



Full wwPDB NMR Structure Validation Report ⓘ

Mar 17, 2026 – 12:54 AM UTC

PDB ID : 2MLR / pdb_00002mlr
BMRB ID : 7089
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Alpha-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.

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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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.48.1

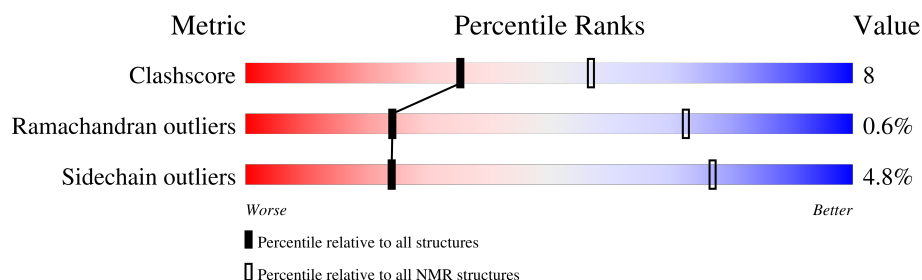
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	164	

2 Ensemble composition and analysis

This entry contains 14 models. Model 3 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:100-A:187, A:192-A:263 (160)	0.66	3

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

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

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

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

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

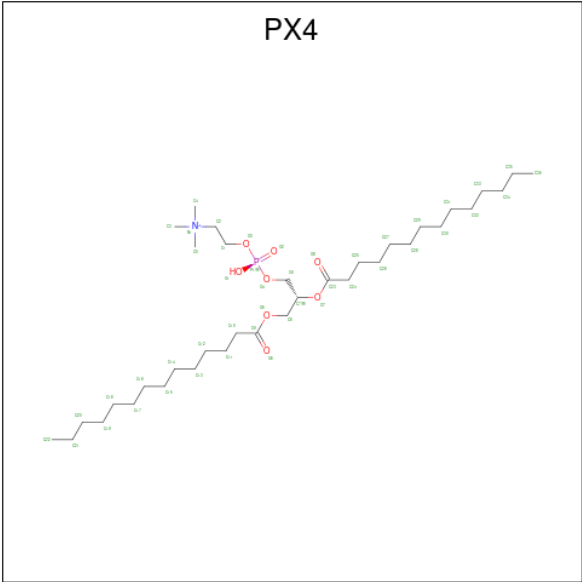
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	3	Total	Ca
			3	3

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



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

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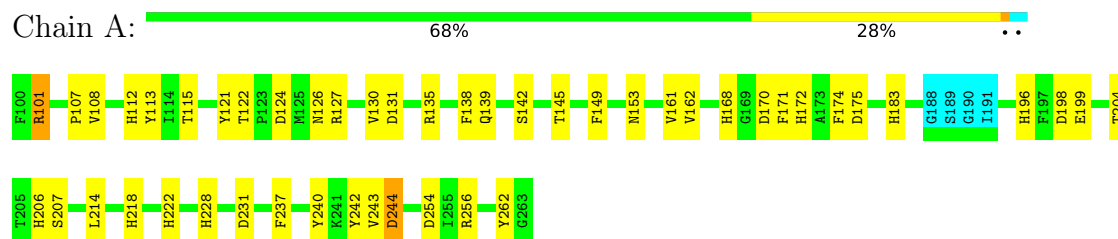
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Macrophage metalloelastase

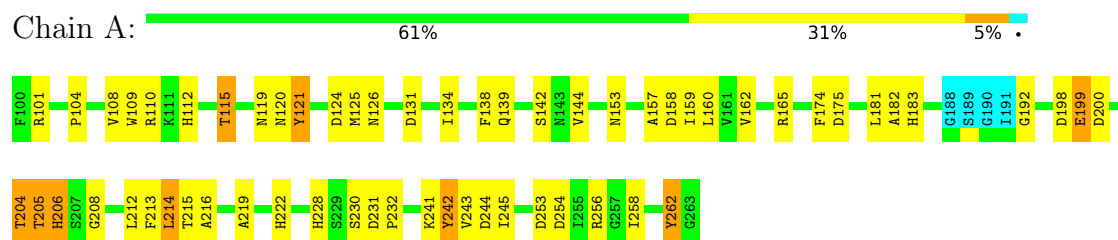


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

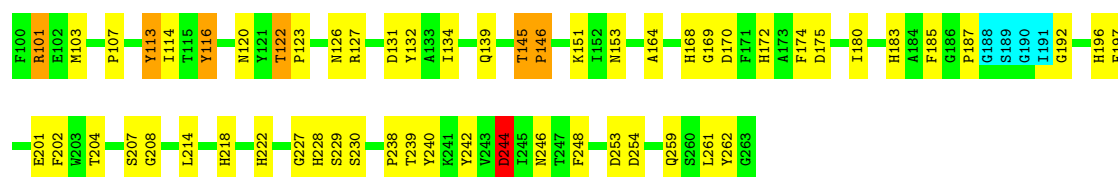
- Molecule 1: Macrophage metalloelastase



