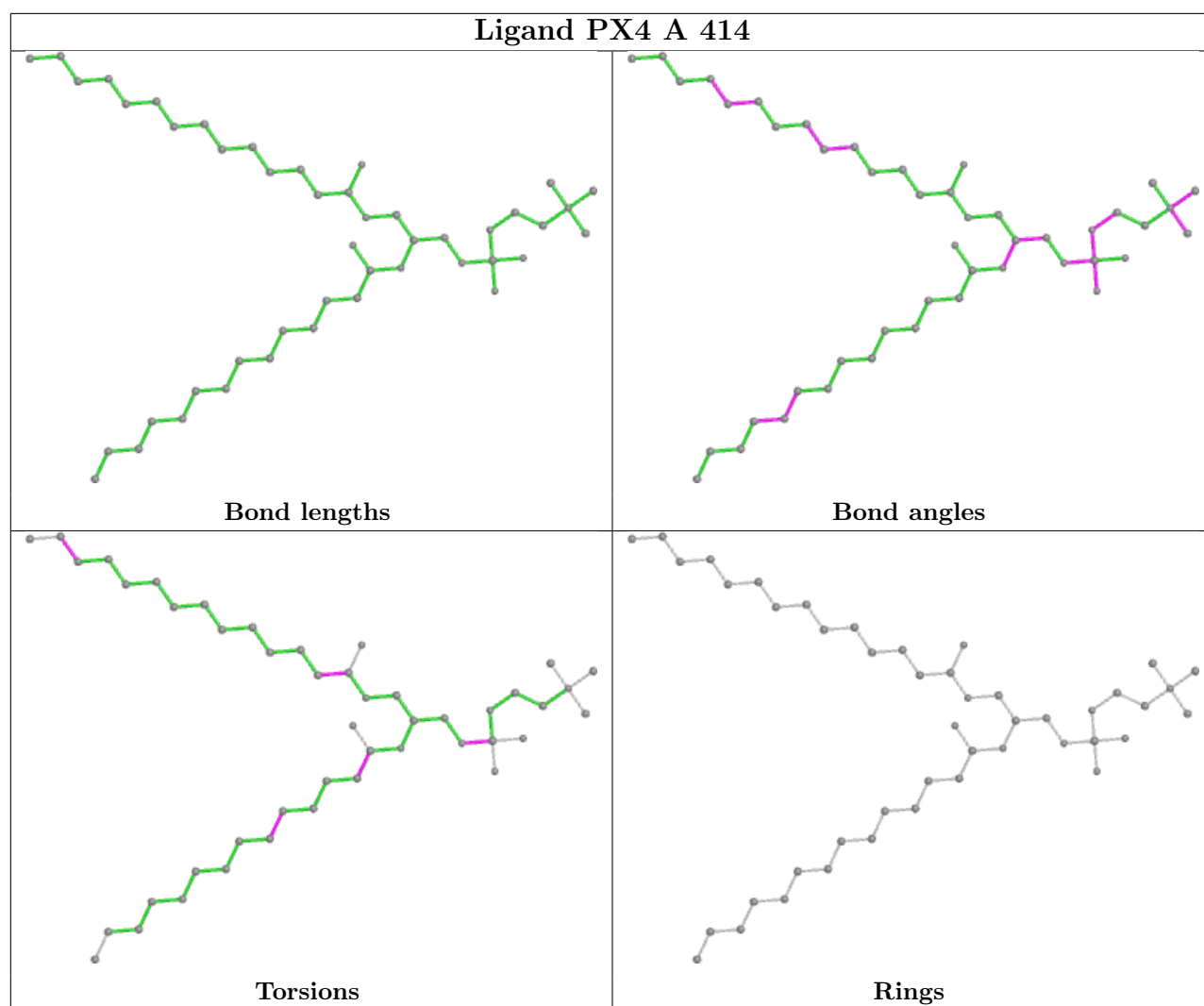


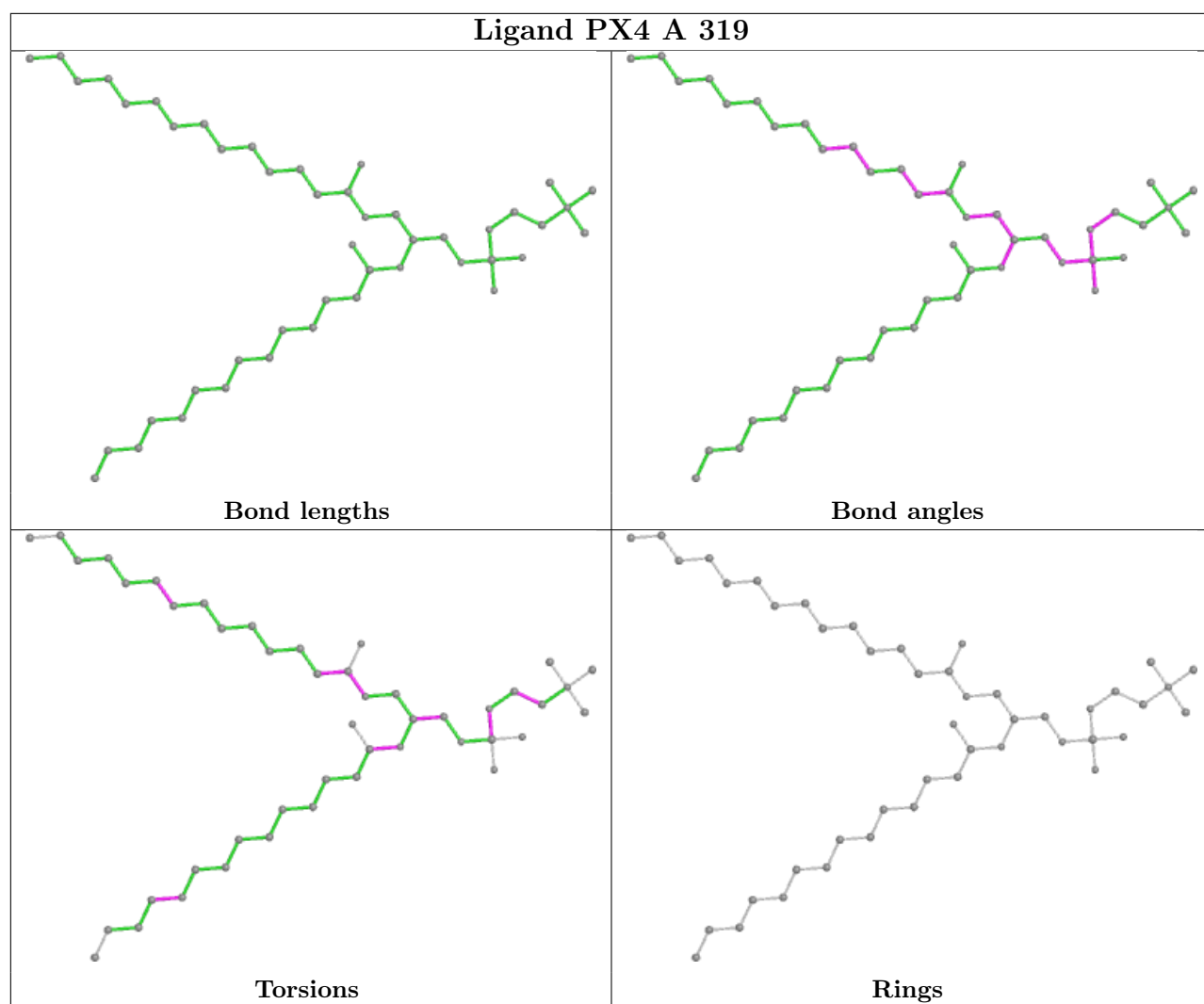


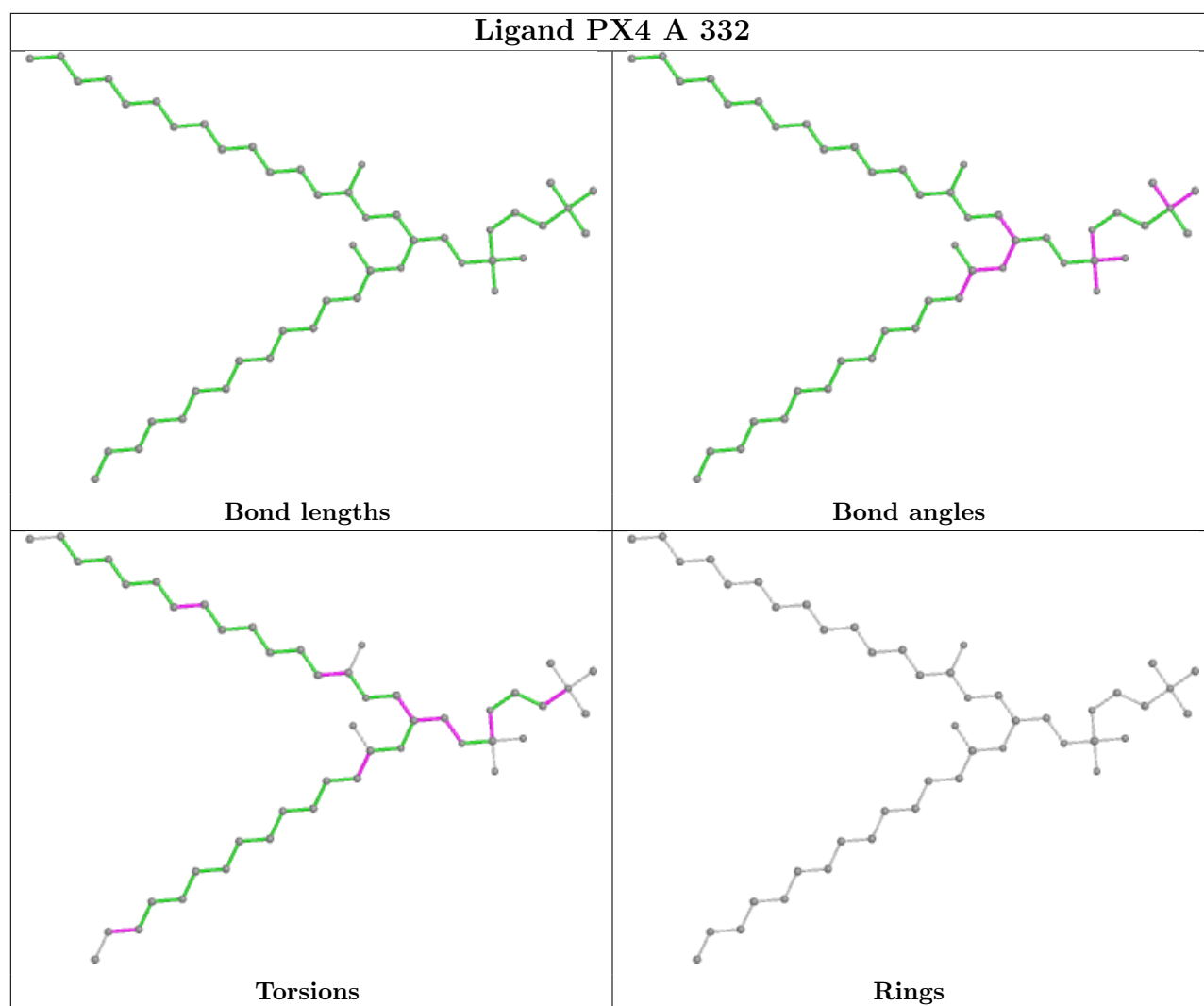


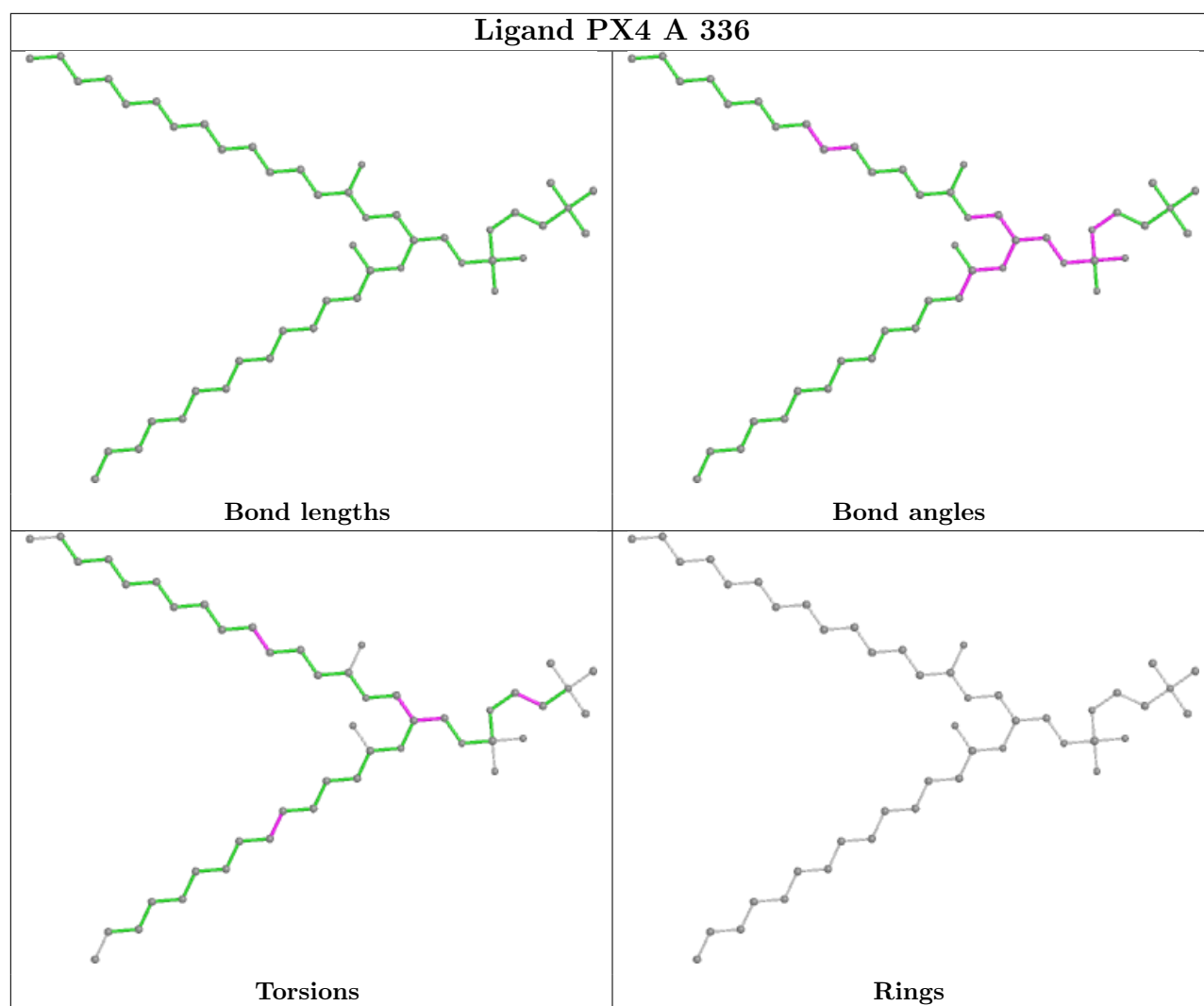


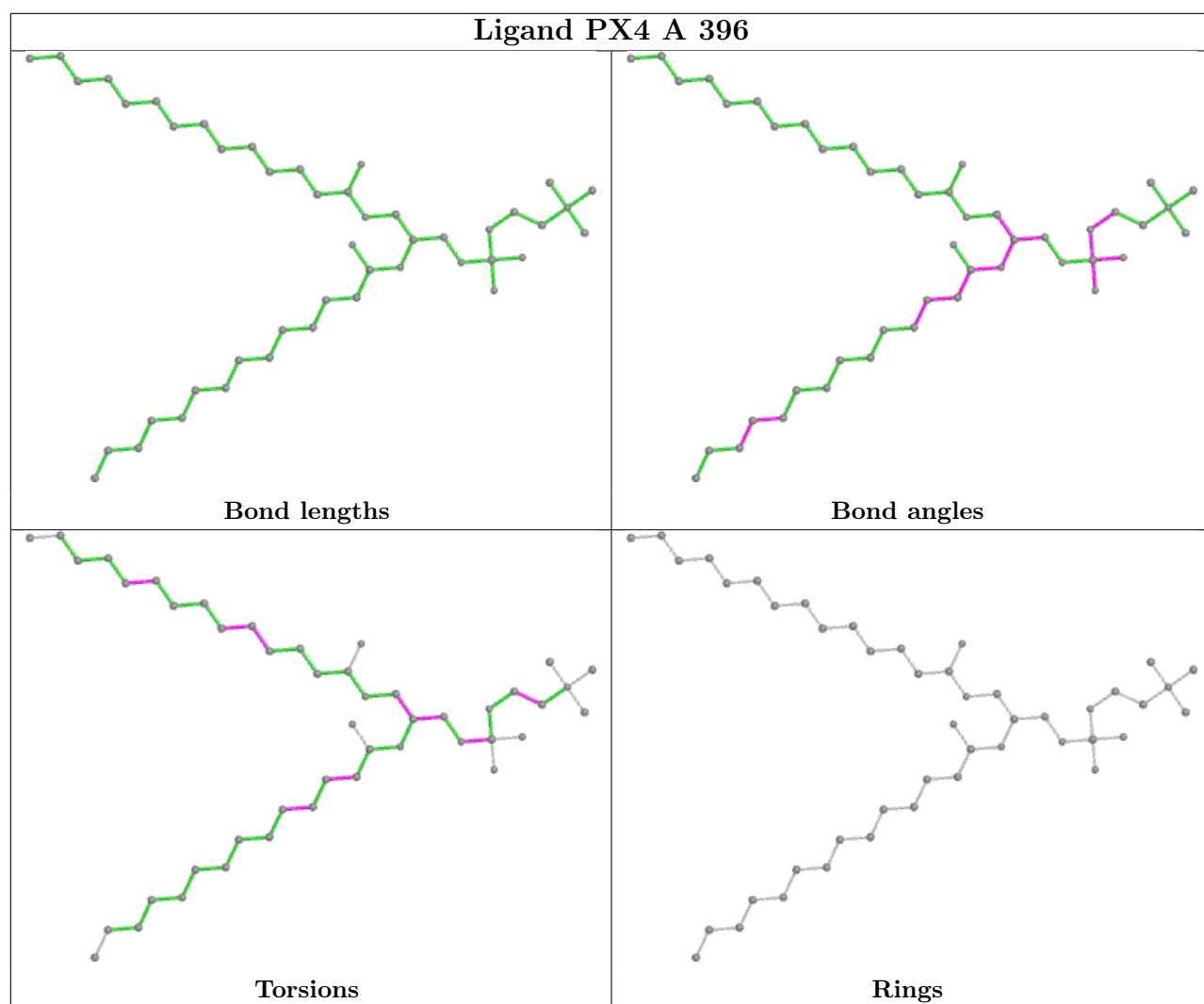


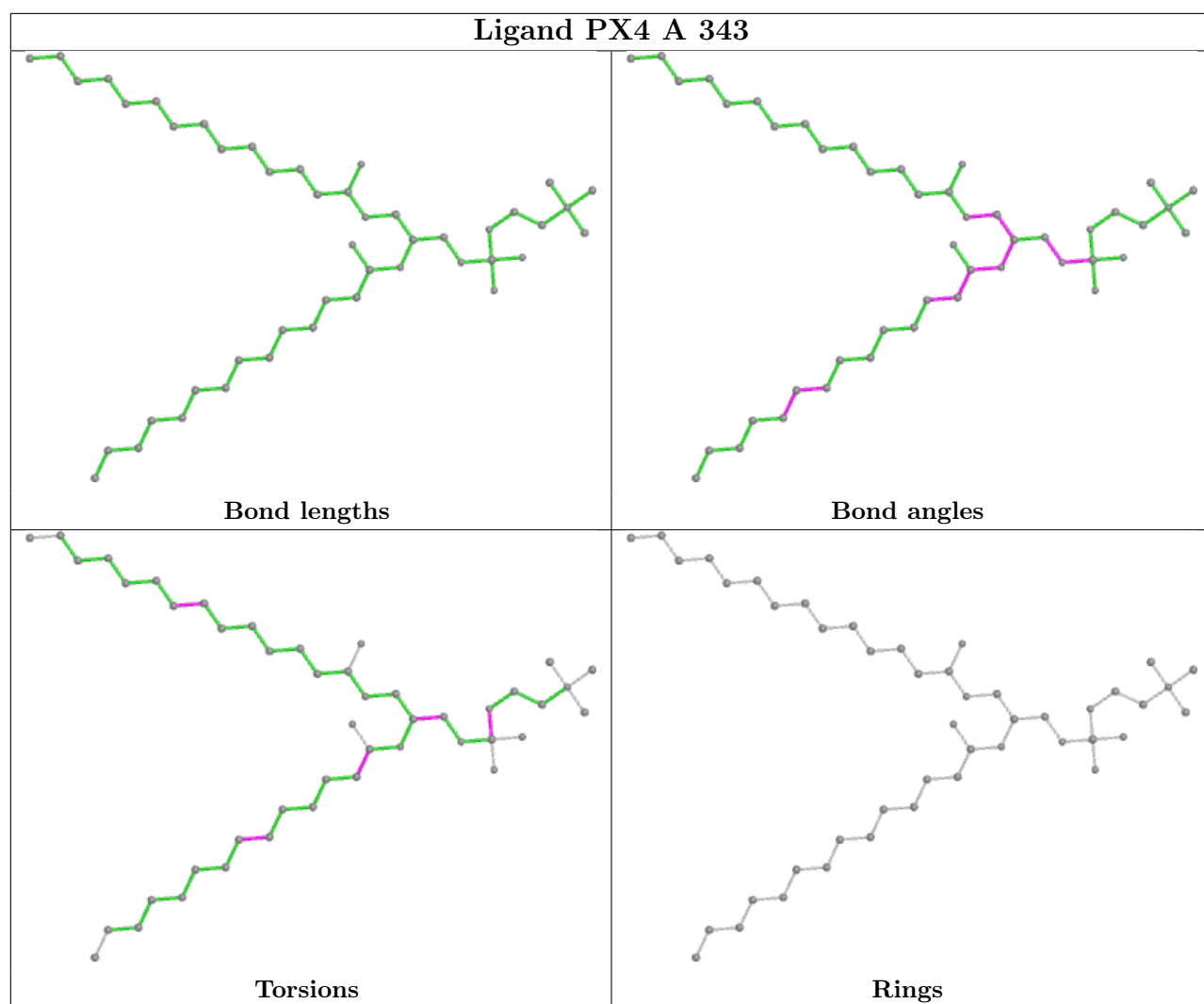