4.2.2 Score per residue for model 2

- Molecule 1: Macrophage metalloelastase





4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Macrophage metalloelastase

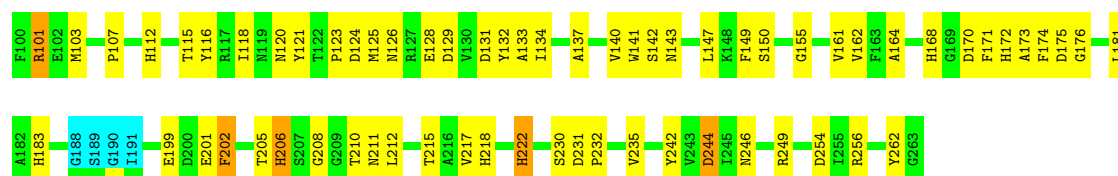
Chain A: 57% 38%



4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase

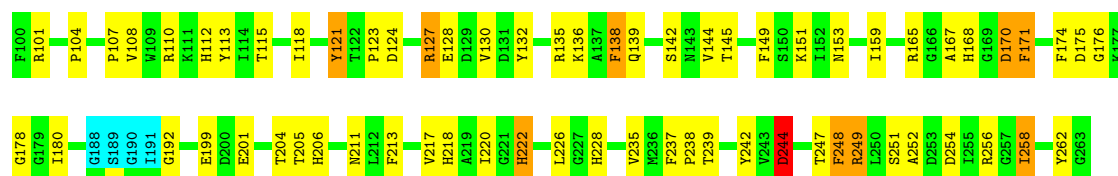
Chain A: 58% 37%



4.2.5 Score per residue for model 5

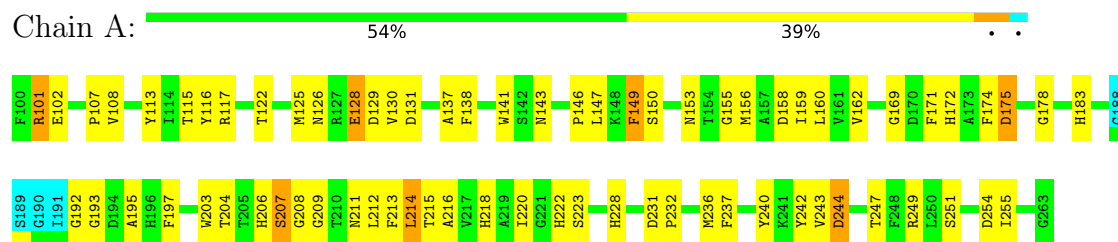
- Molecule 1: Macrophage metalloelastase

Chain A: 57% 34% 5%



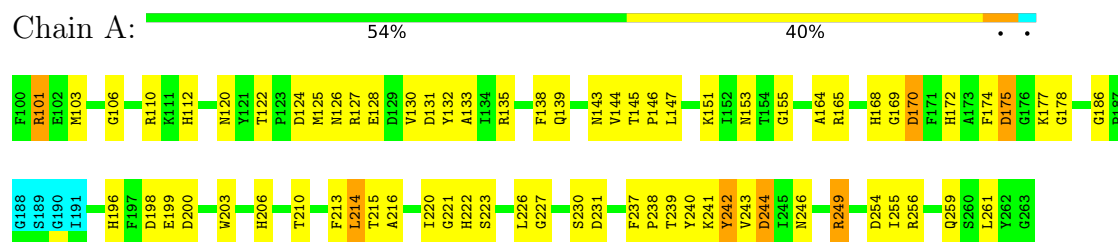
4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



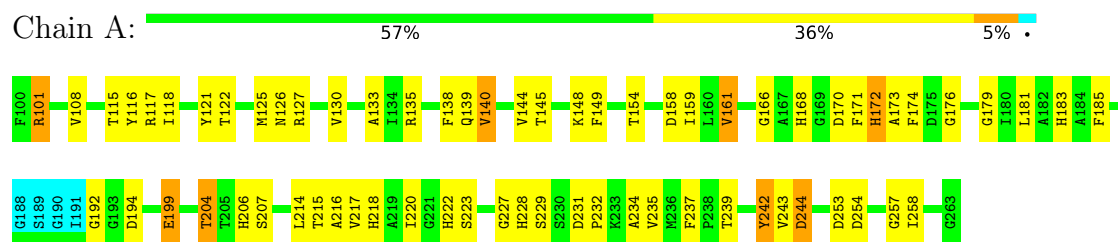
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



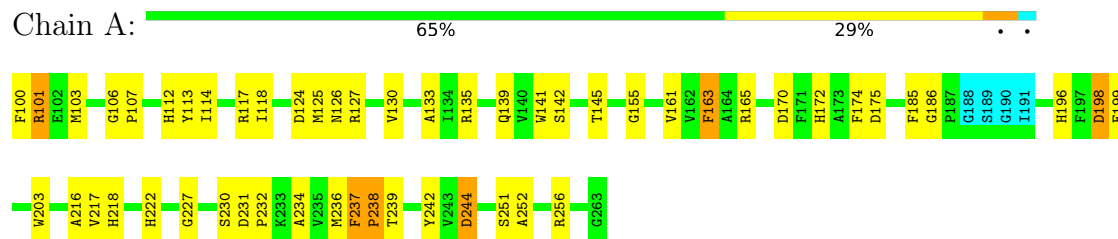
4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase



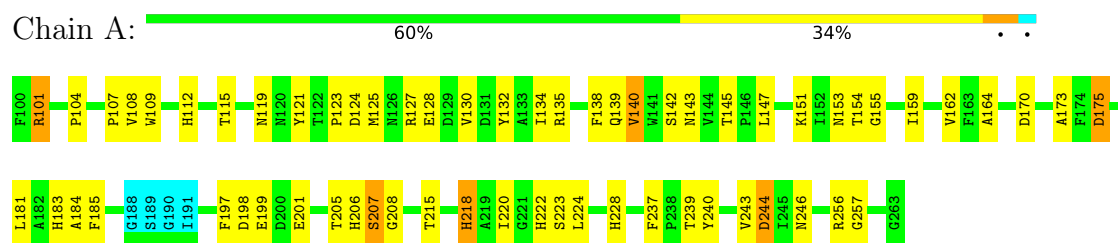
4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase



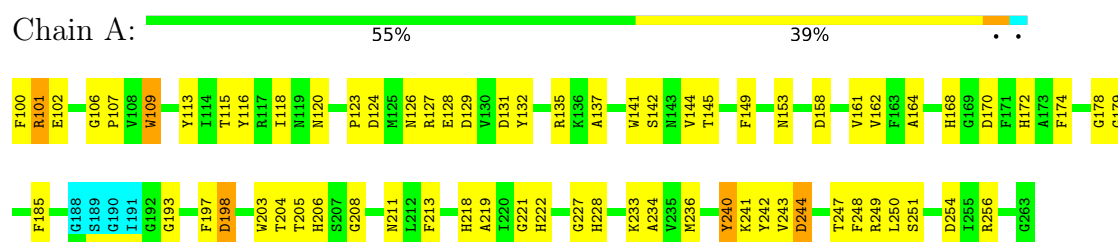
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



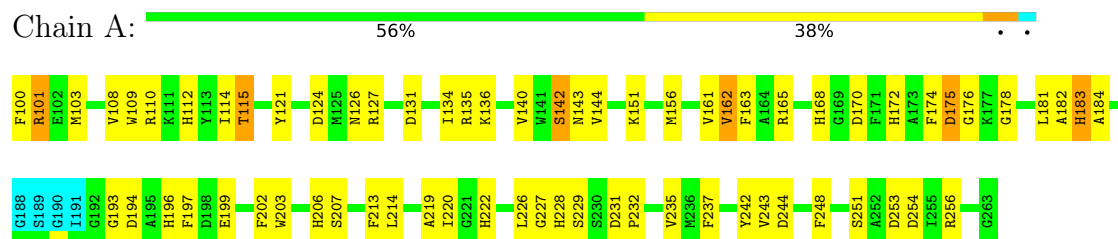
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



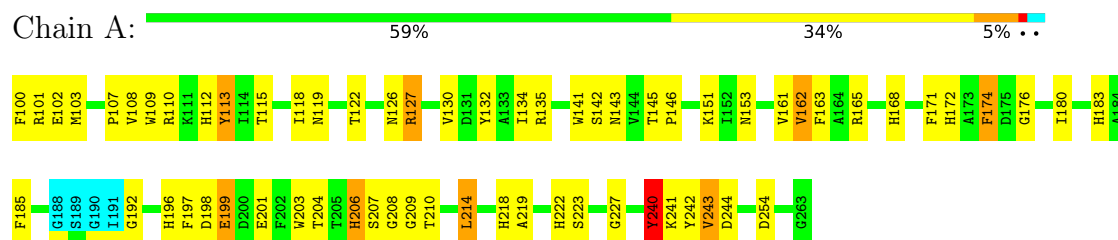
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