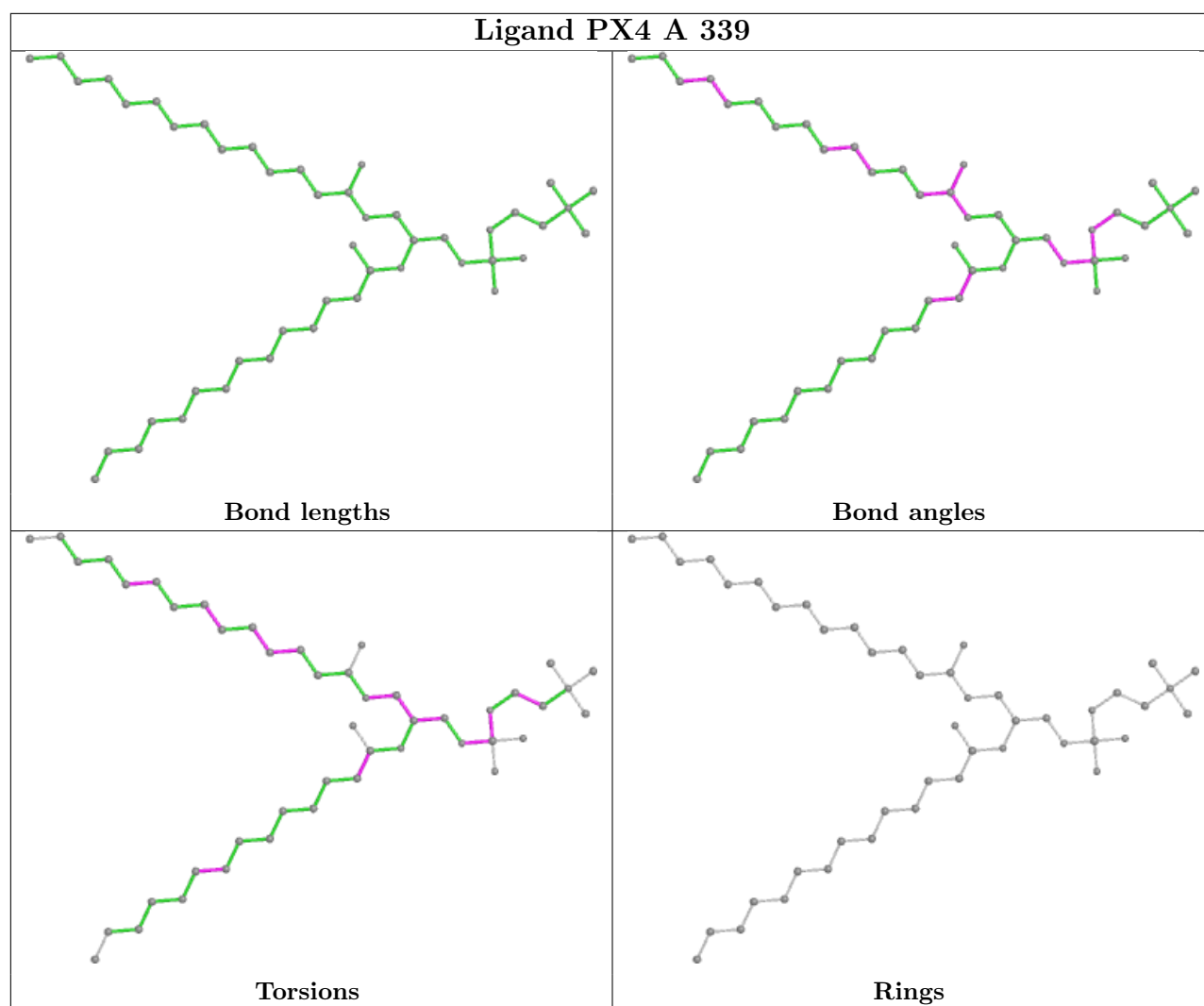


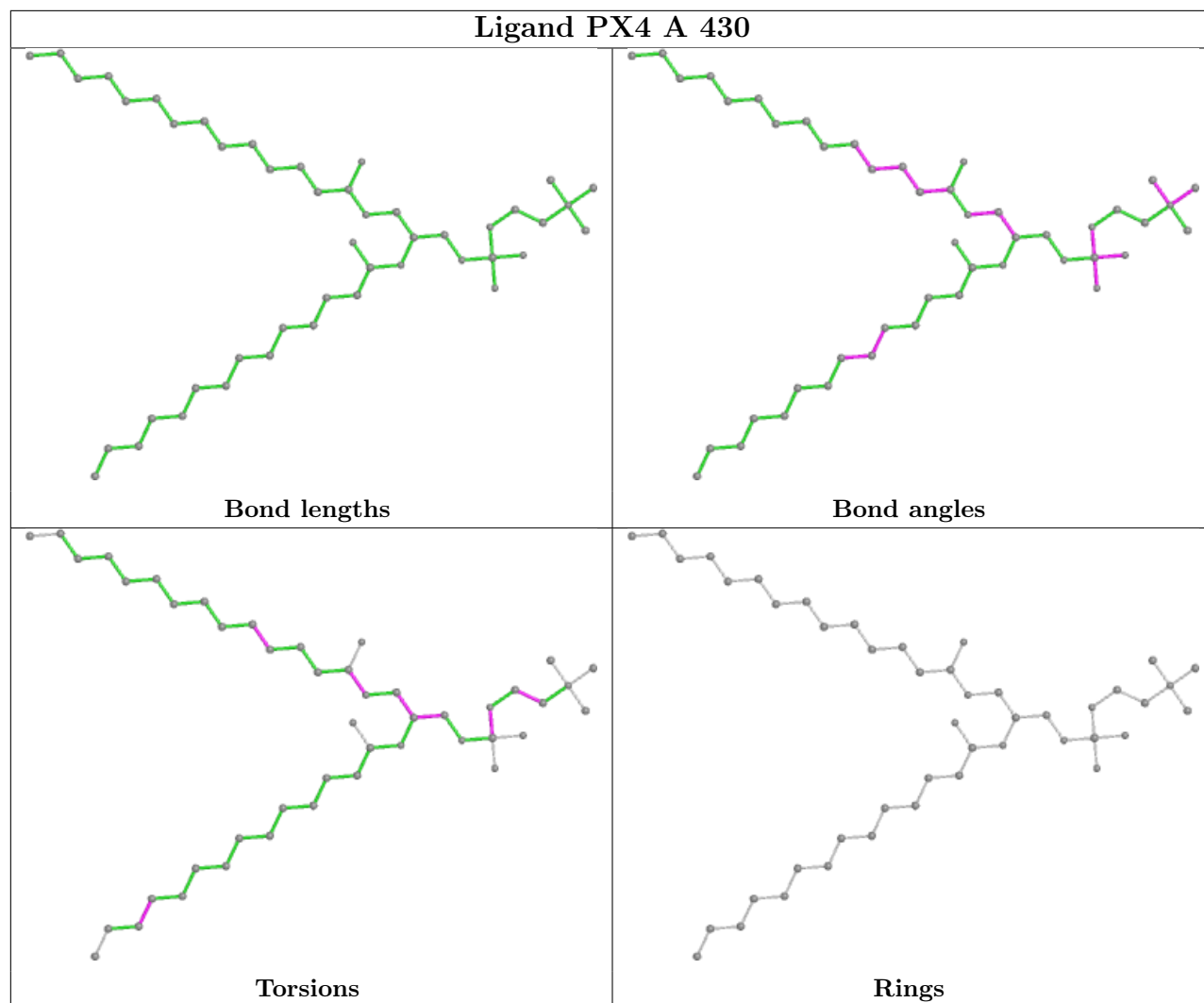


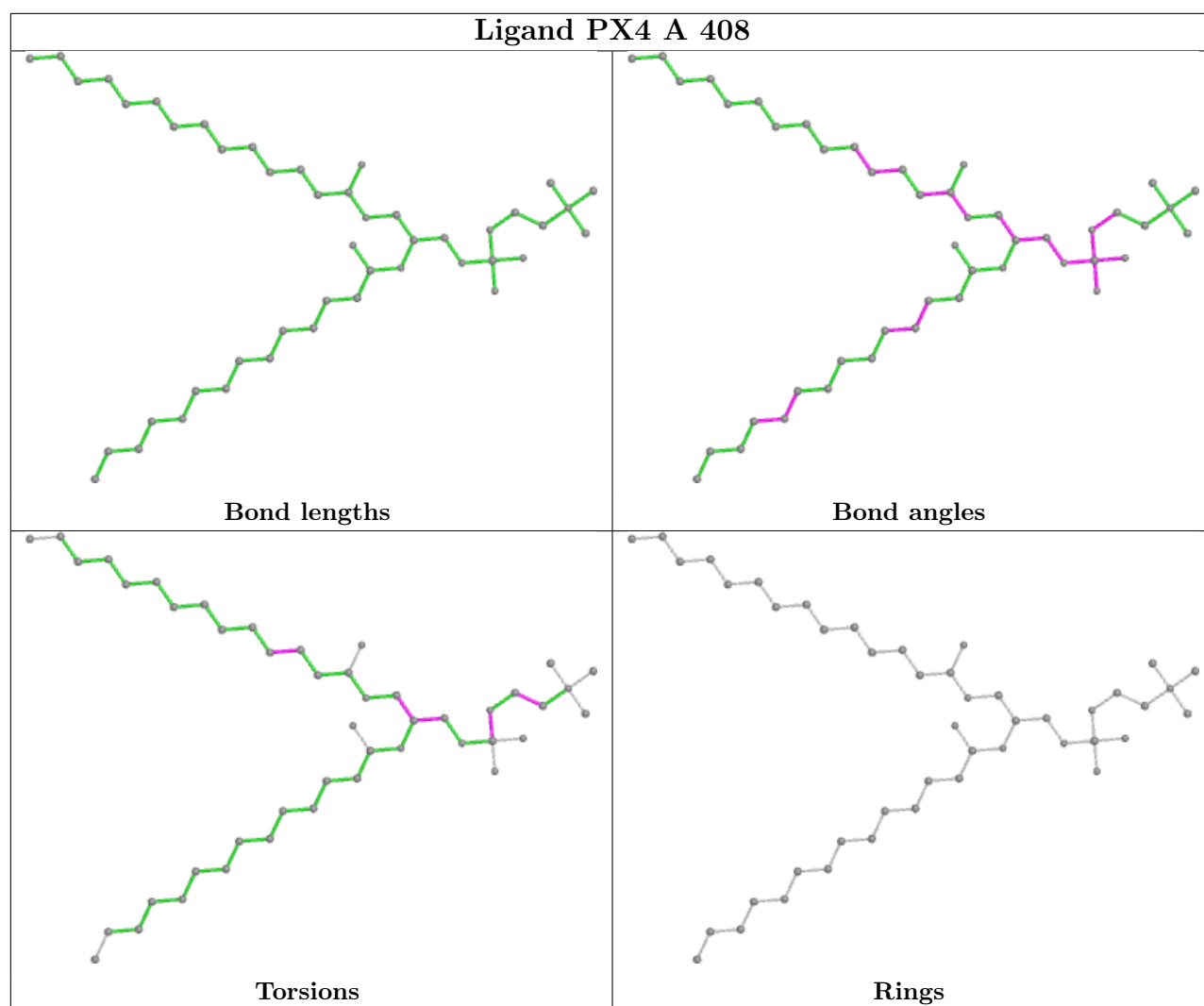


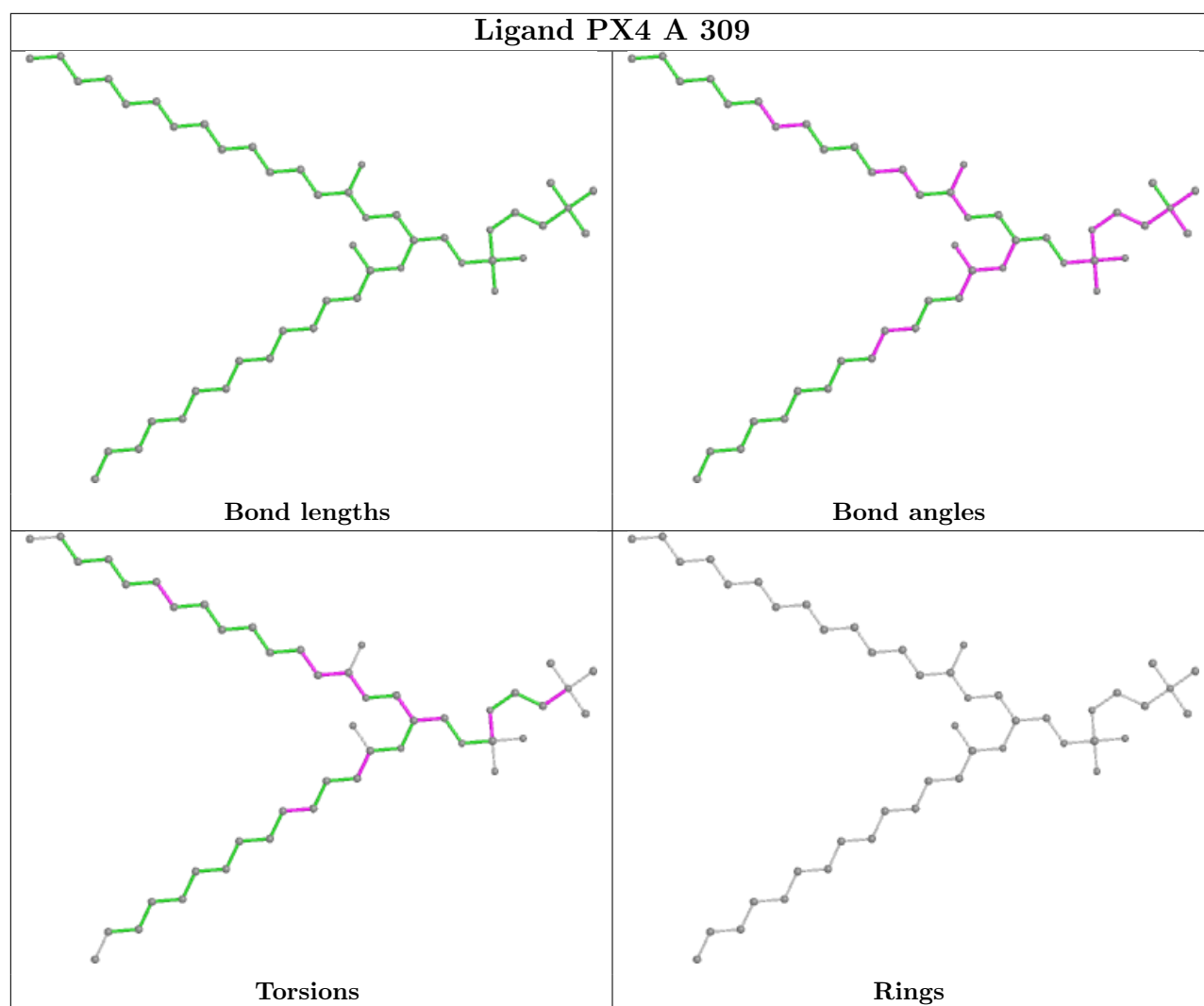


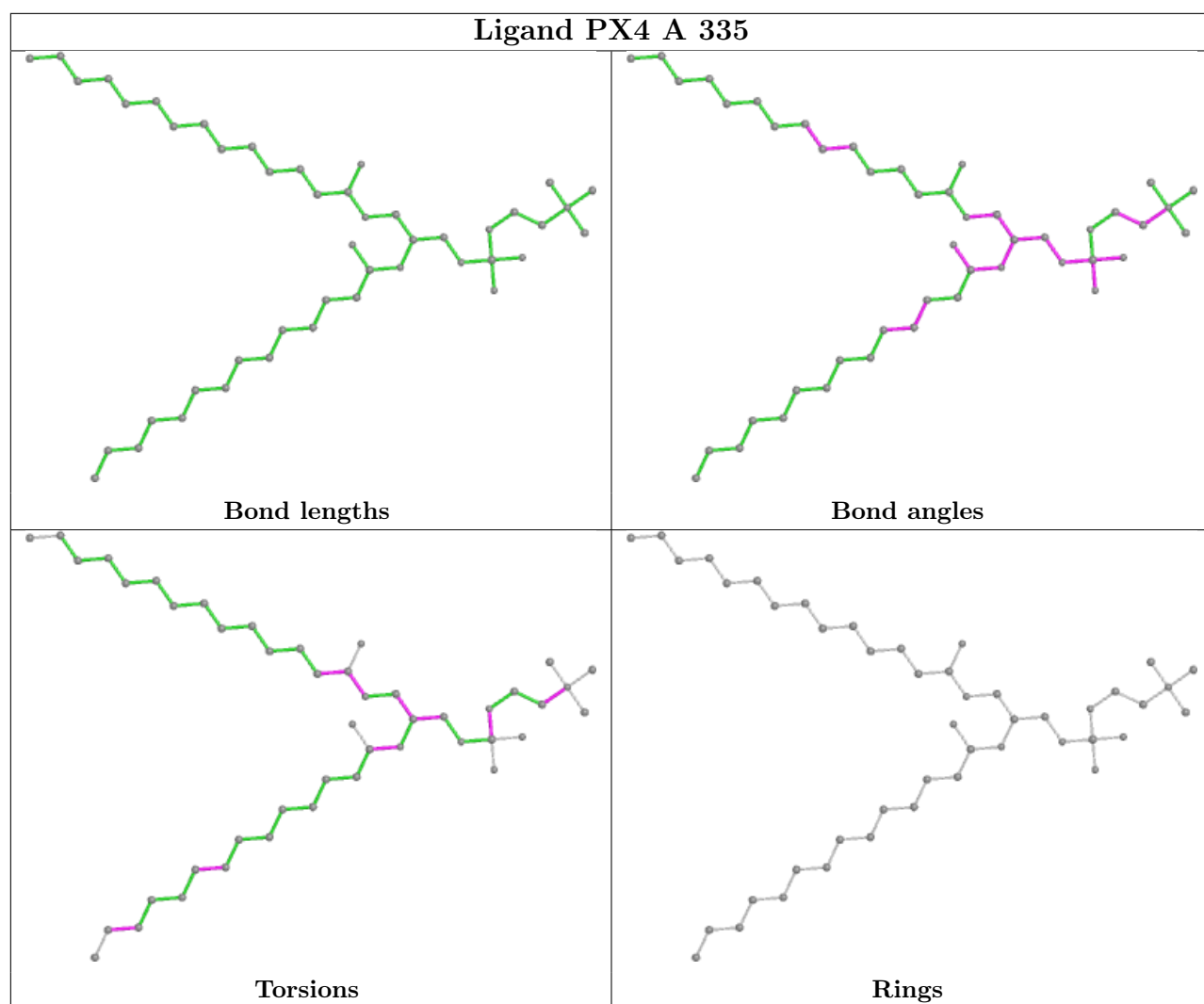




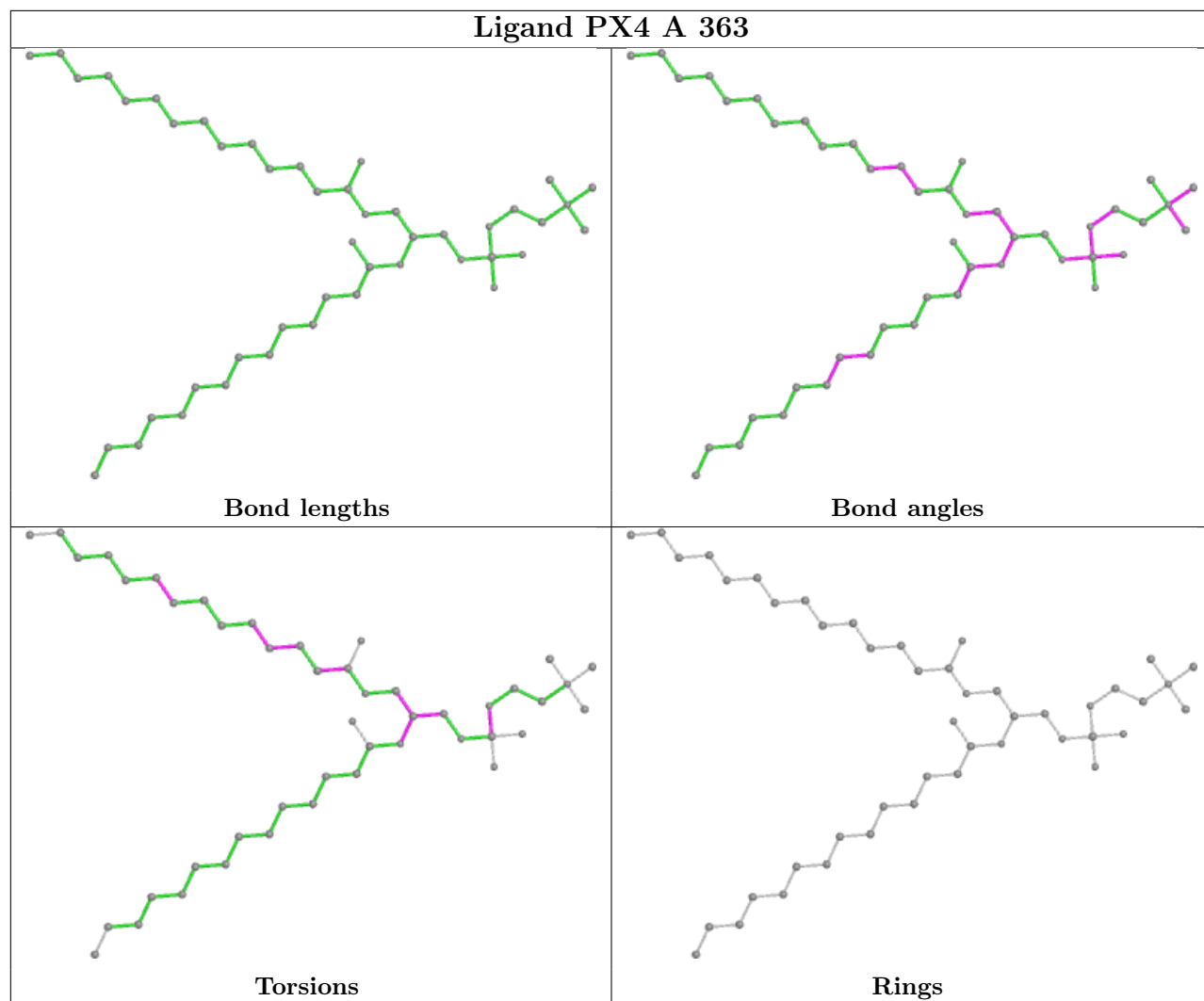