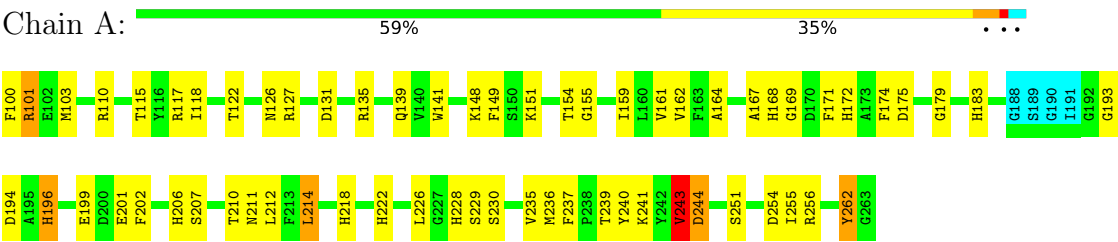
4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



4.2.14 Score per residue for model 14

● Molecule 1: Macrophage metalloelastase



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)	81%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, 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	0.65±0.01	0±0/1305 (0.0± 0.0%)	2.52±0.06	95±11/1768 (5.3± 0.6%)
All	All	0.65	0/18270 (0.0%)	2.52	1324/24752 (5.3%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.1±1.9
All	All	0	71

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	254	ASP	CA-CB-CG	14.39	126.99	112.60	4	9
1	A	100	PHE	CA-CB-CG	11.75	125.55	113.80	3	3
1	A	155	GLY	CA-C-O	-11.58	112.95	122.33	14	2
1	A	222	HIS	CA-CB-CG	11.52	125.32	113.80	4	4
1	A	151	LYS	CA-C-N	11.36	137.27	123.19	7	4
1	A	151	LYS	C-N-CA	11.36	137.27	123.19	7	4
1	A	172	HIS	CA-CB-CG	11.35	125.15	113.80	7	5
1	A	213	PHE	N-CA-C	11.30	123.29	110.97	5	2
1	A	185	PHE	CA-CB-CG	11.25	125.05	113.80	13	2
1	A	227	GLY	N-CA-C	-11.16	97.41	112.81	12	3
1	A	222	HIS	ND1-CE1-NE2	11.10	119.50	108.40	12	4
1	A	218	HIS	CA-CB-CG	10.91	124.71	113.80	13	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	153	ASN	CA-CB-CG	10.31	122.92	112.60	6	2
1	A	183	HIS	CA-CB-CG	10.30	124.10	113.80	13	5
1	A	145	THR	CA-C-N	10.17	132.55	119.84	7	2
1	A	145	THR	C-N-CA	10.17	132.55	119.84	7	2
1	A	244	ASP	CA-CB-CG	9.74	122.34	112.60	5	6
1	A	122	THR	CA-C-O	-9.73	110.31	120.23	3	1
1	A	174	PHE	CA-C-N	9.70	133.62	120.44	2	10
1	A	174	PHE	C-N-CA	9.70	133.62	120.44	2	10
1	A	124	ASP	CA-CB-CG	9.66	122.26	112.60	9	5
1	A	132	TYR	CA-C-N	9.45	133.30	120.54	10	4
1	A	132	TYR	C-N-CA	9.45	133.30	120.54	10	4
1	A	181	LEU	CA-C-O	9.44	129.25	118.77	10	4
1	A	234	ALA	CA-C-N	9.41	134.20	120.74	11	3
1	A	234	ALA	C-N-CA	9.41	134.20	120.74	11	3
1	A	127	ARG	NE-CZ-NH2	-9.22	110.91	119.20	11	5
1	A	239	THR	N-CA-CB	-9.15	97.36	110.44	7	3
1	A	172	HIS	ND1-CE1-NE2	9.14	117.54	108.40	3	4
1	A	112	HIS	CA-C-N	9.10	135.50	122.85	13	5
1	A	112	HIS	C-N-CA	9.10	135.50	122.85	13	5
1	A	123	PRO	CA-C-N	9.04	135.07	120.60	4	4
1	A	123	PRO	C-N-CA	9.04	135.07	120.60	4	4
1	A	210	THR	O-C-N	-9.03	112.47	123.04	4	1
1	A	157	ALA	CA-C-N	8.91	134.10	121.71	1	1
1	A	157	ALA	C-N-CA	8.91	134.10	121.71	1	1
1	A	127	ARG	N-CA-C	8.85	121.89	111.71	2	2
1	A	165