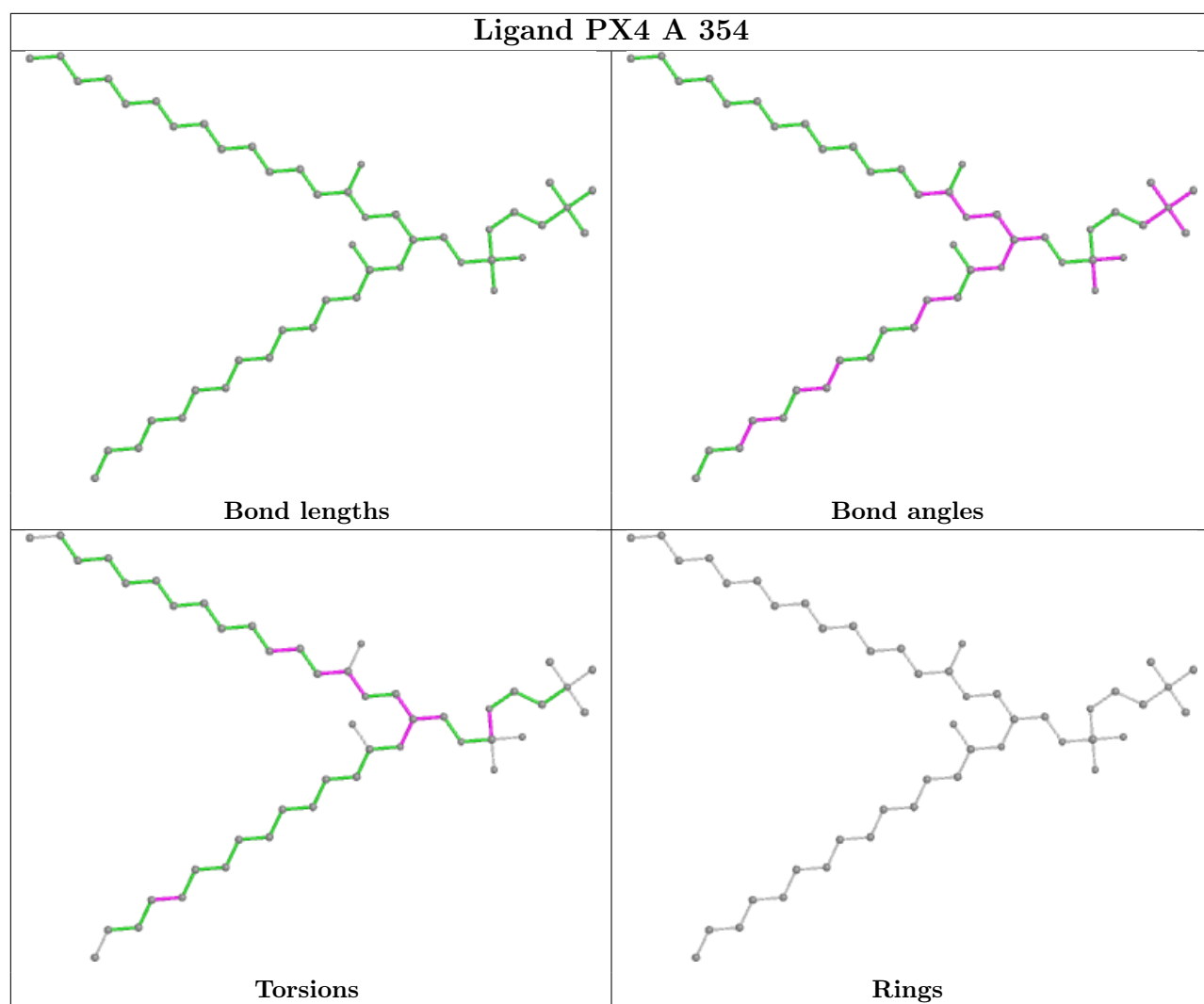


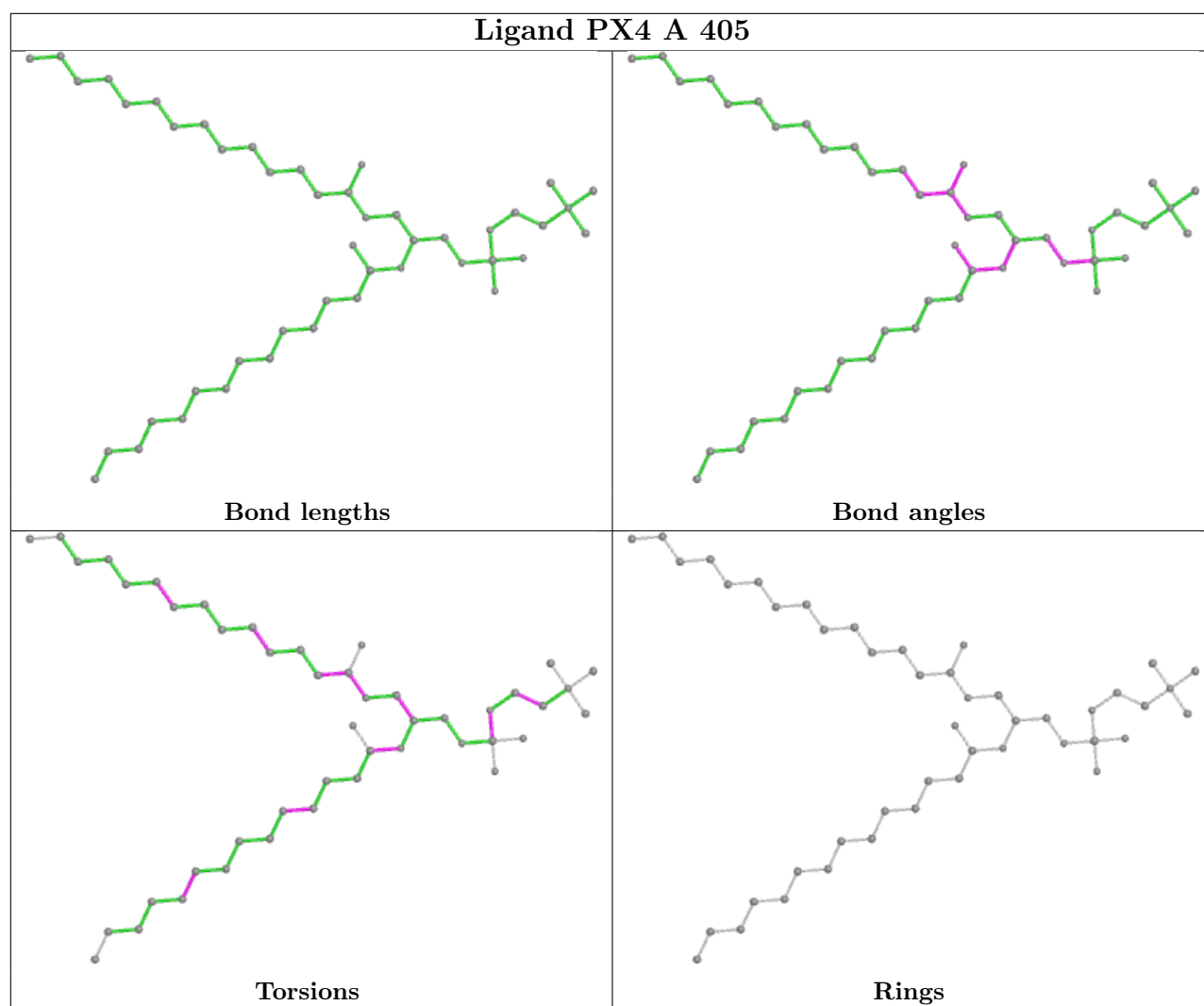


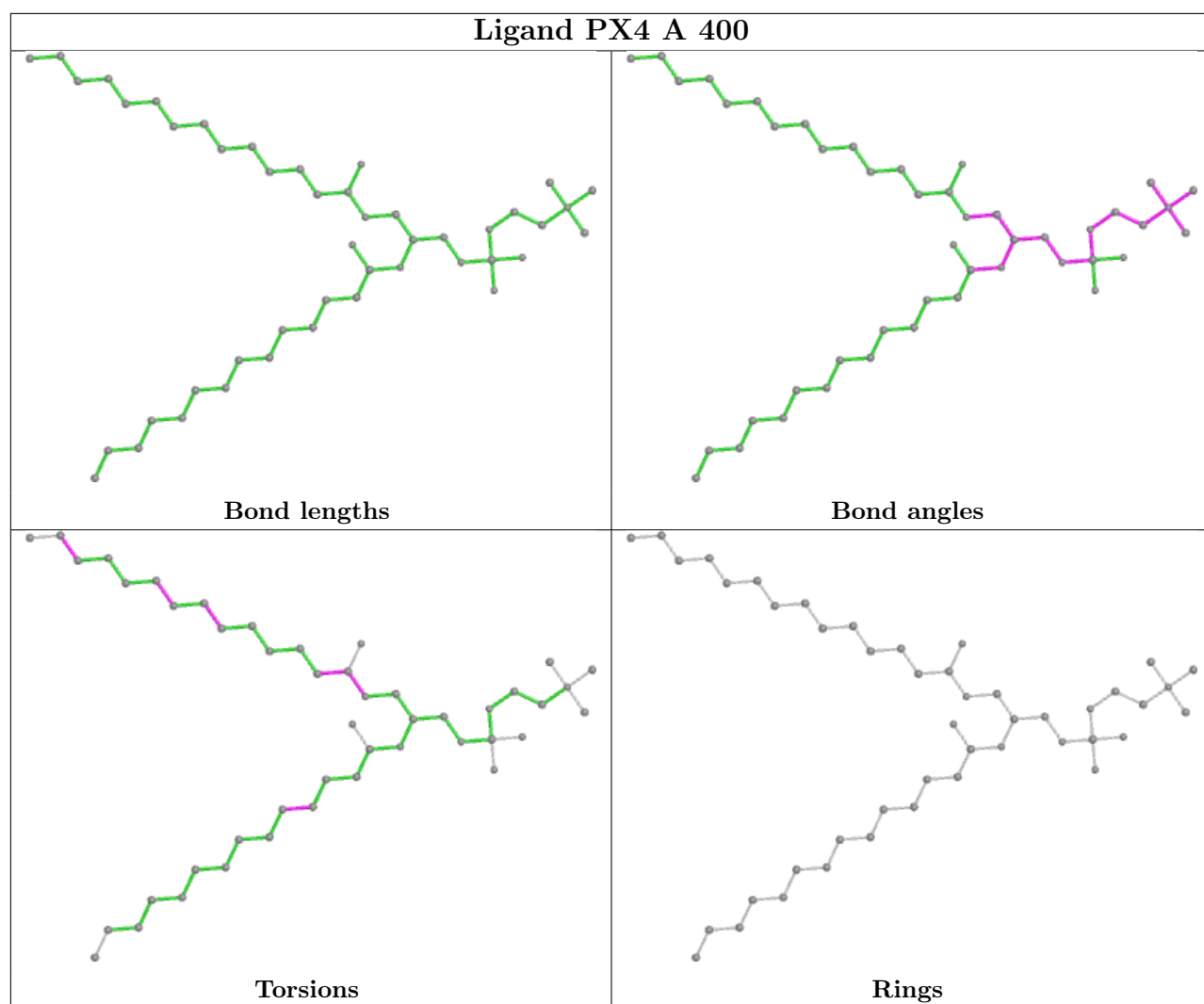


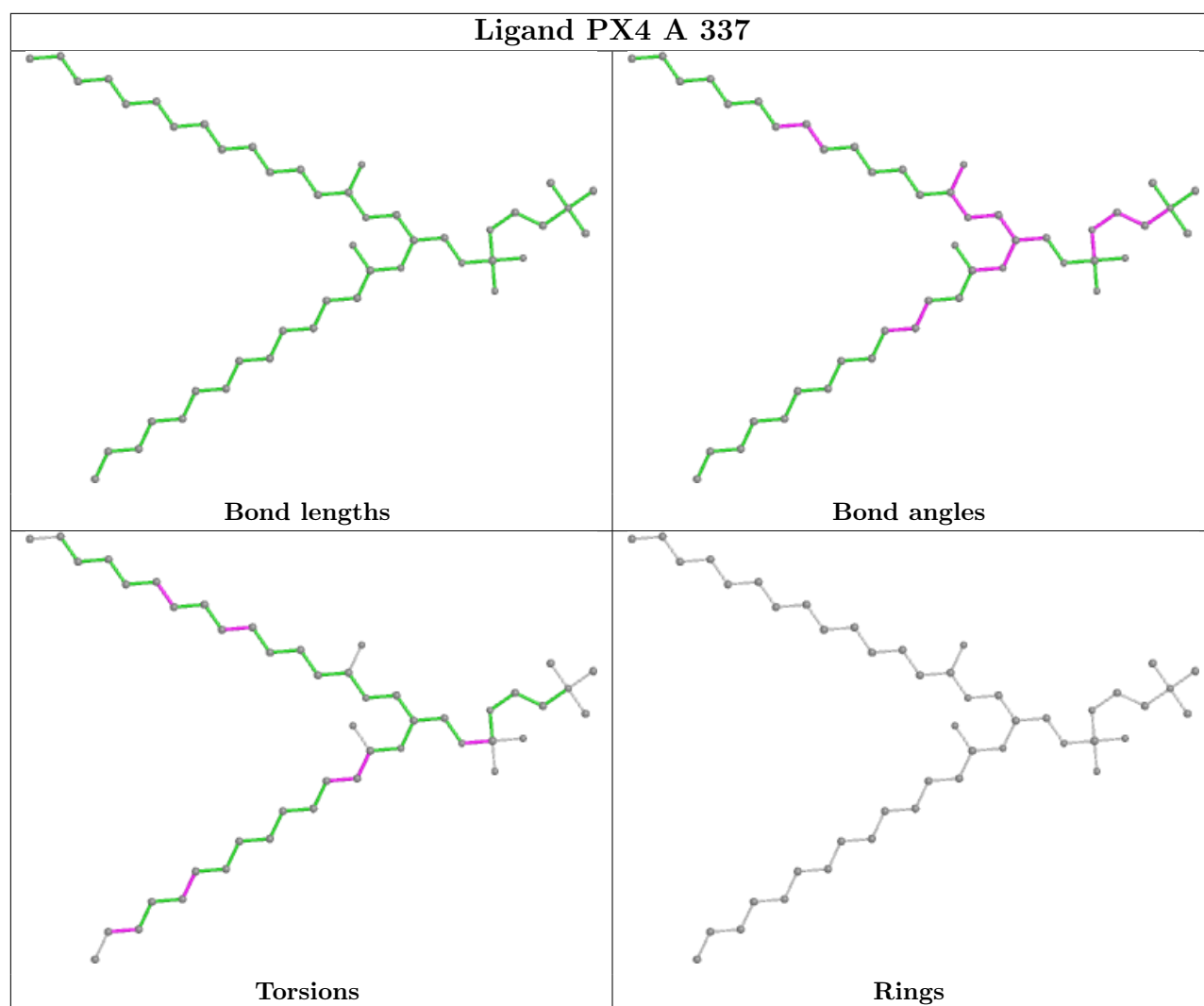
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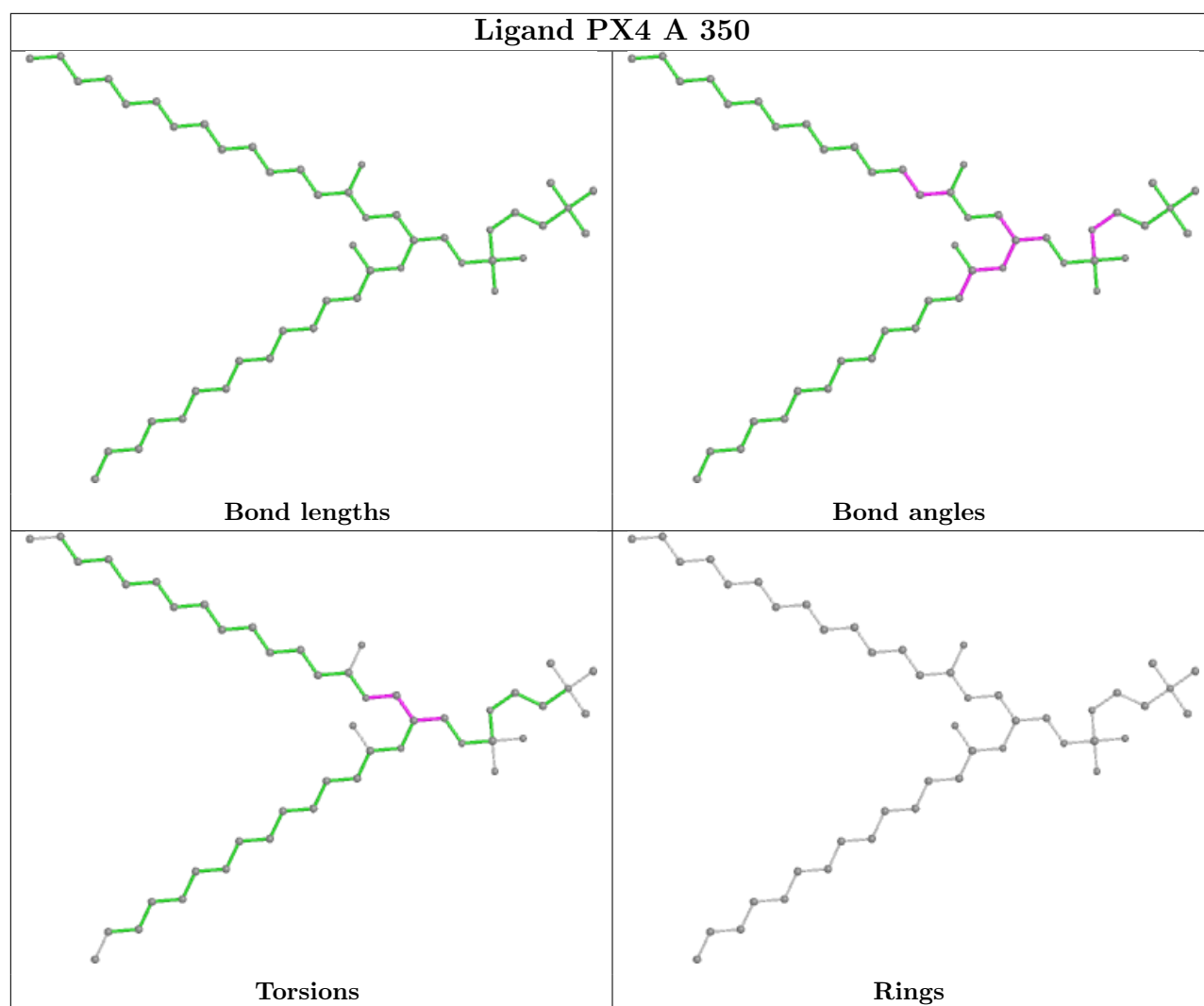


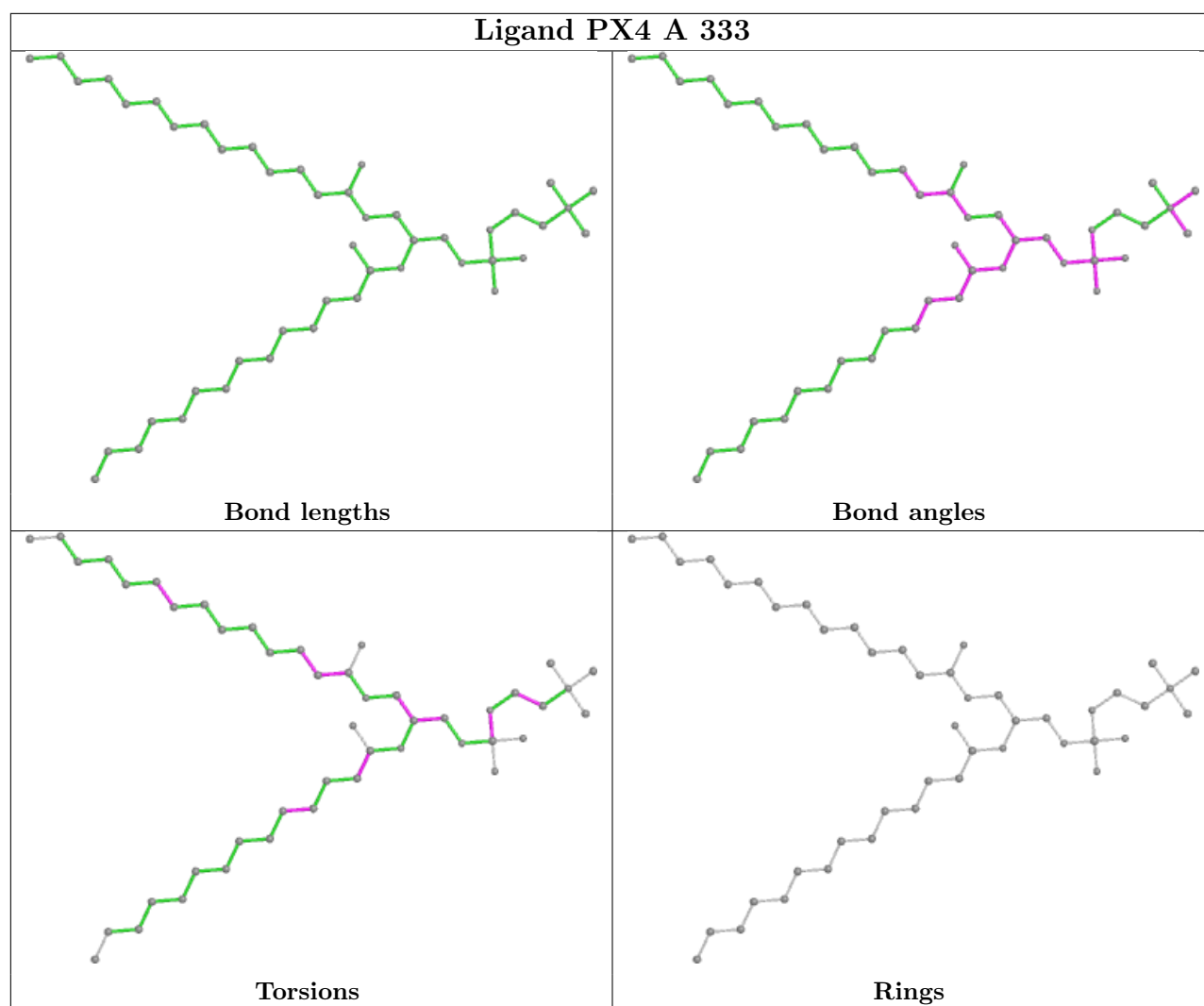


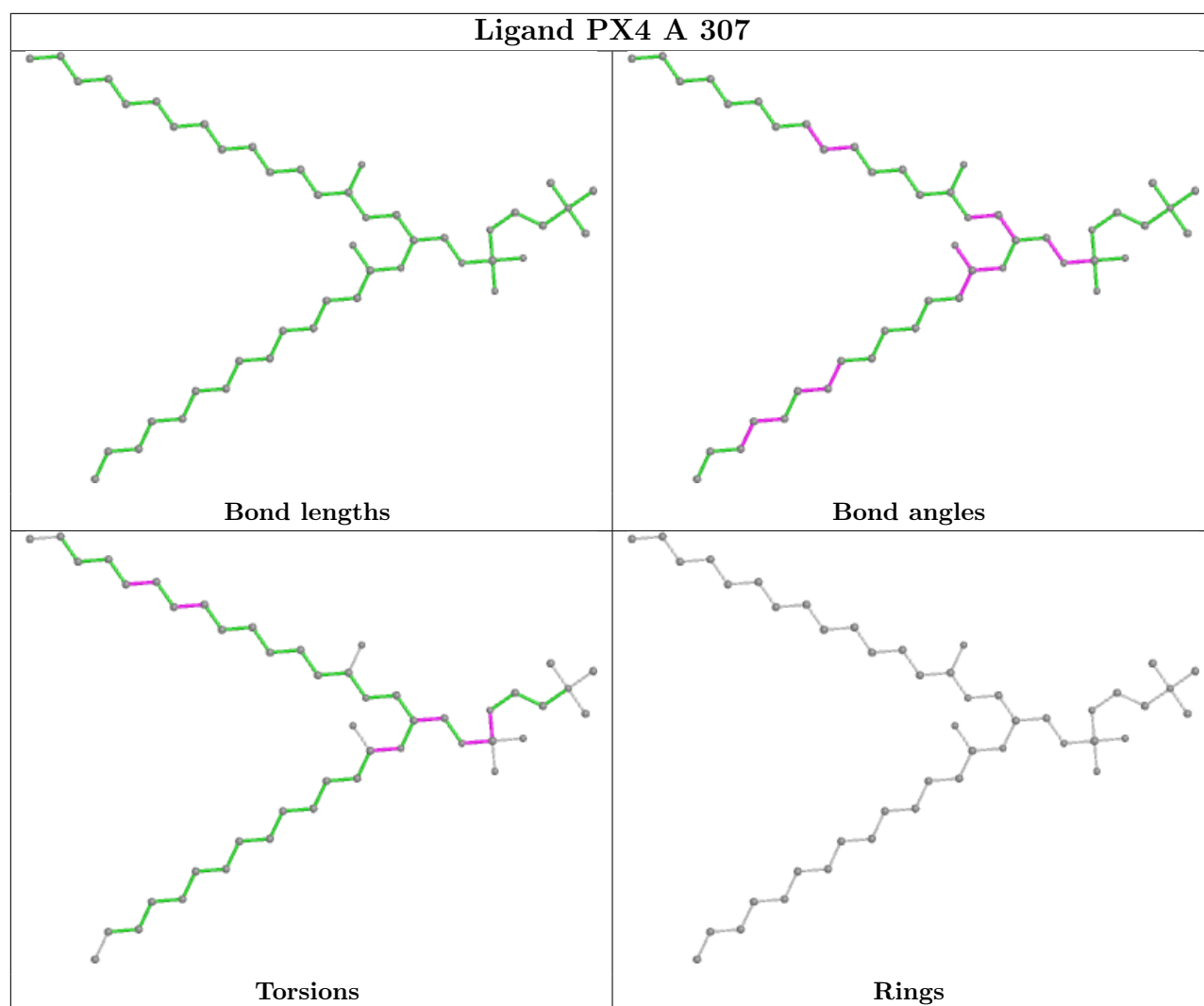


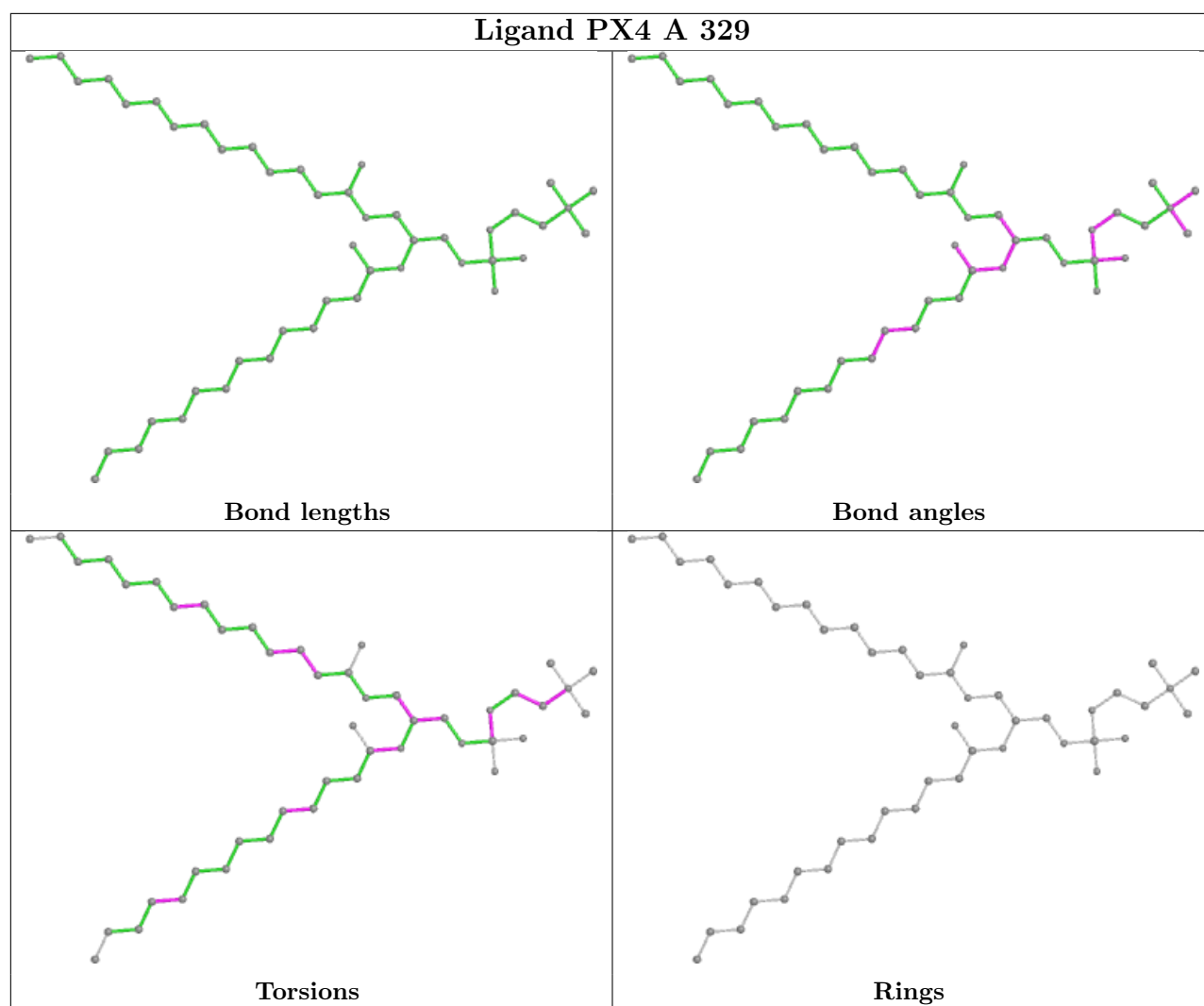


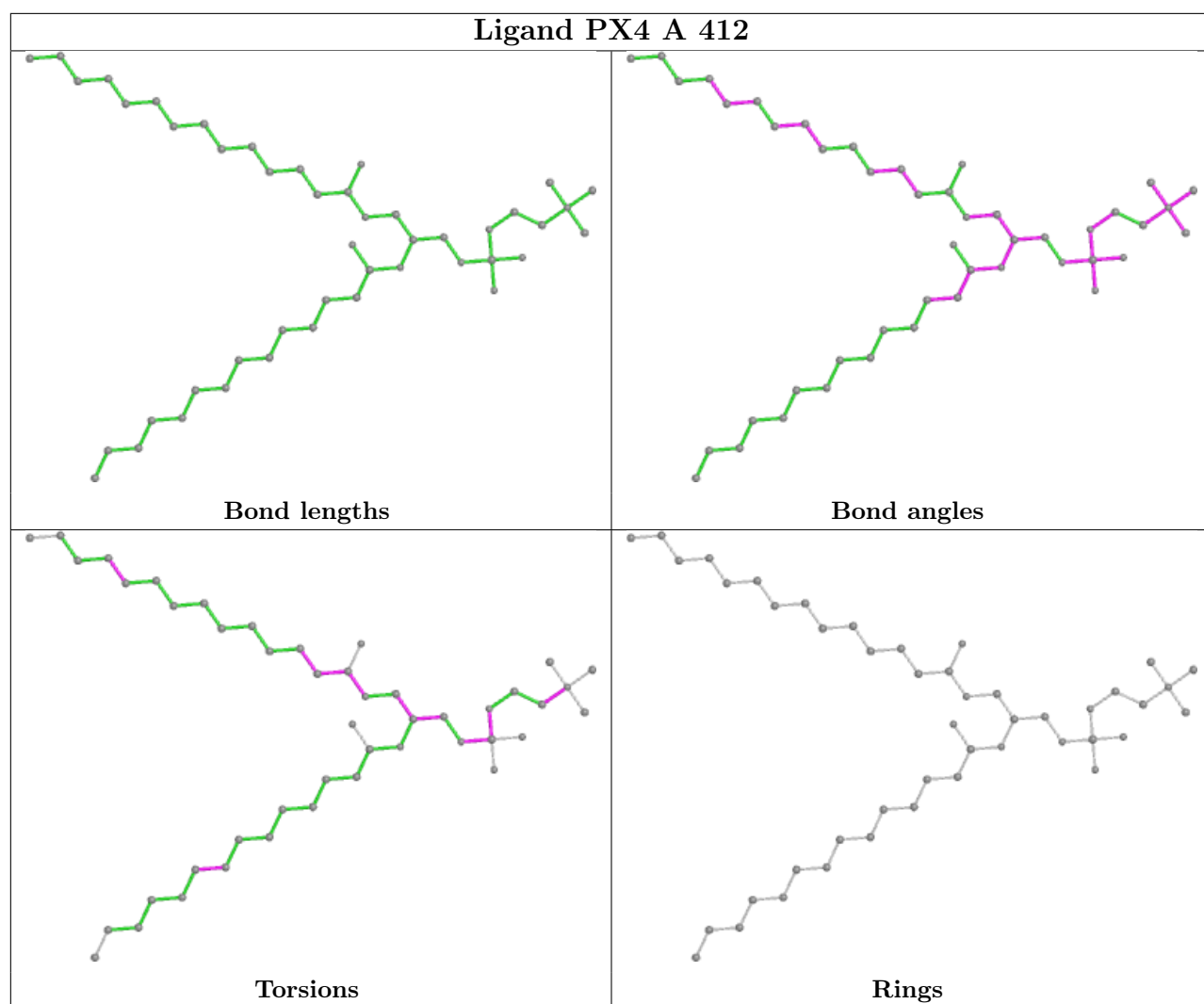


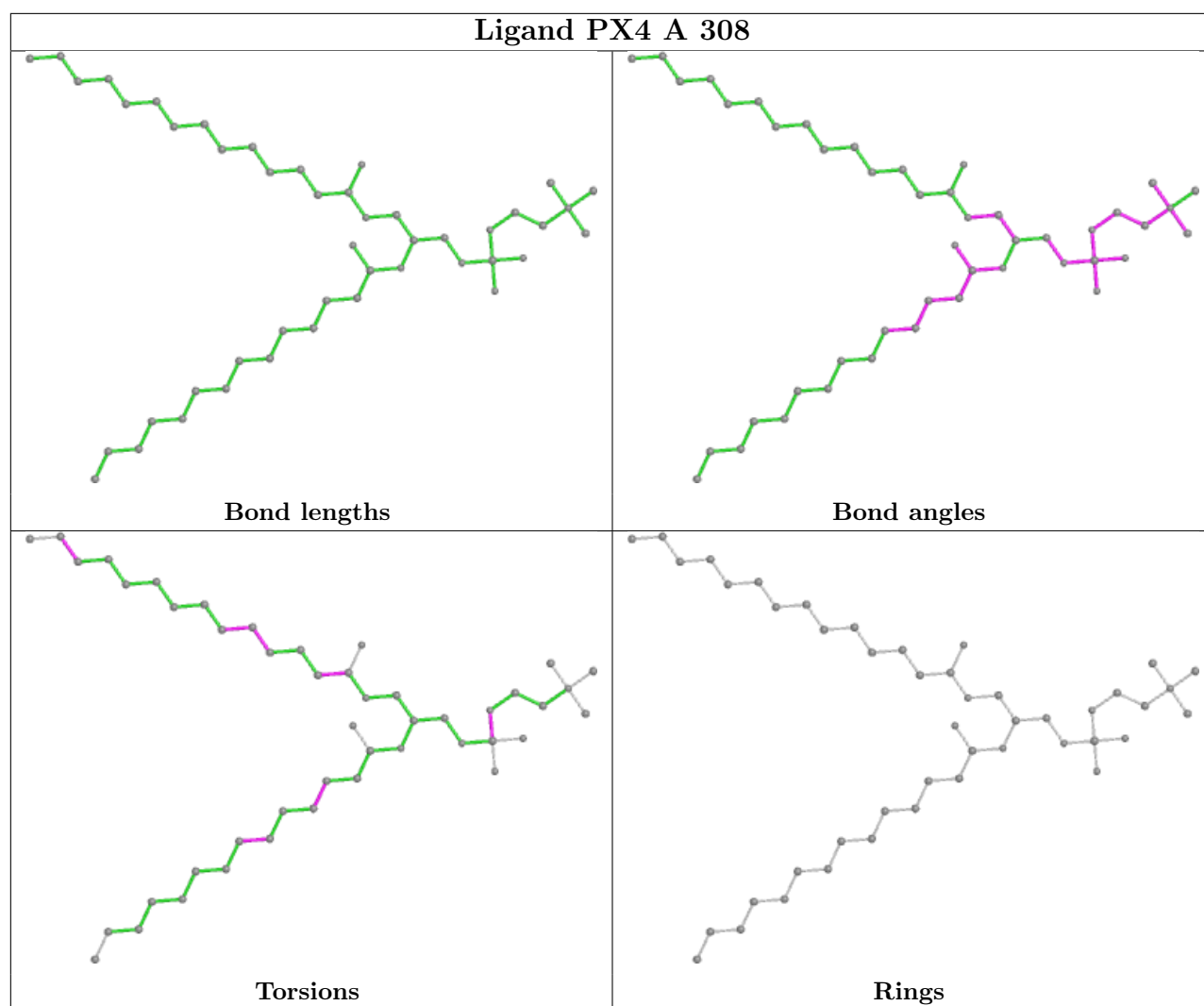


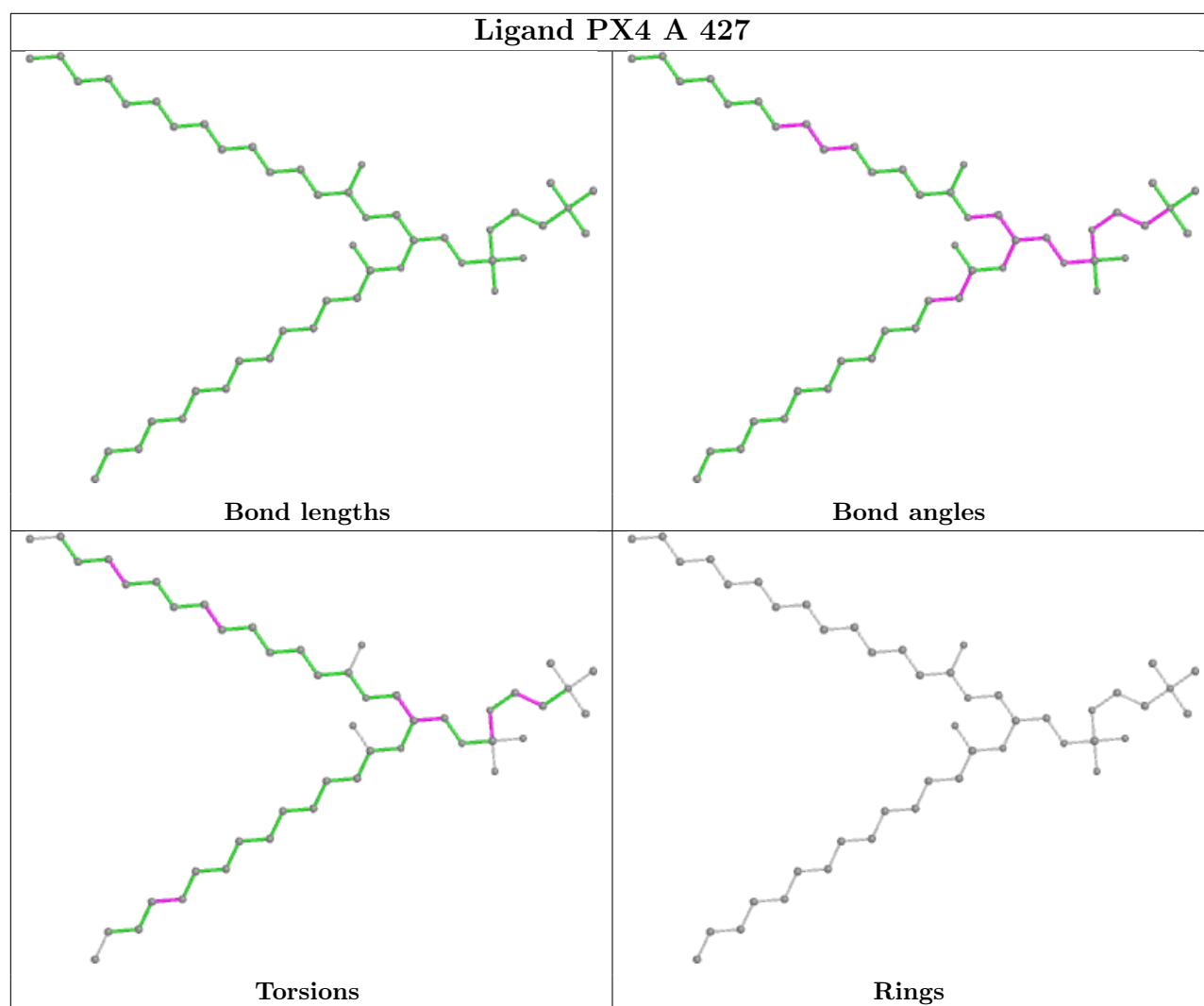


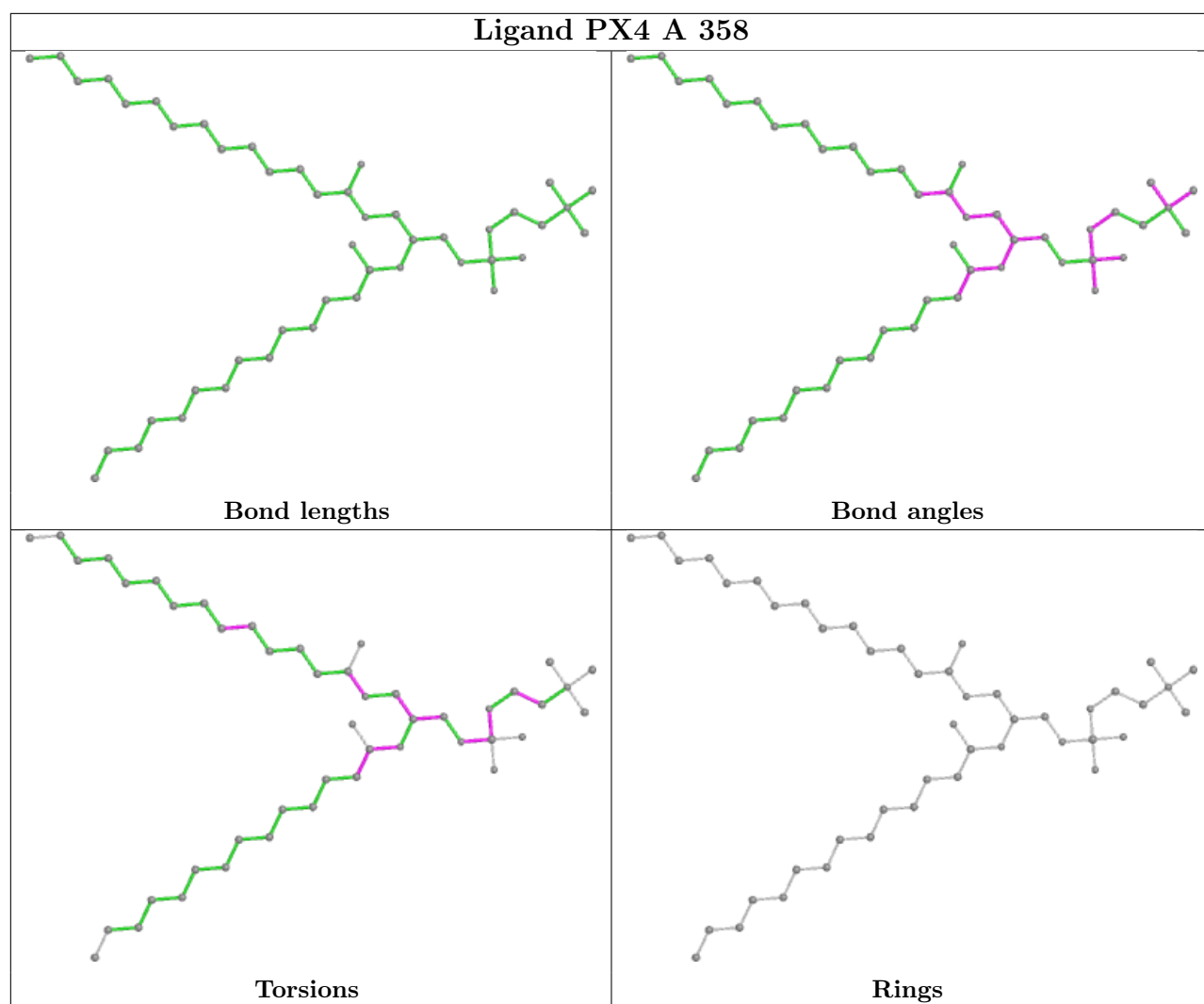


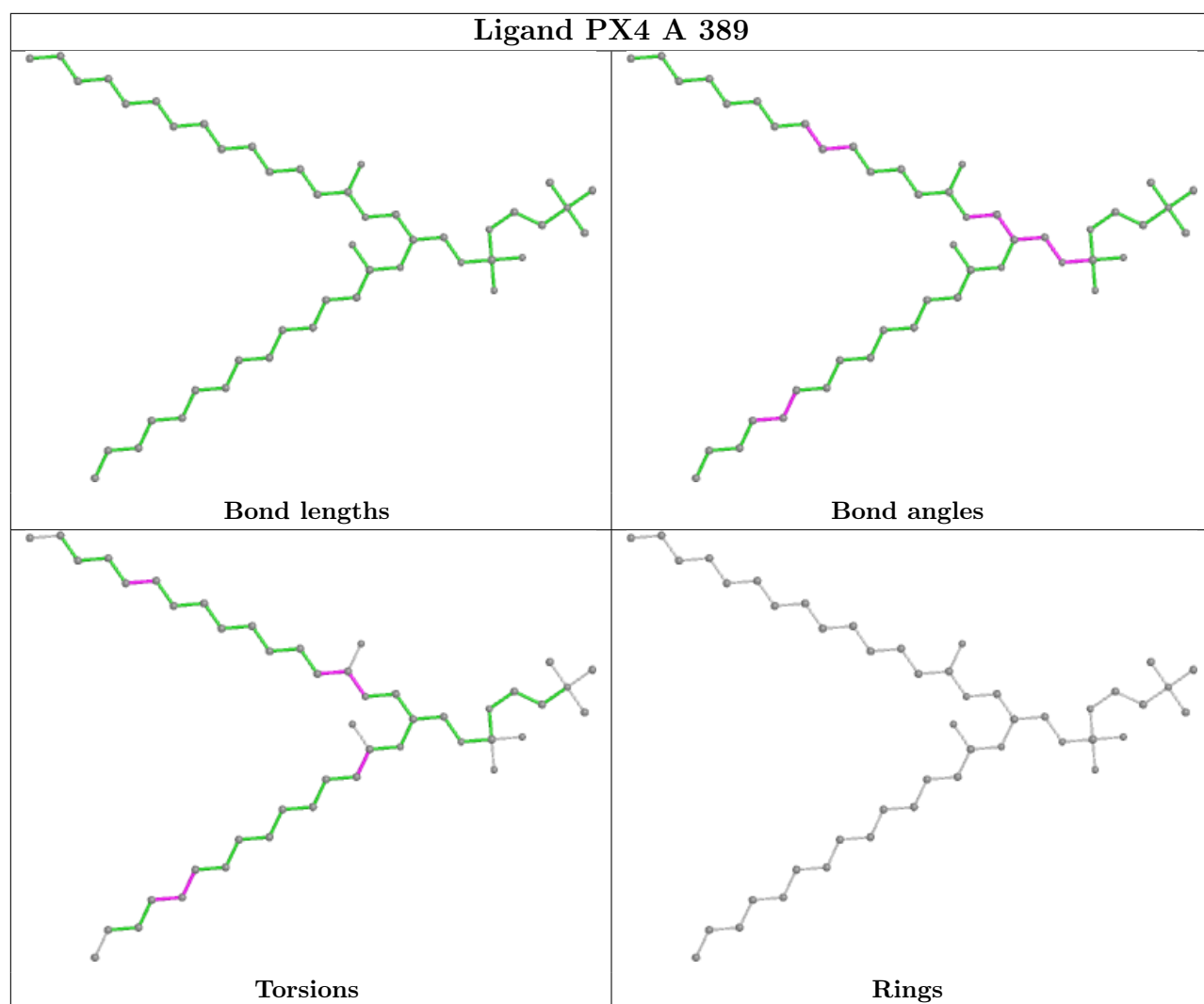


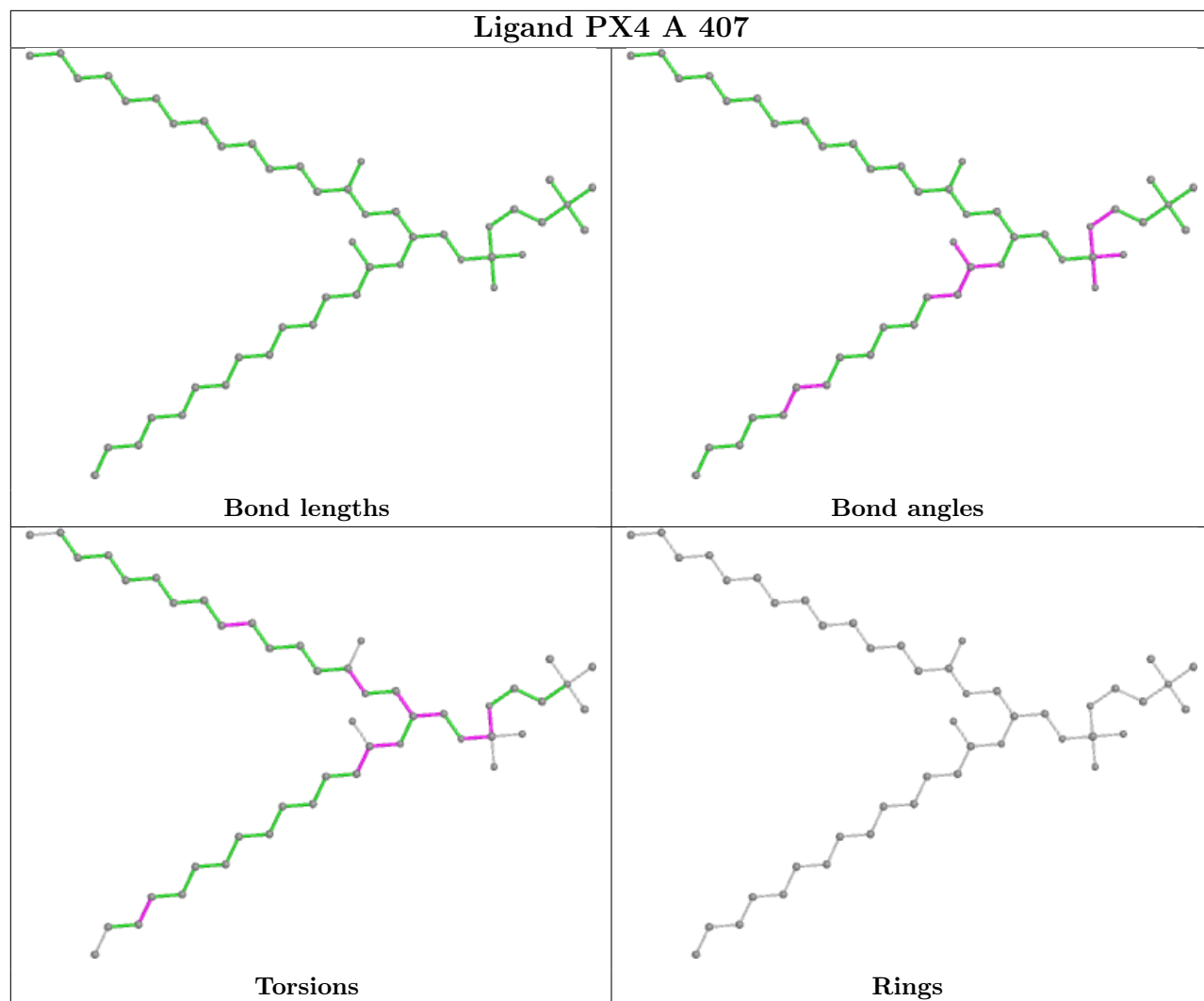


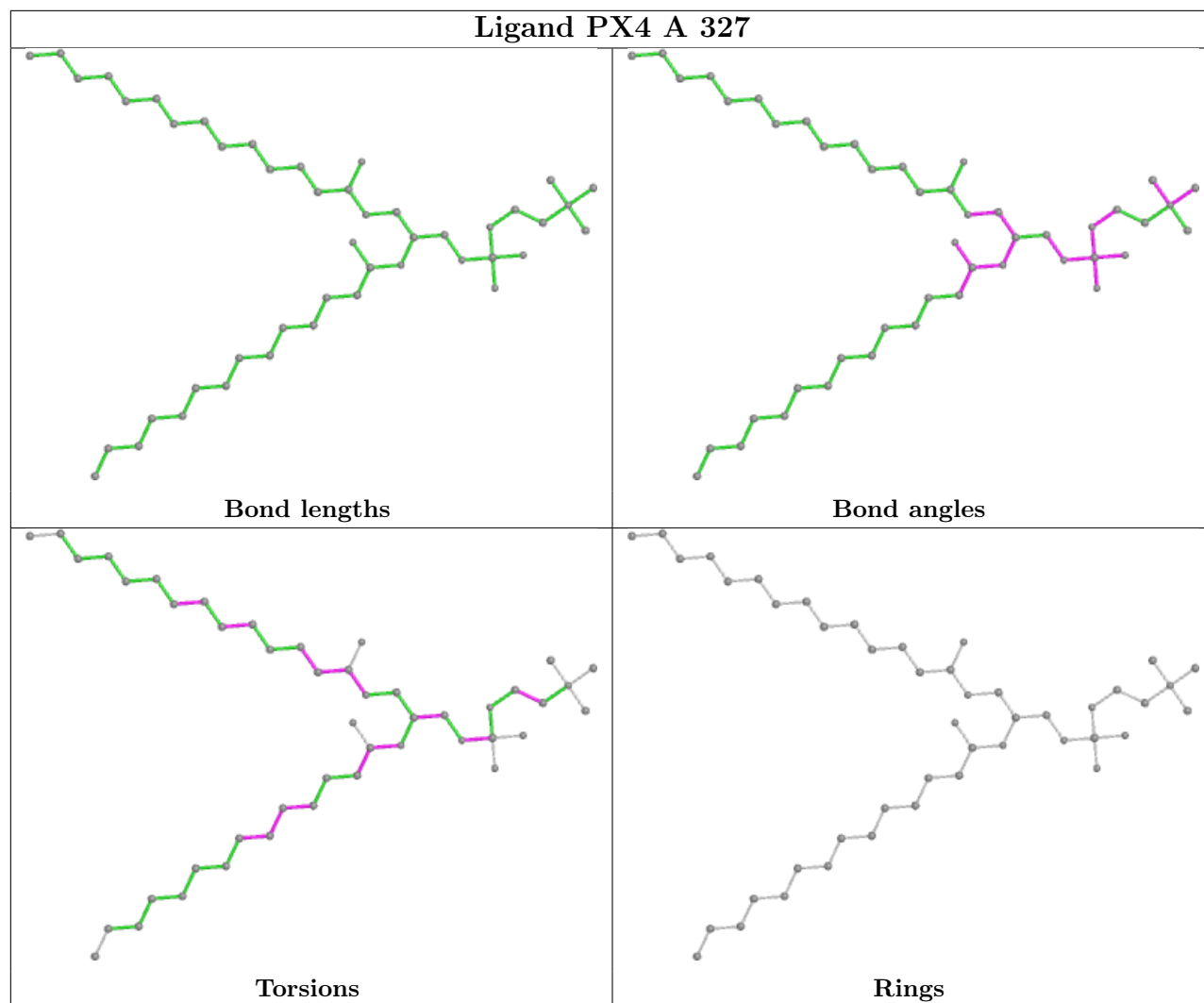


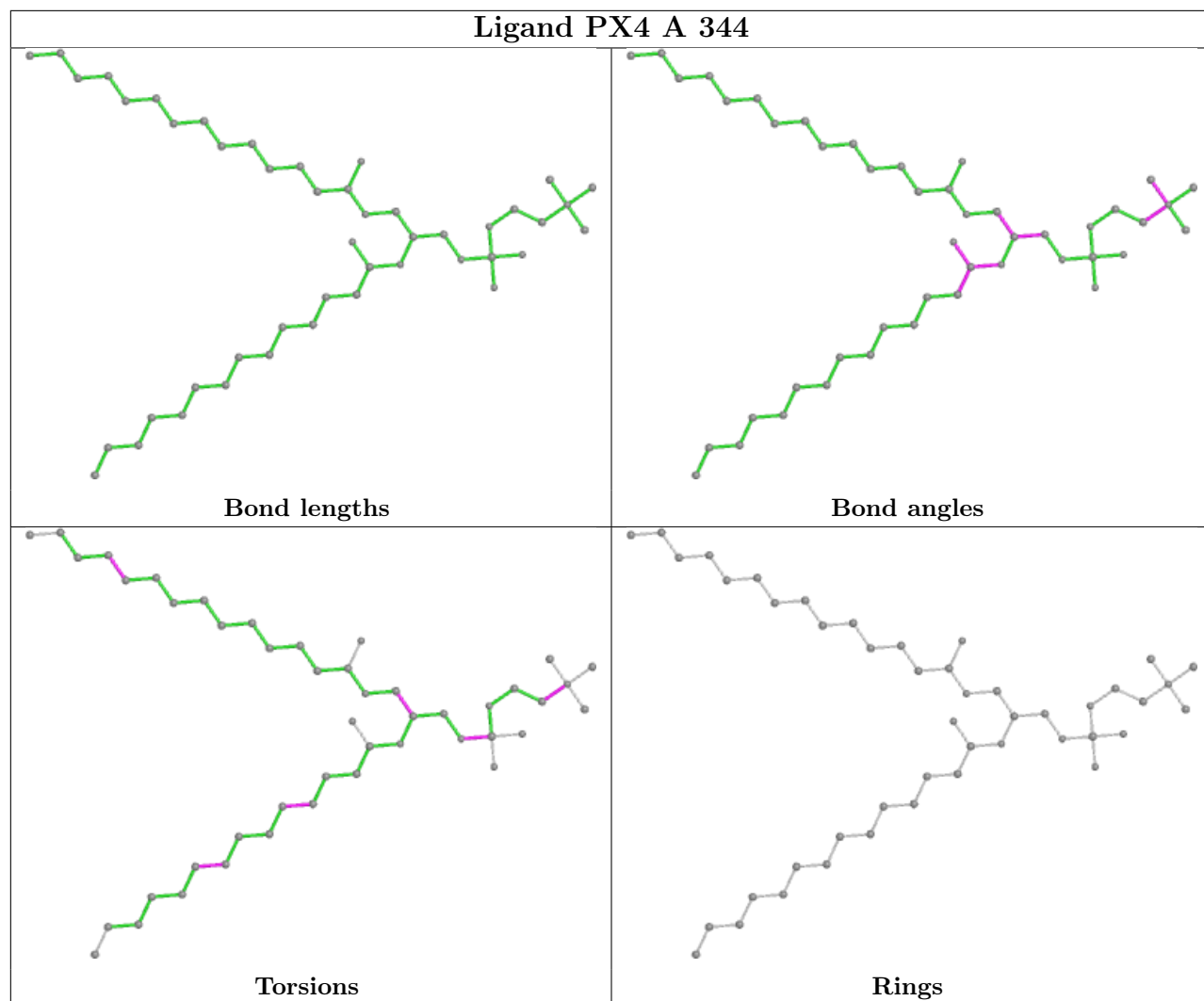


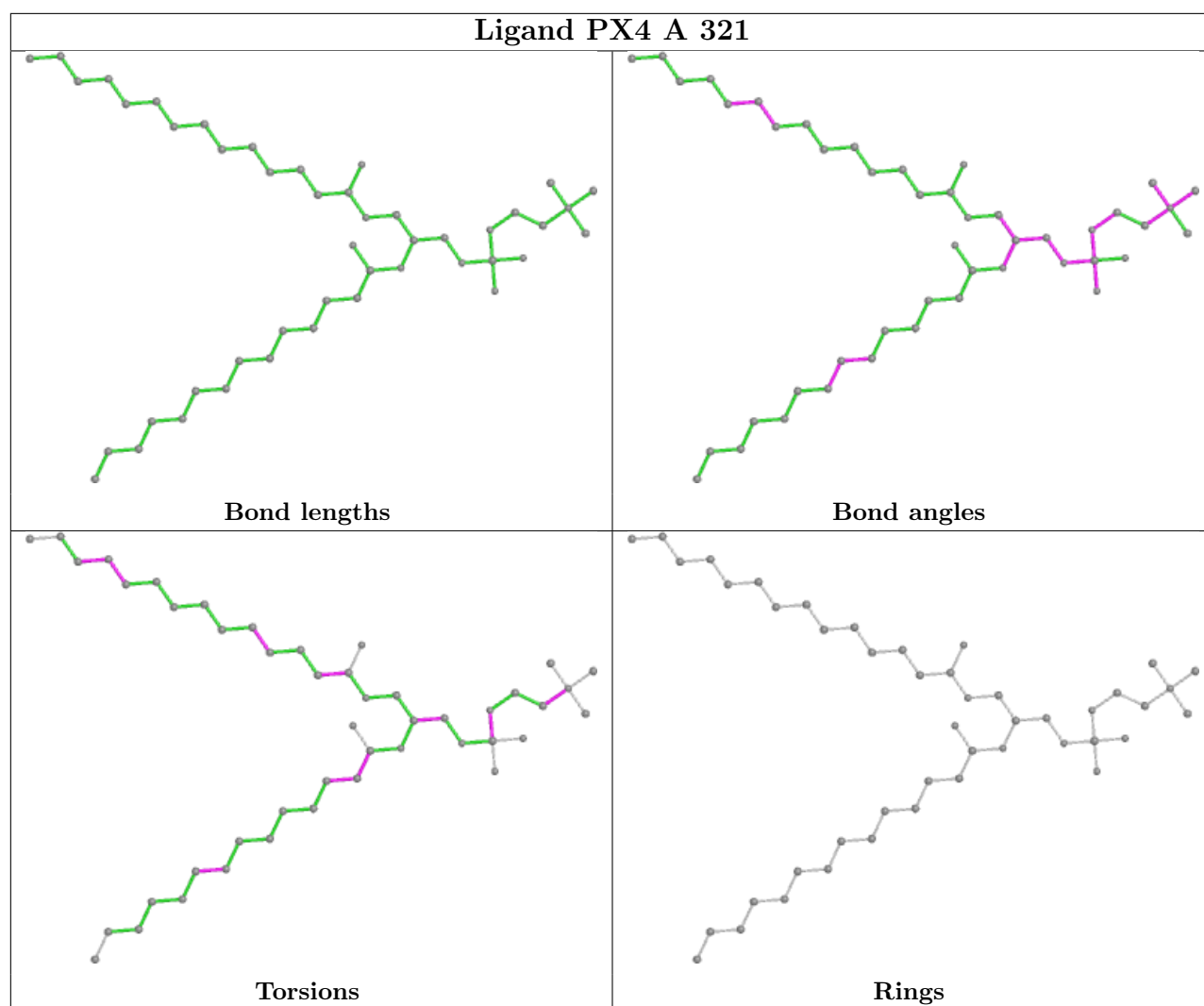


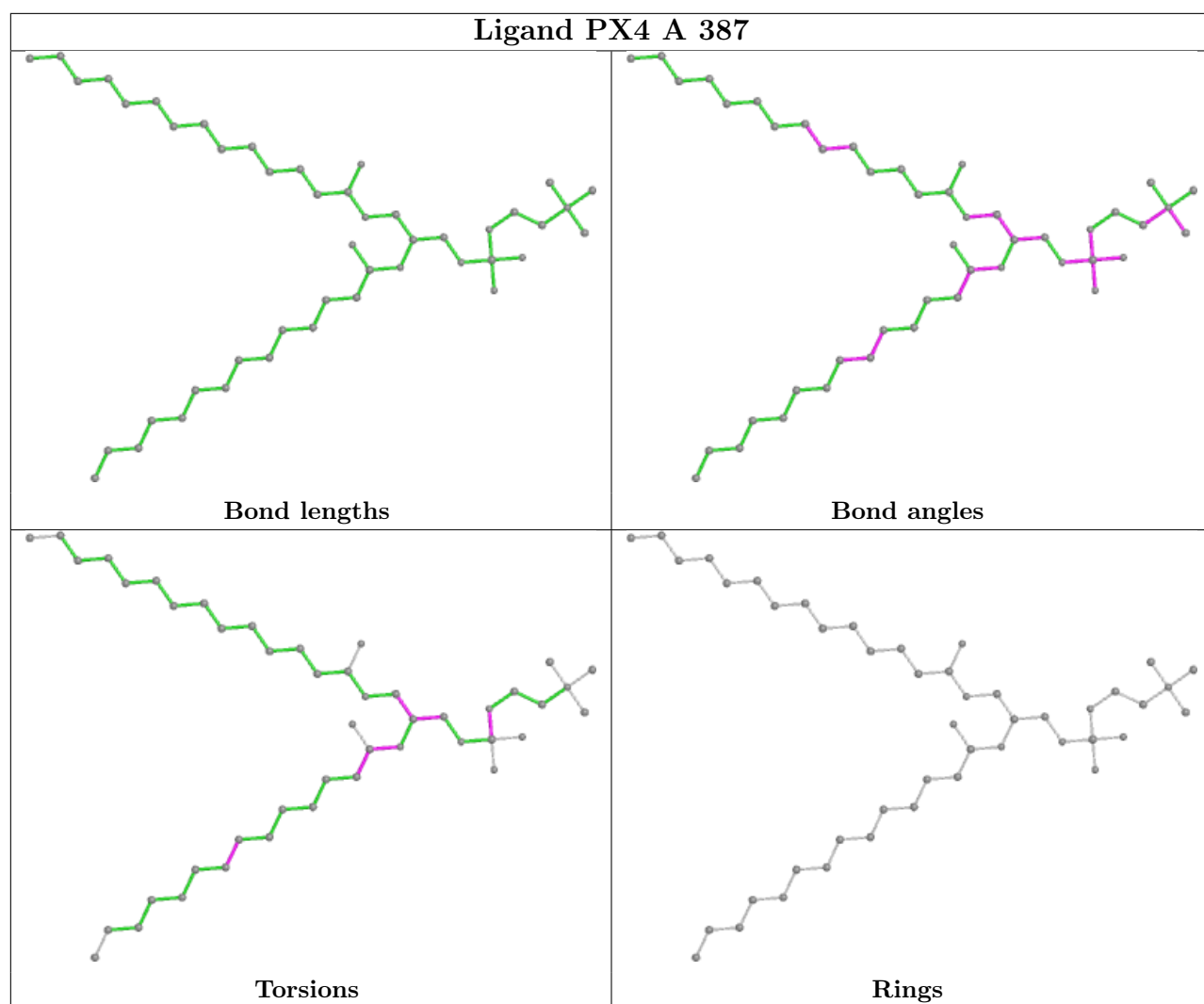


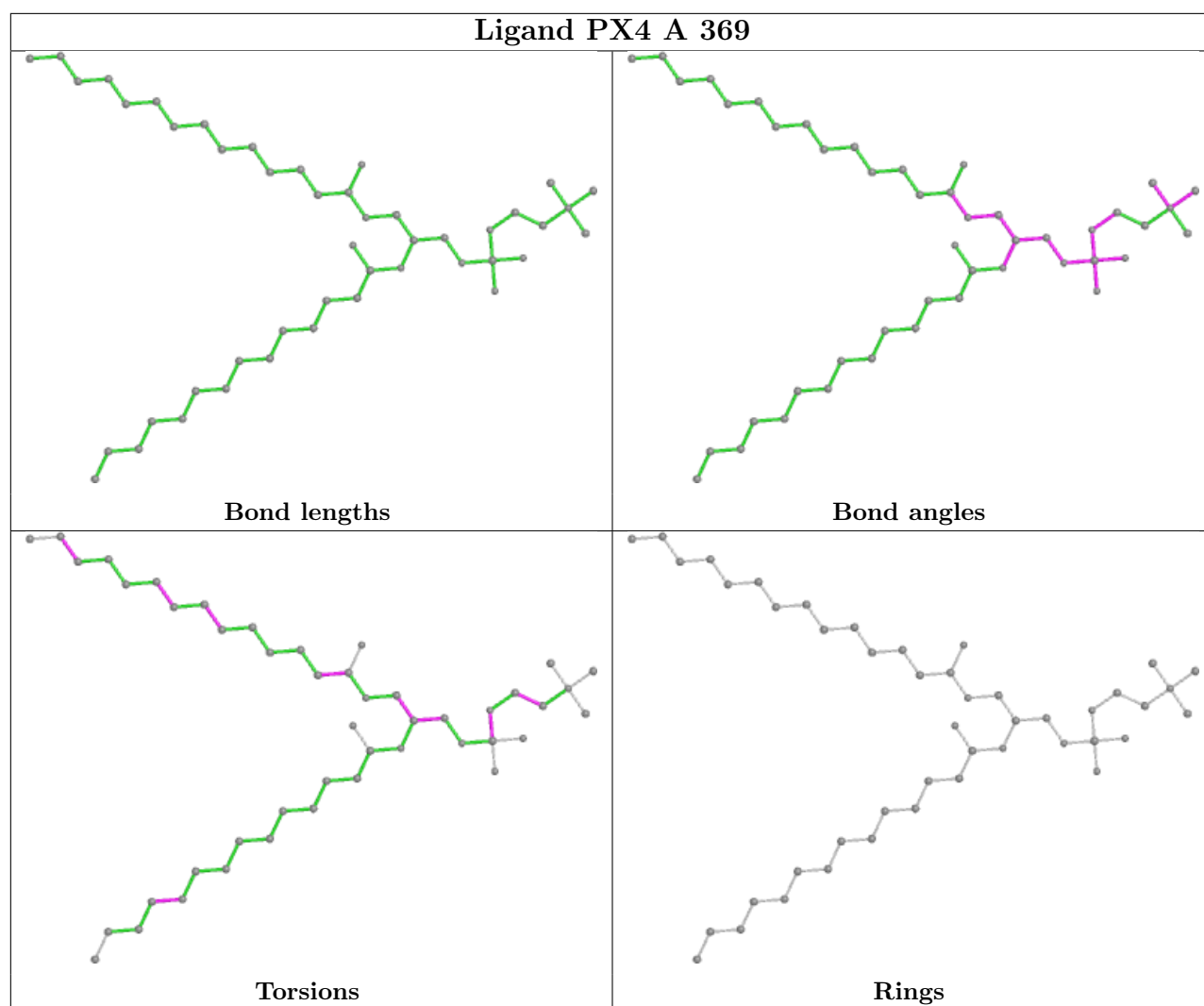




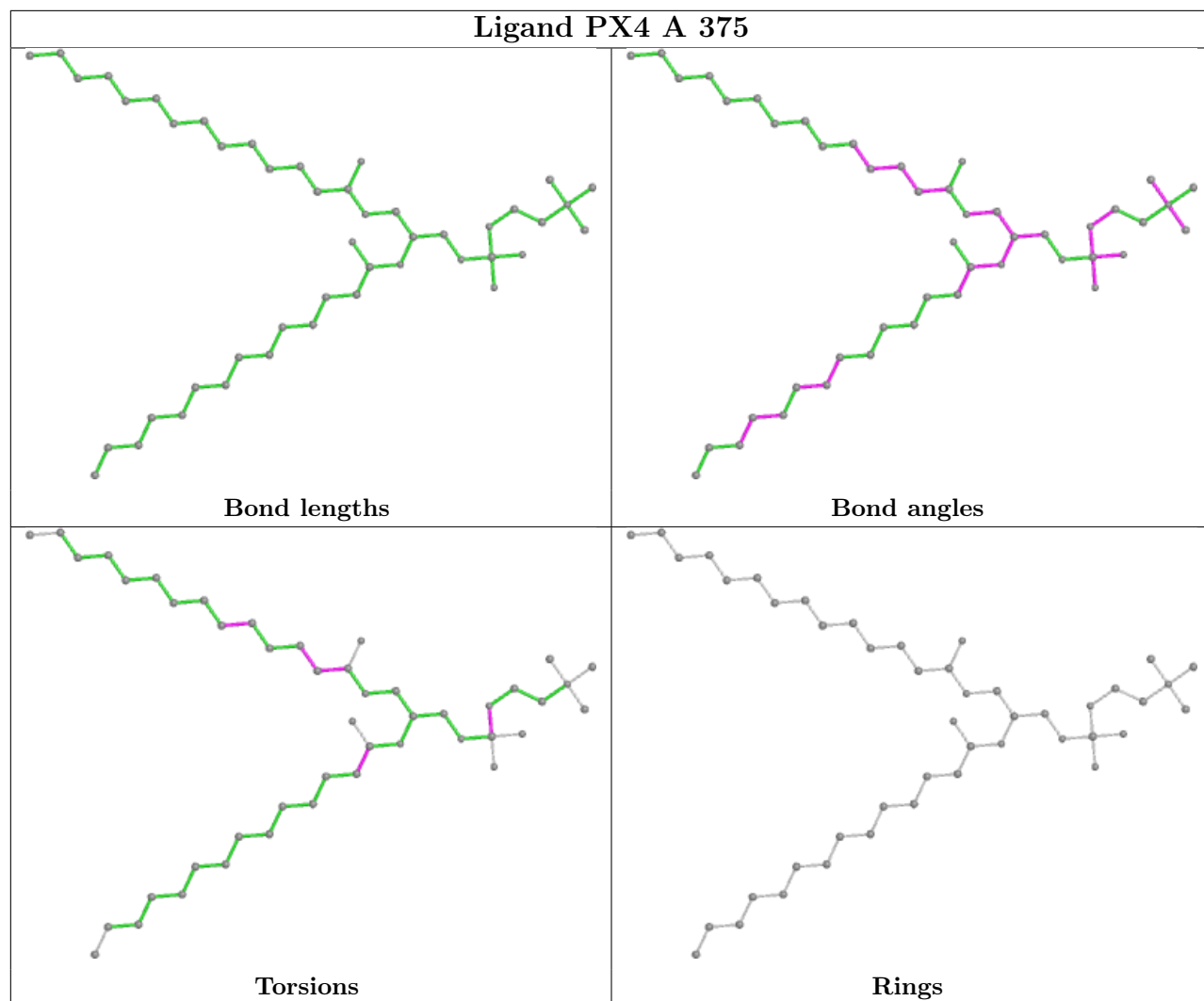


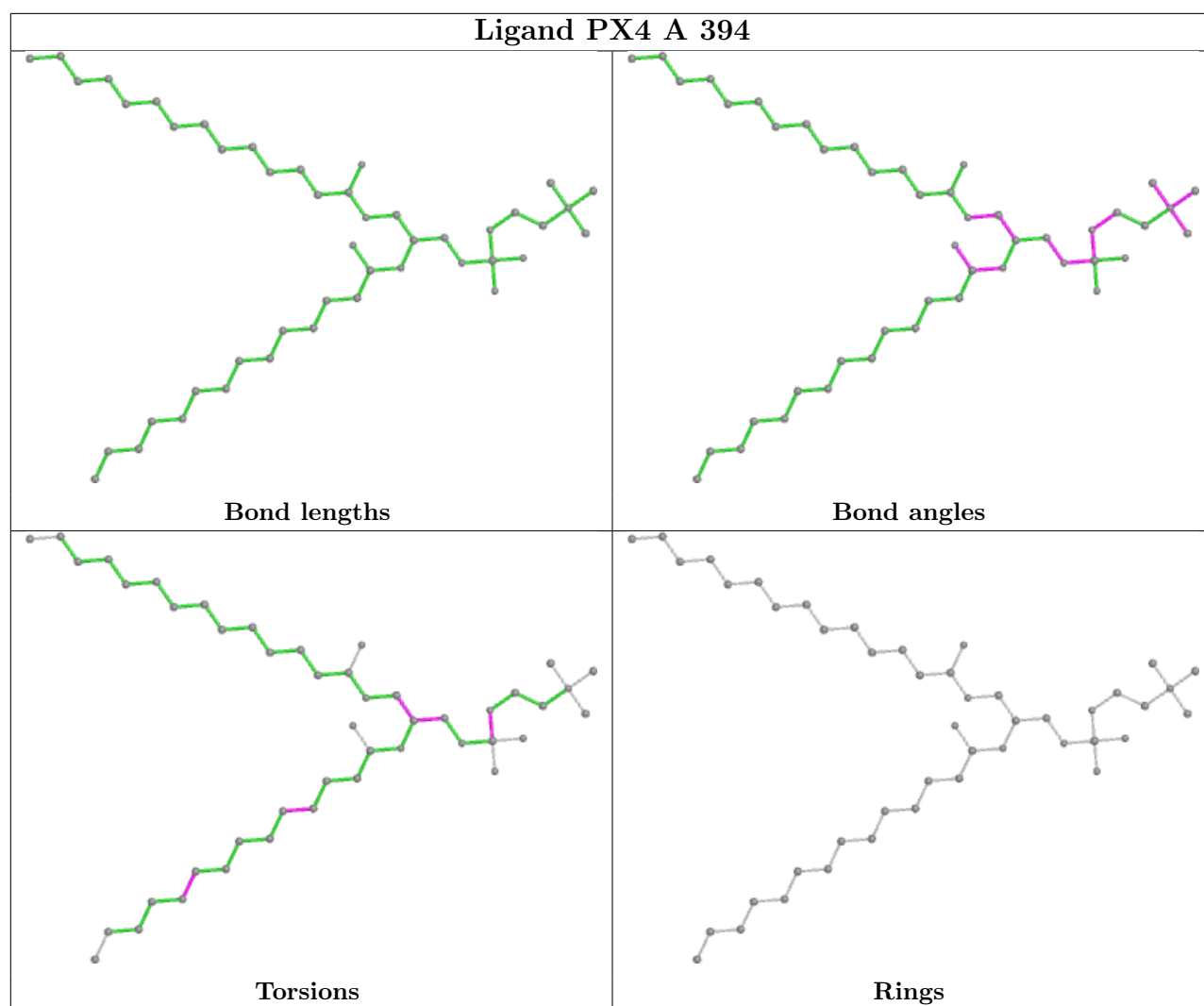


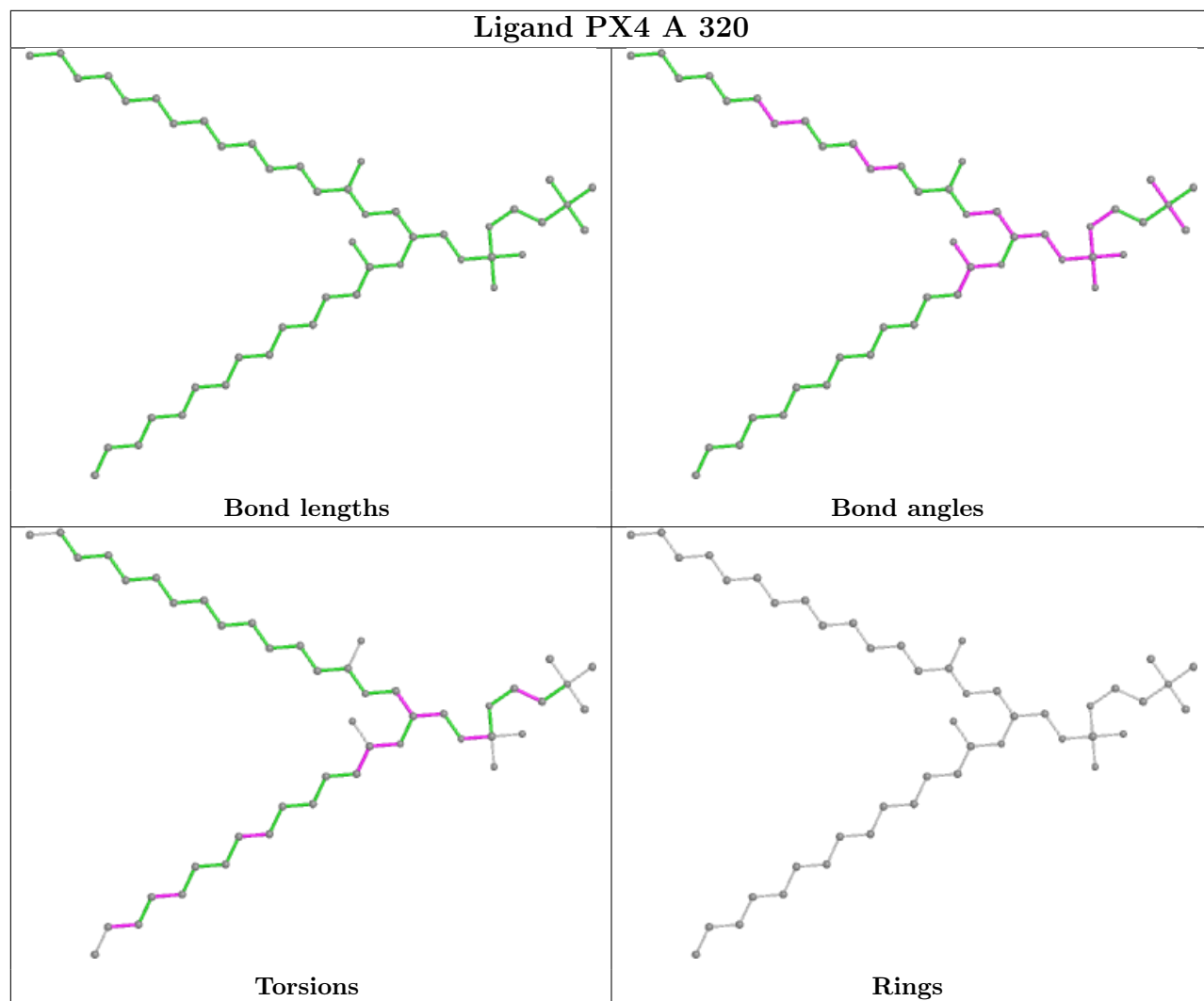


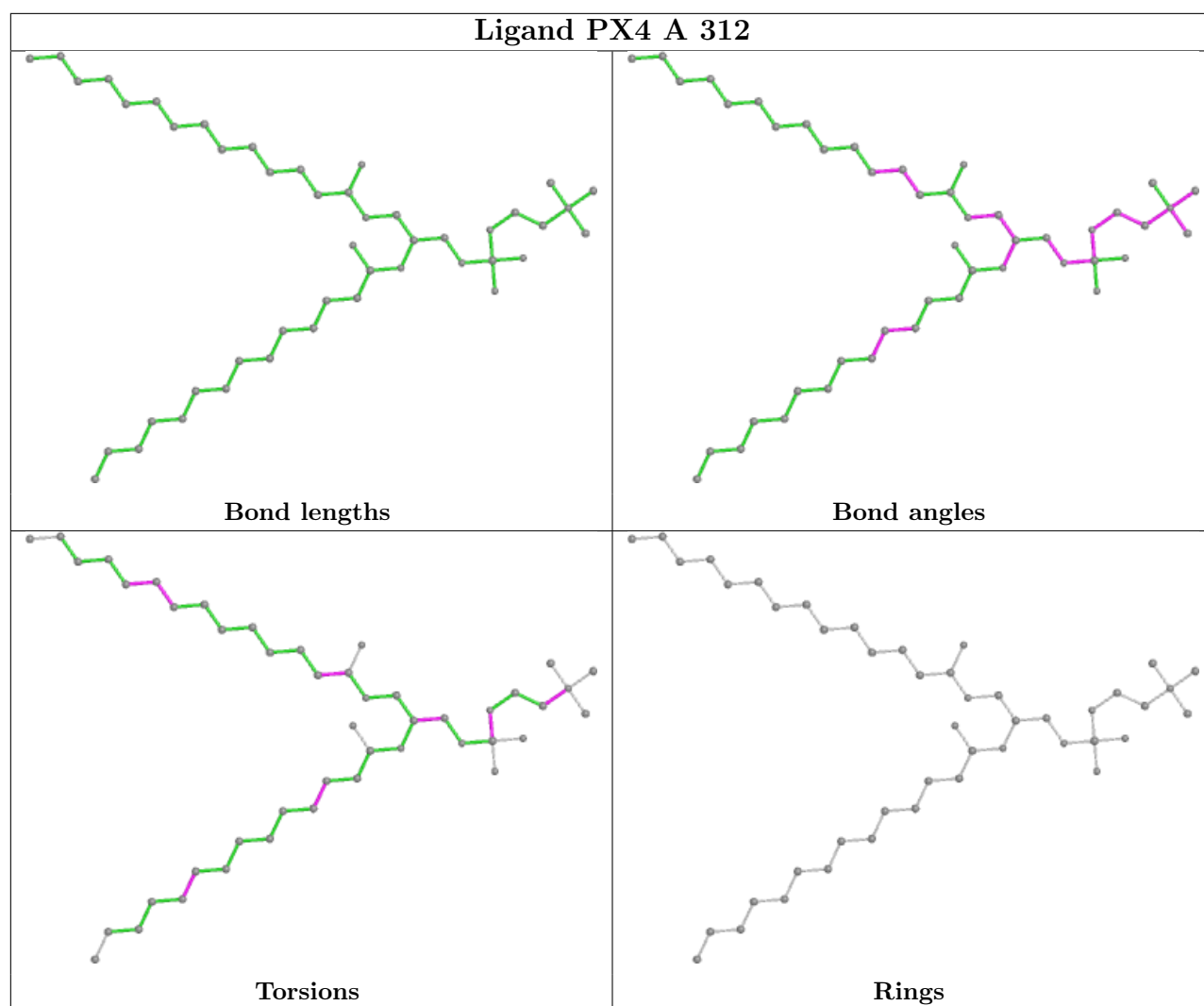


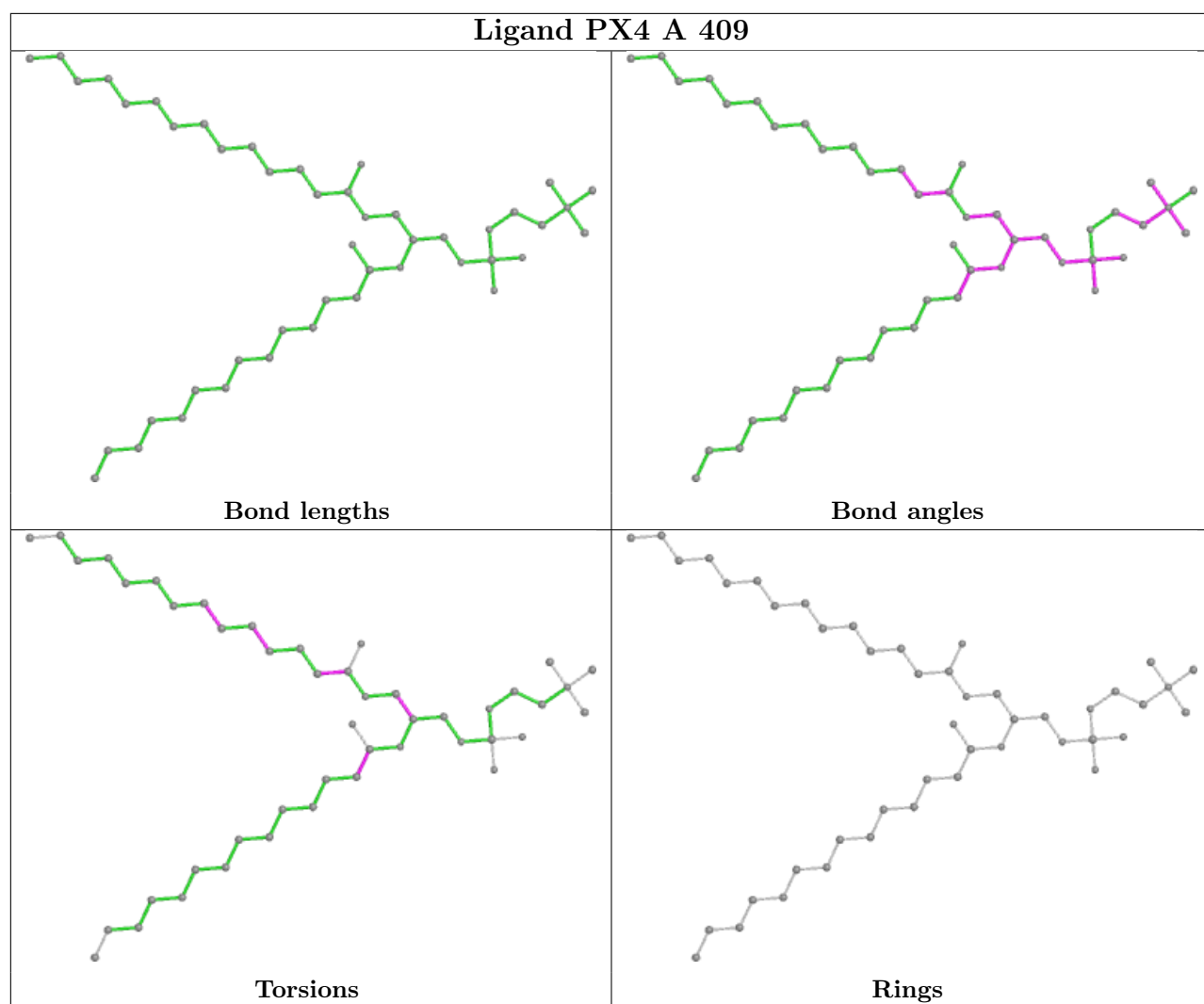
## Ligand PX4 A 375

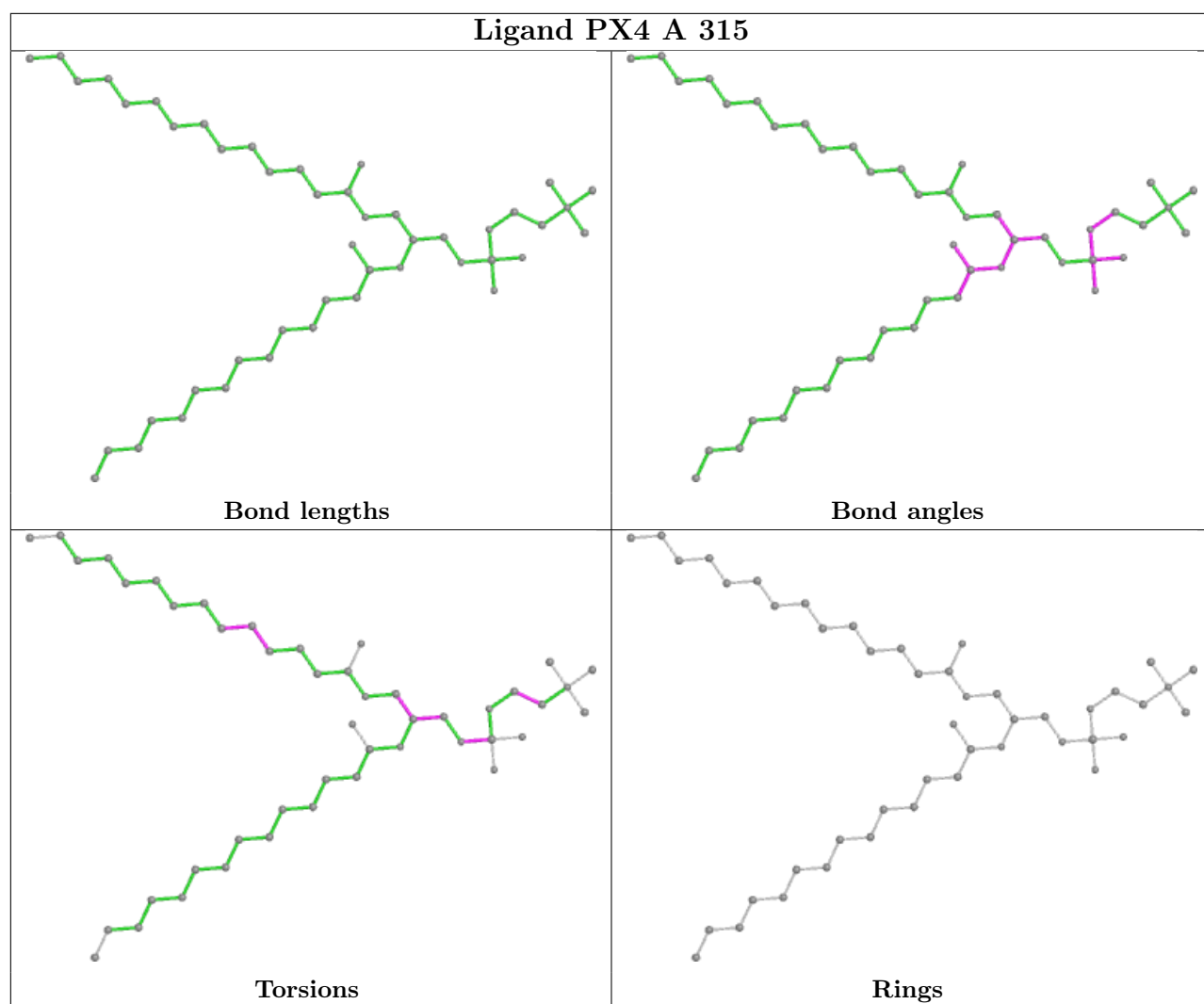


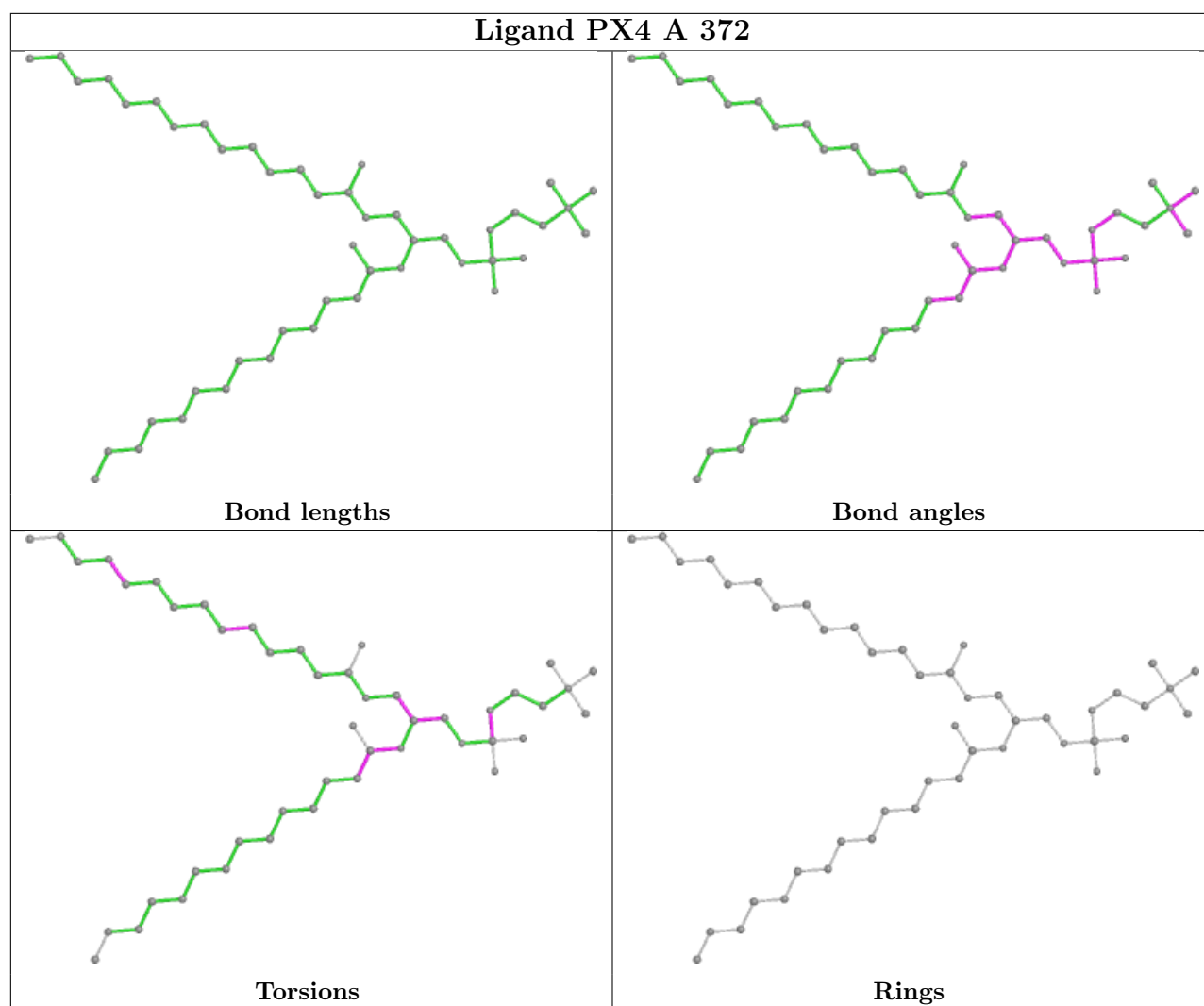


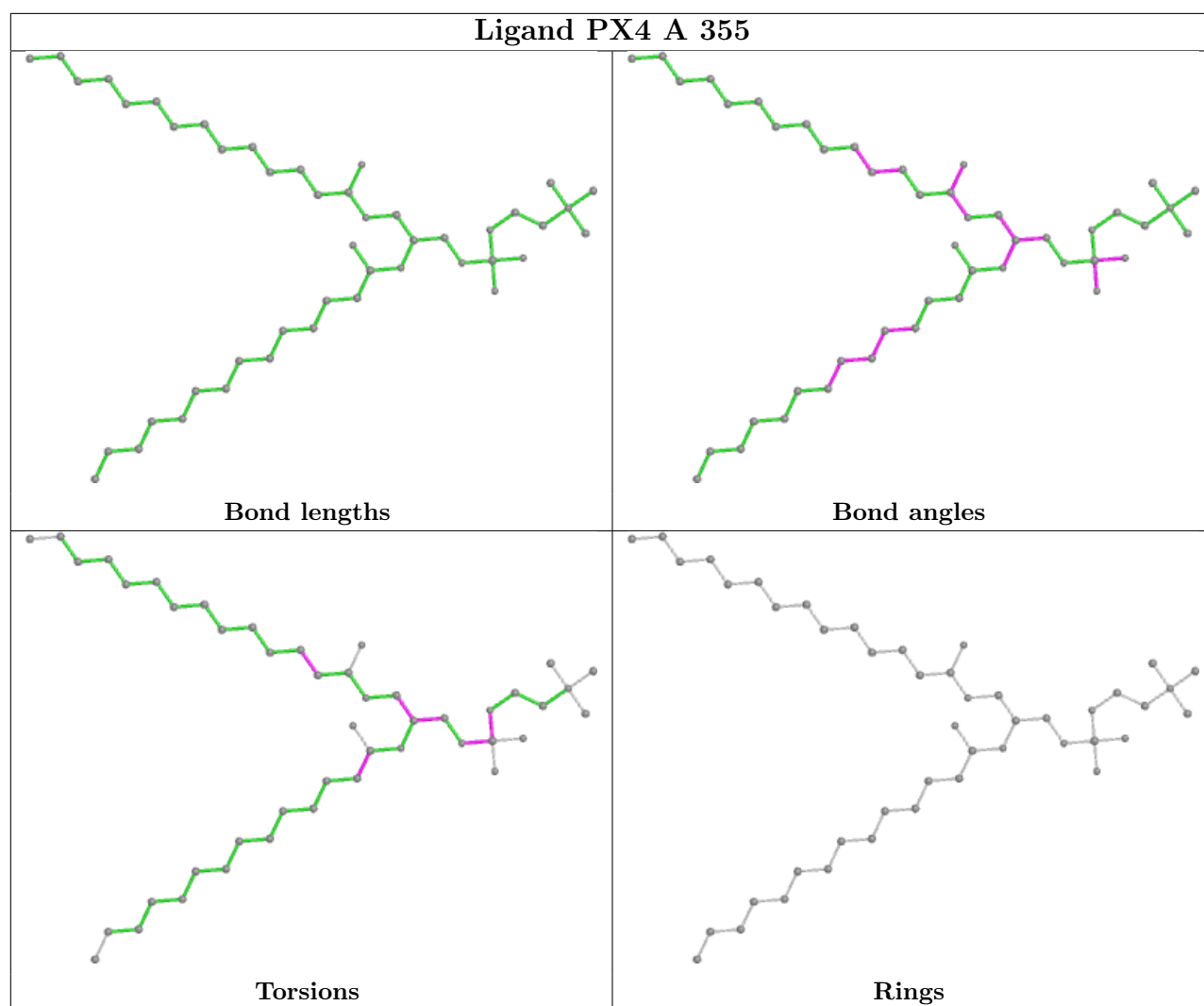




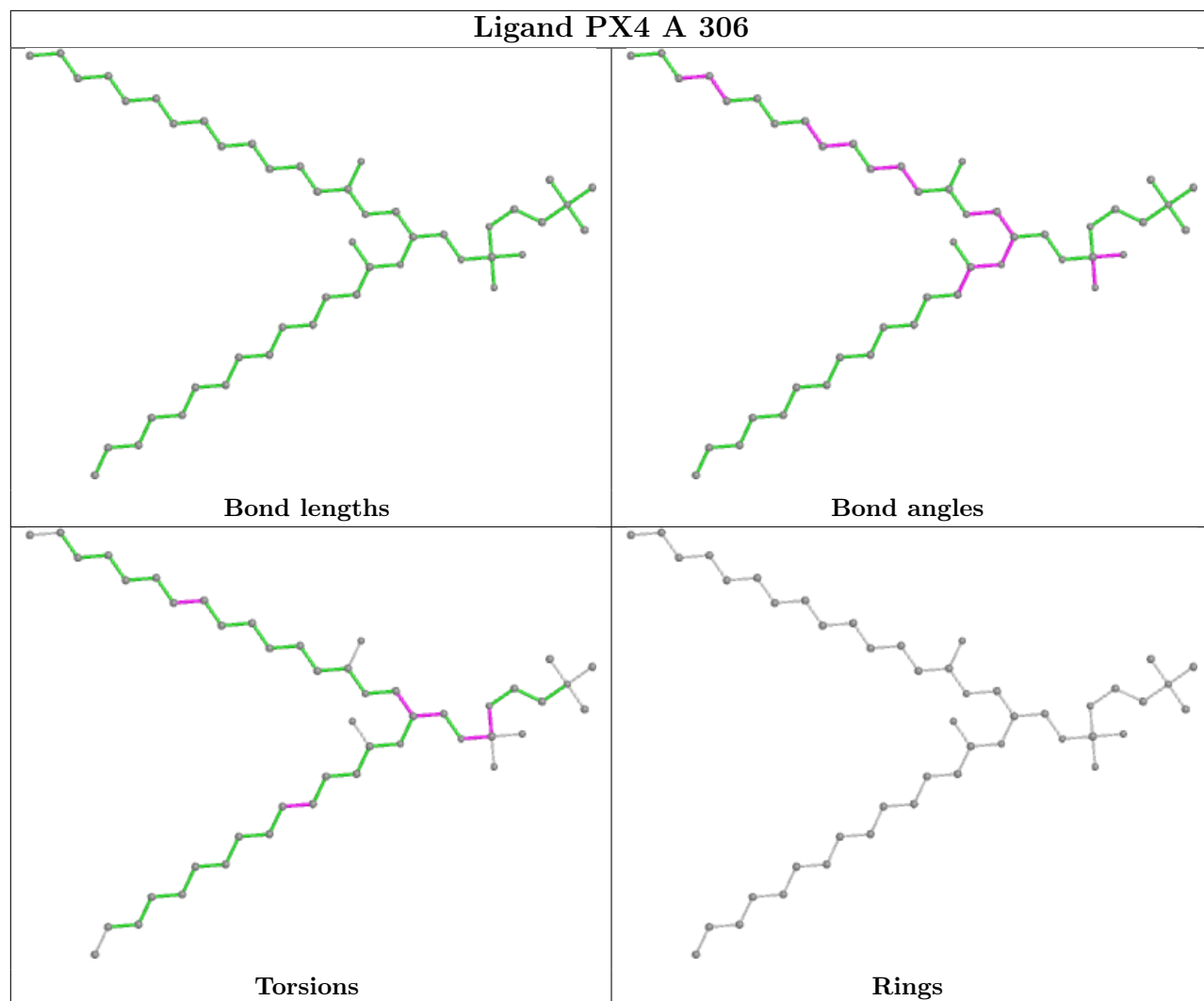


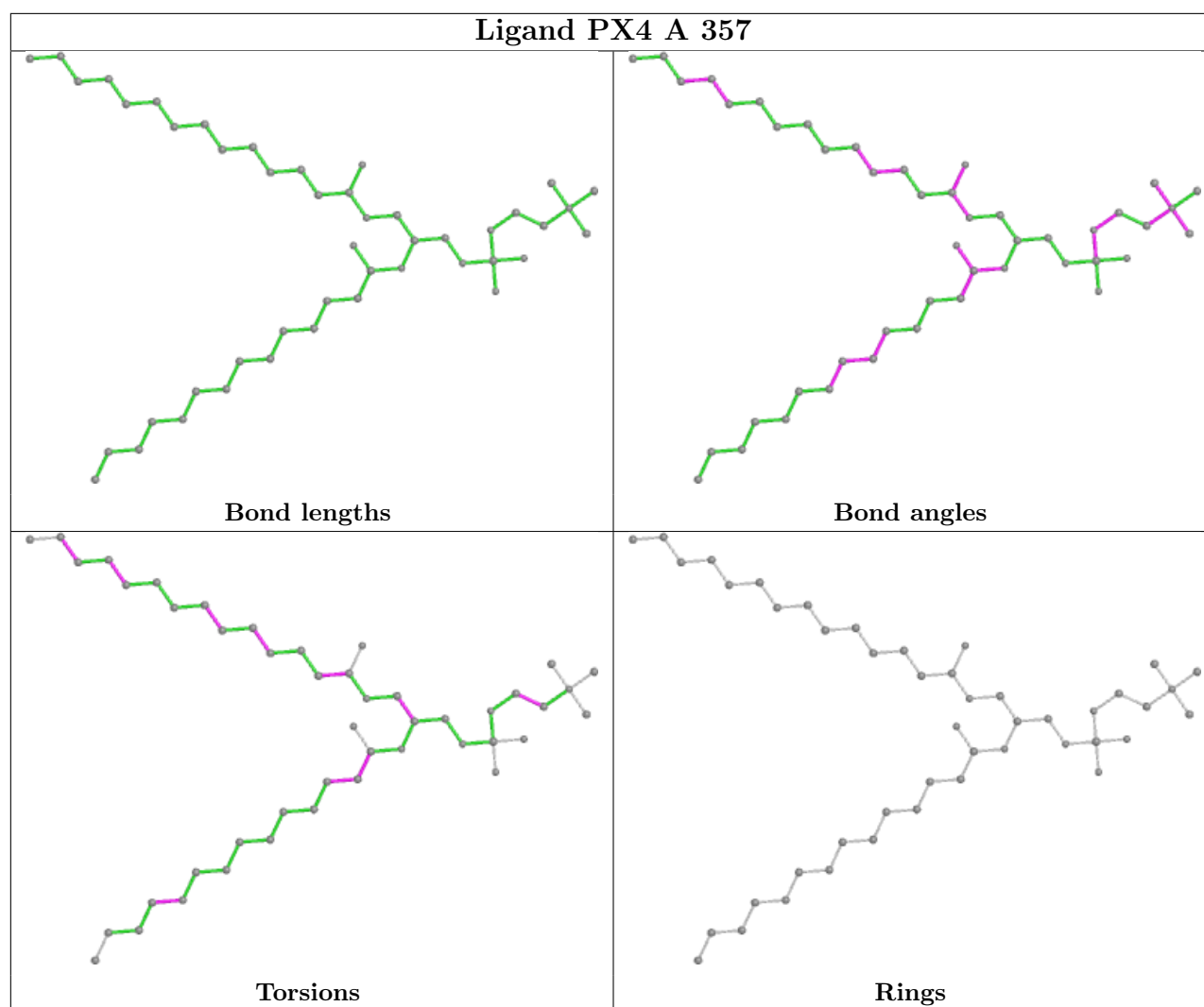


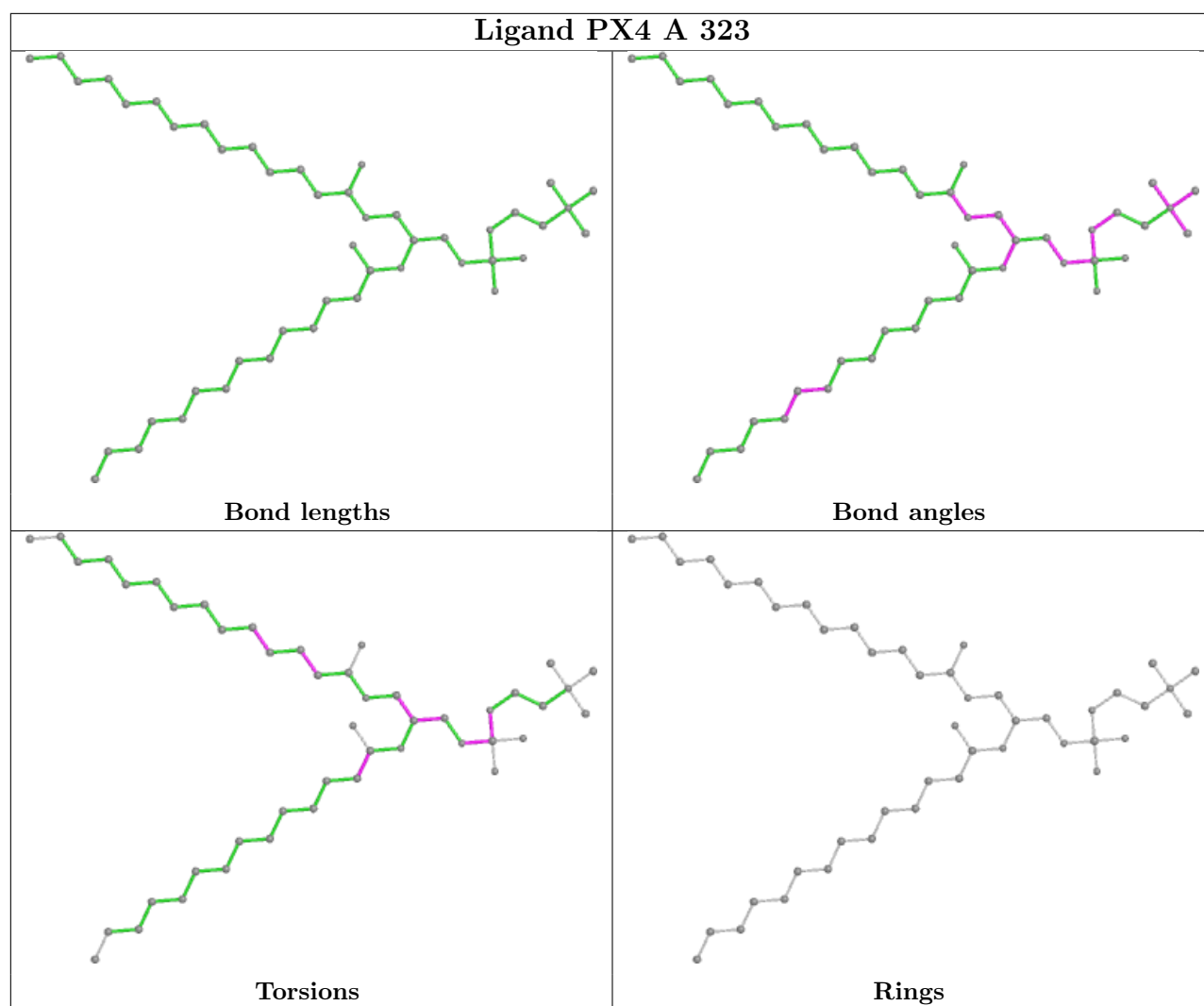


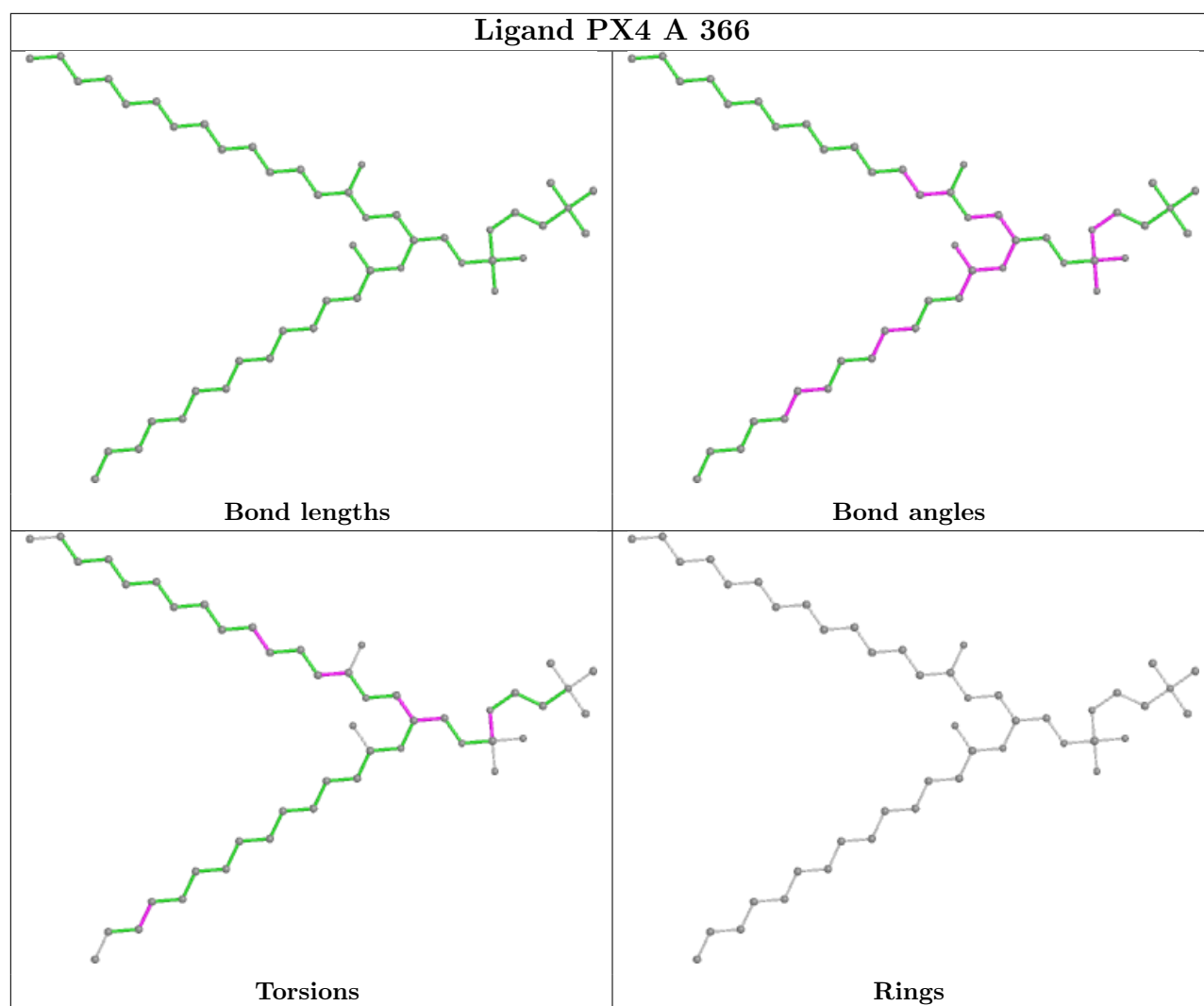


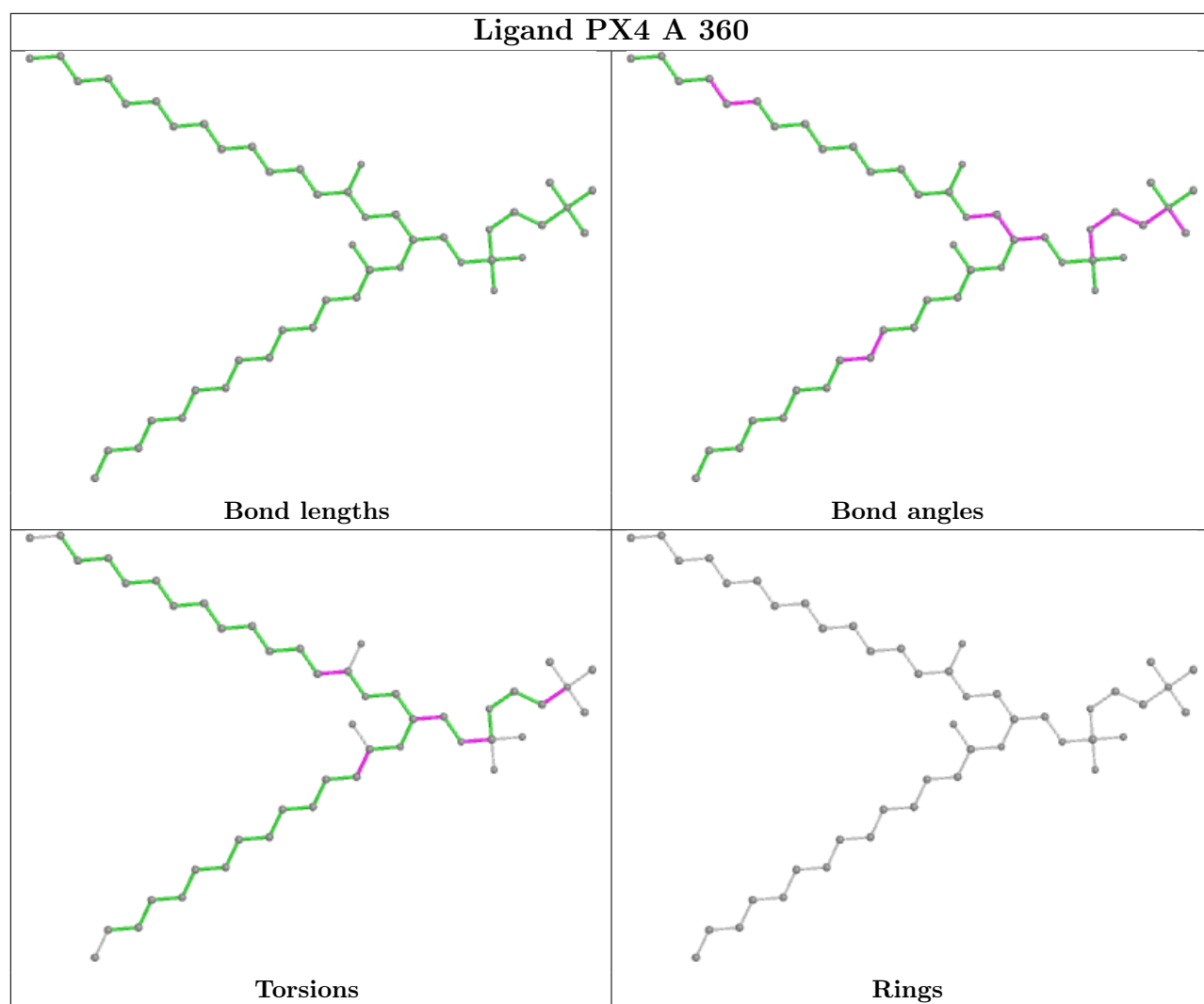
## Ligand PX4 A 306

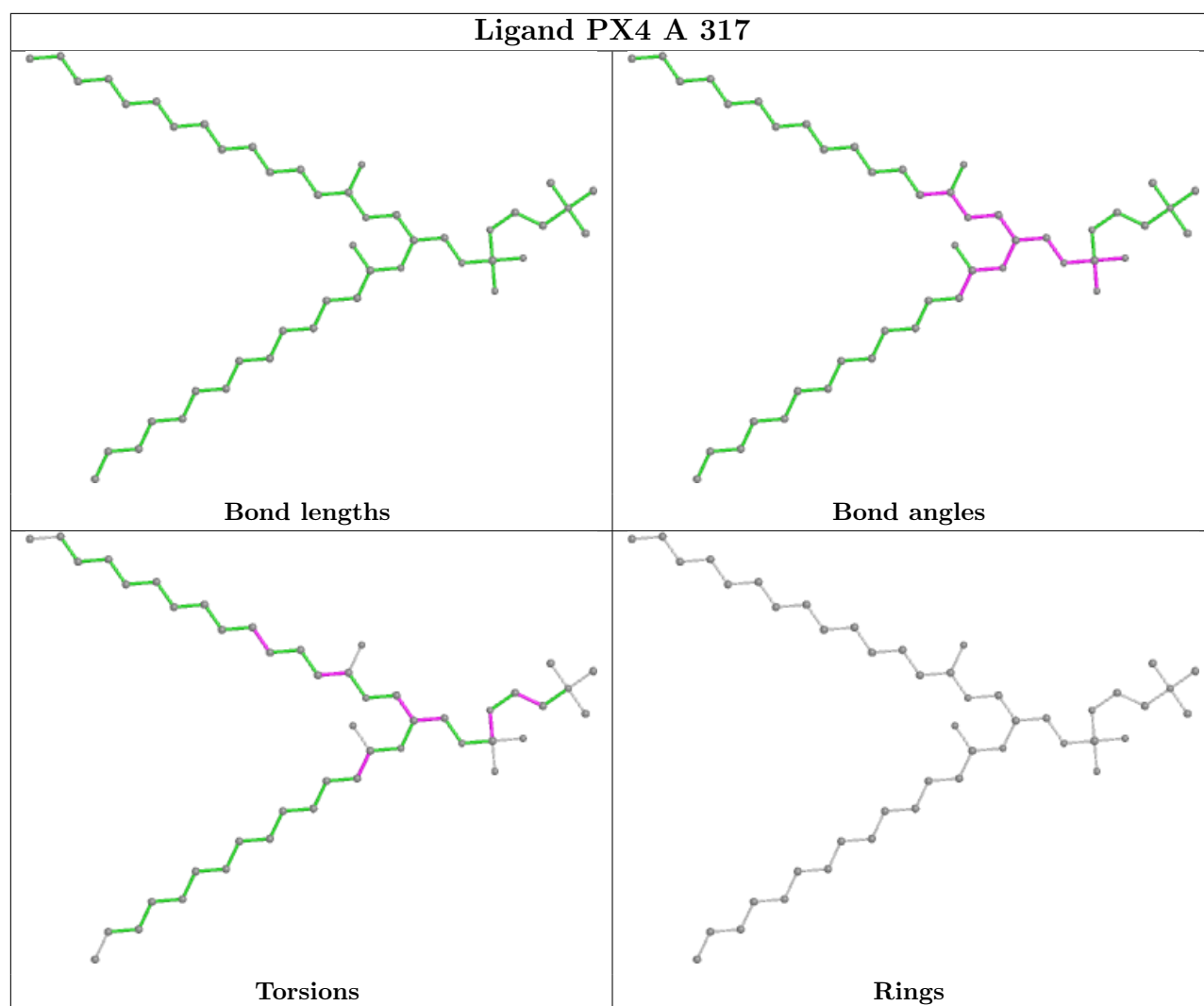


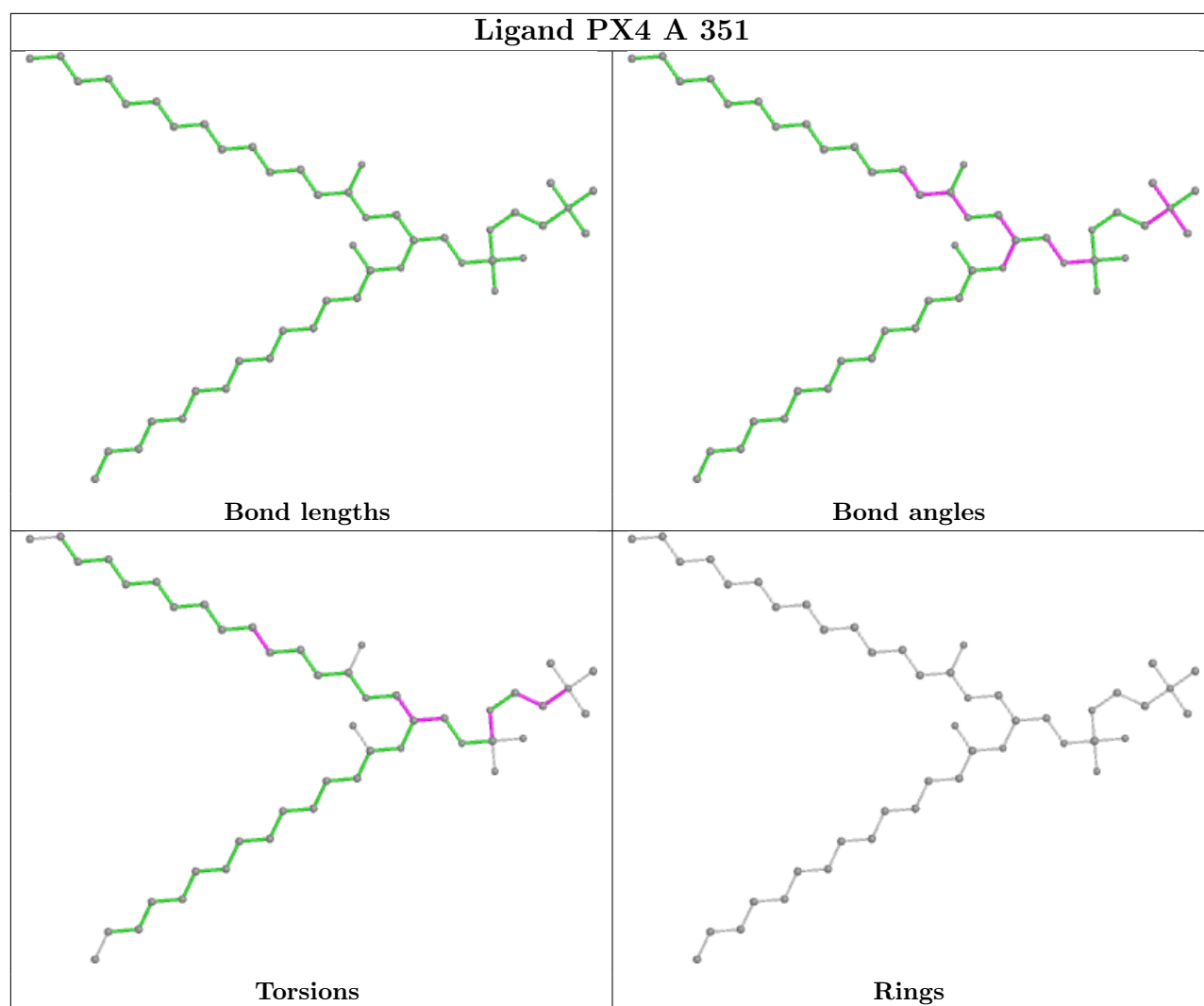


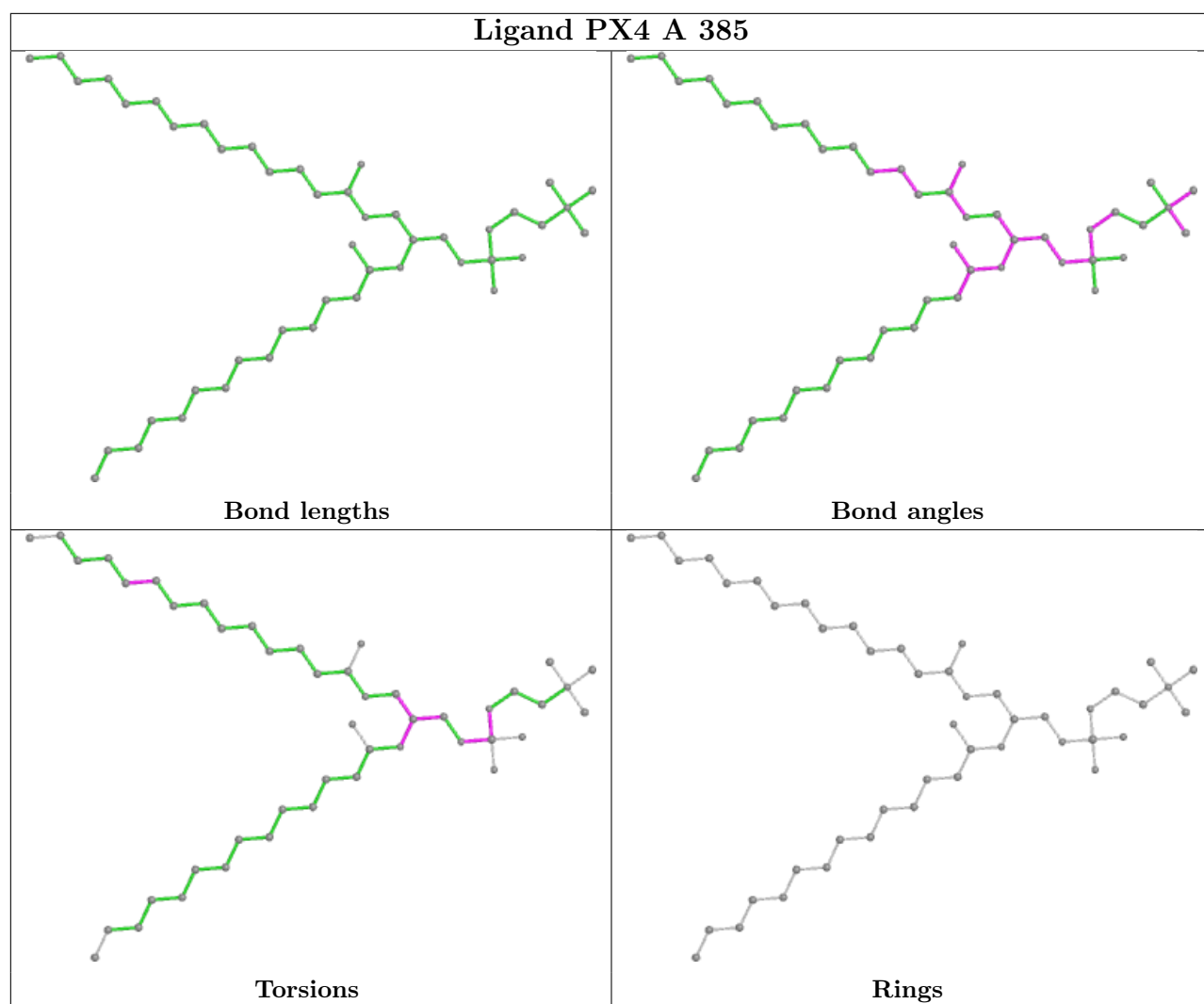


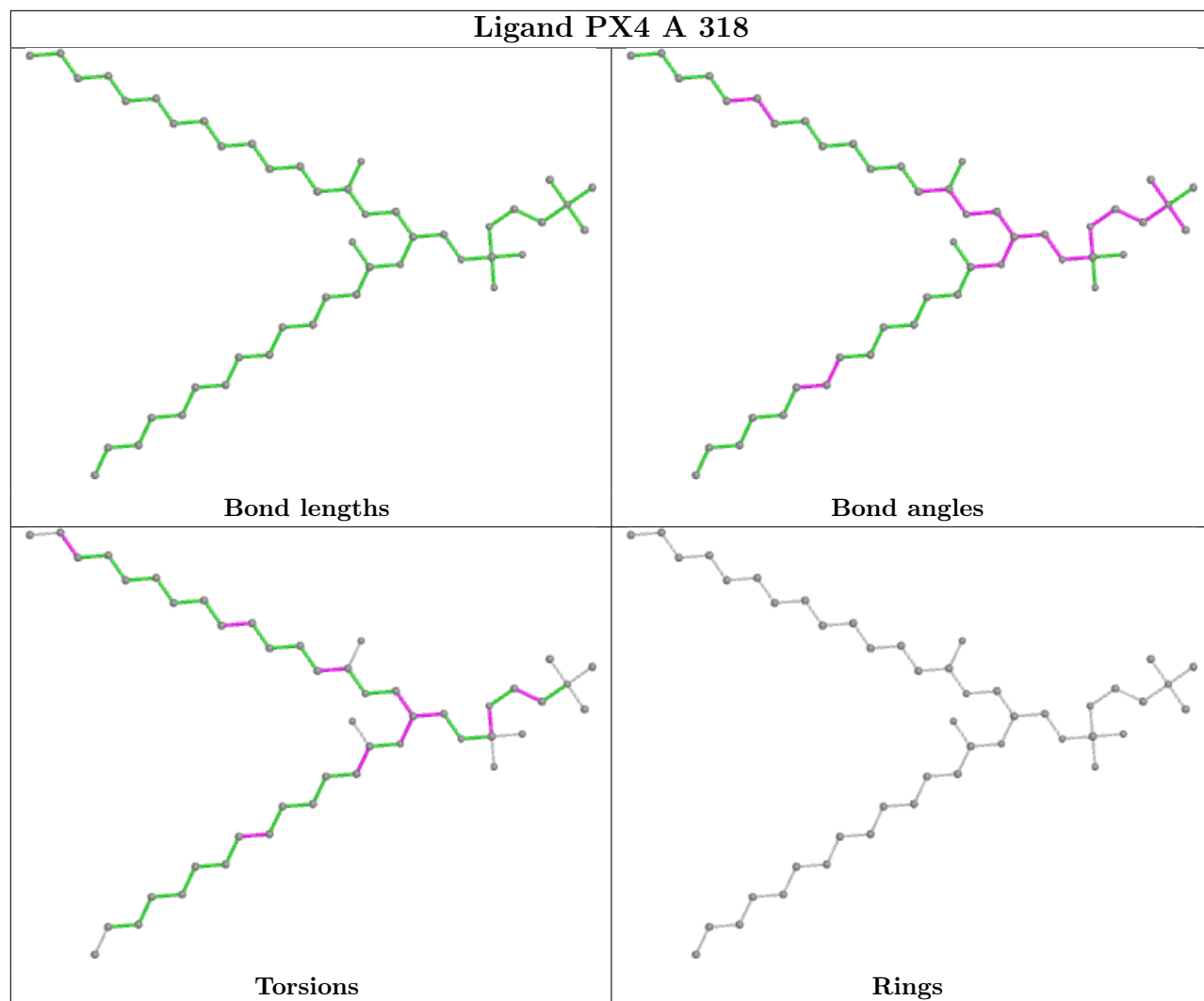


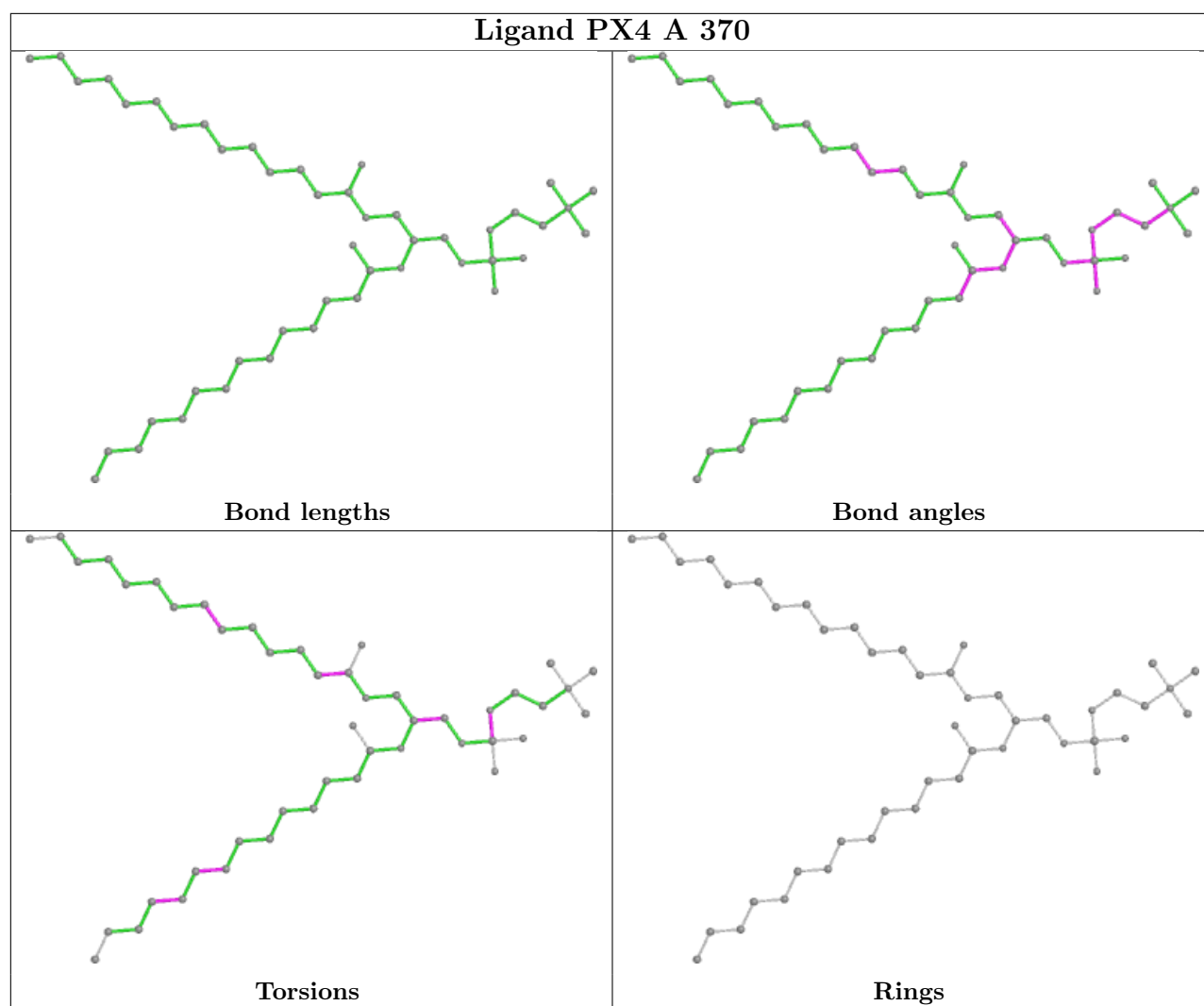


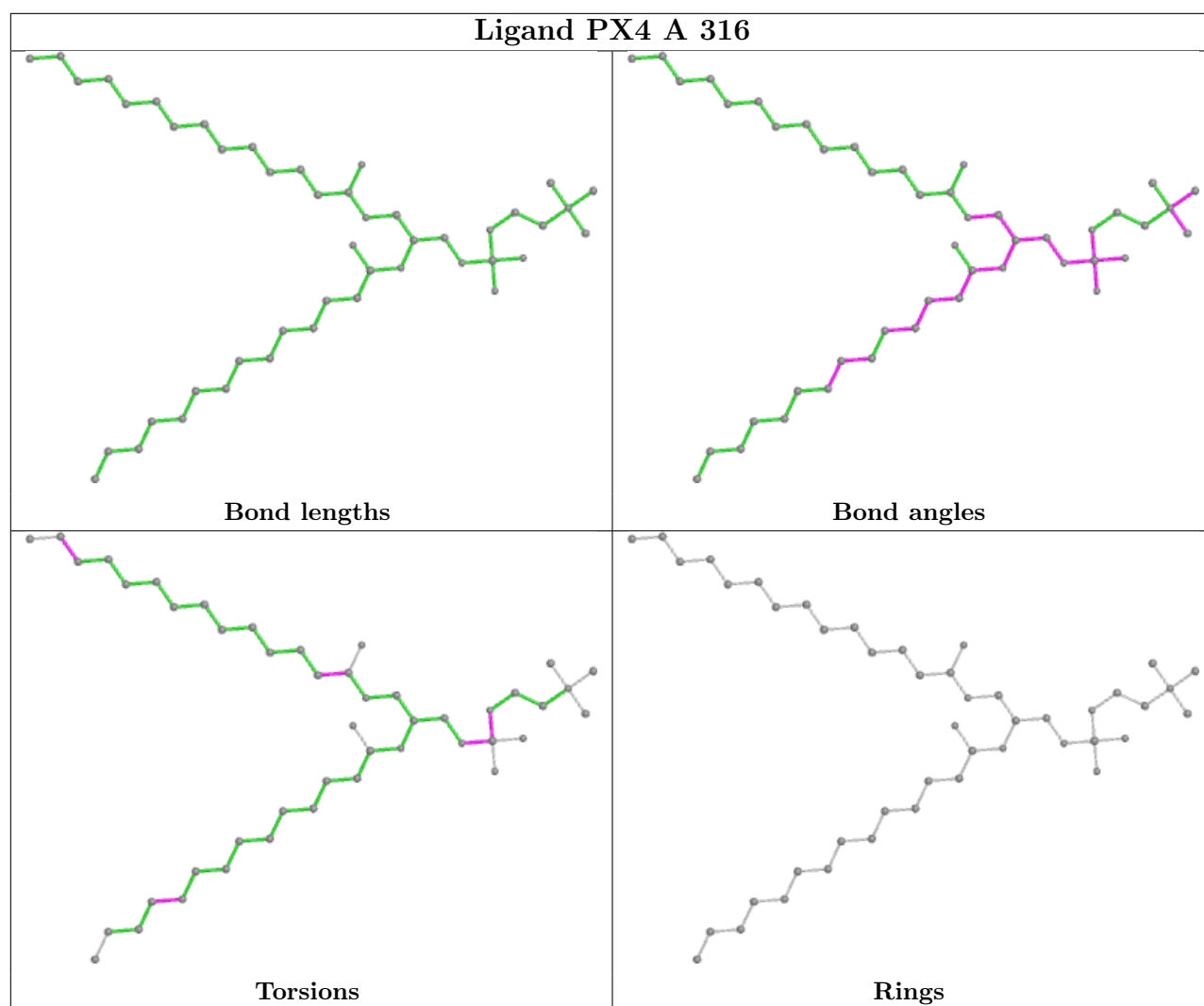


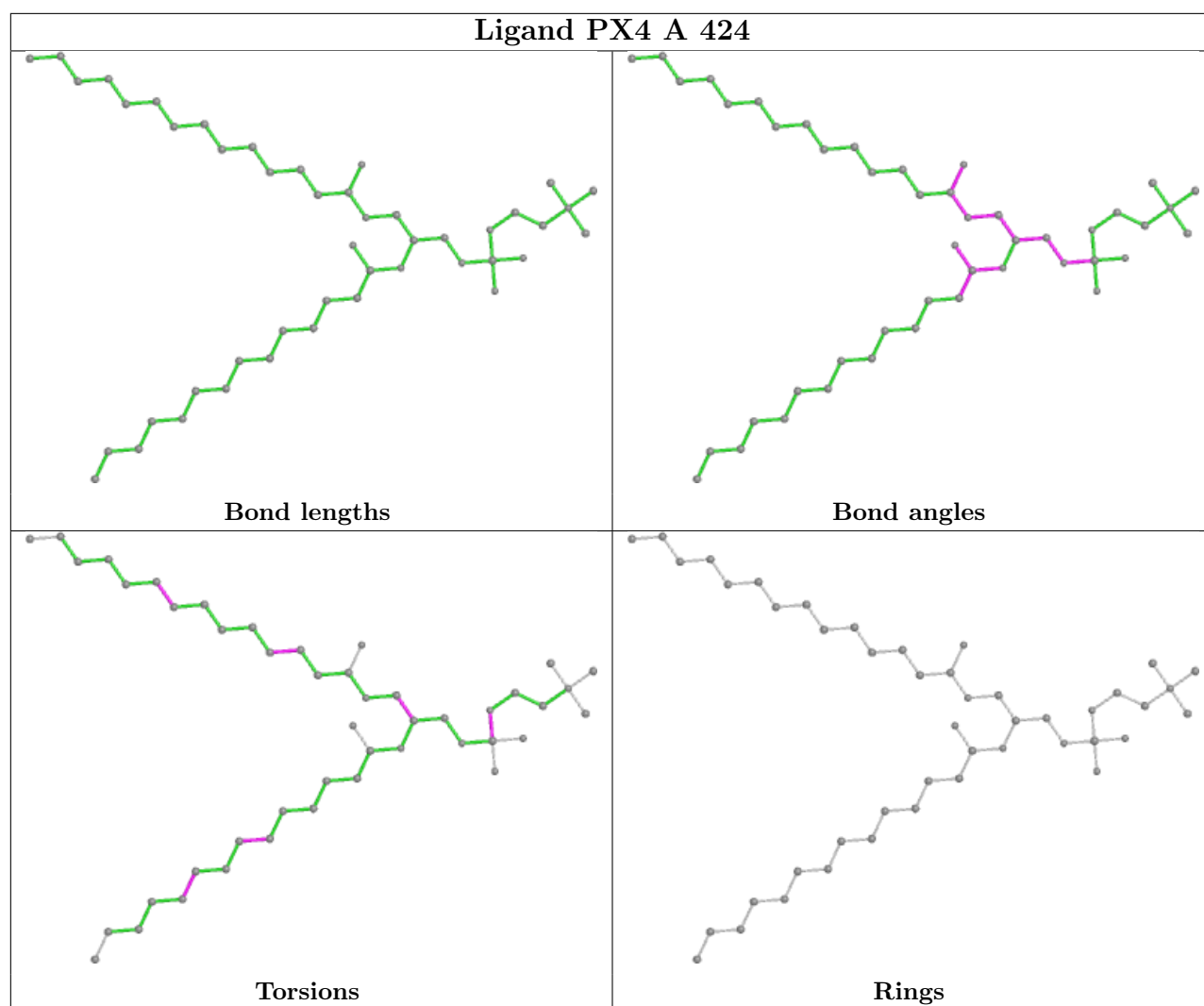












## 6.7 Other polymers [i](#)

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 82% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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

#### 7.1.1 Bookkeeping

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	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	160	$-0.25 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	138	$0.12 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	129	$-0.17 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	154	$-0.67 \pm 0.35$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1756 atoms were assigned a chemical shift out of a possible 2153. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	769/815 (94%)	329/336 (98%)	287/324 (89%)	153/155 (99%)
Sidechain	829/1066 (78%)	547/696 (79%)	273/330 (83%)	9/40 (22%)

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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	158/272 (58%)	79/137 (58%)	76/123 (62%)	3/12 (25%)
Overall	1756/2153 (82%)	955/1169 (82%)	636/777 (82%)	165/207 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1762 atoms were assigned a chemical shift out of a possible 2177. 0 out of 18 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	775/826 (94%)	332/341 (97%)	289/328 (88%)	154/157 (98%)
Sidechain	829/1069 (78%)	547/698 (78%)	273/331 (82%)	9/40 (22%)
Aromatic	158/282 (56%)	79/142 (56%)	76/128 (59%)	3/12 (25%)
Overall	1762/2177 (81%)	958/1181 (81%)	638/787 (81%)	166/209 (79%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	214	LEU	CG	33.00	21.37 – 32.19	5.8
1	A	226	LEU	CG	33.00	21.37 – 32.19	5.8
1	A	224	LEU	CG	32.30	21.37 – 32.19	5.1

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

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

Random coil index (RCI) for chain A:

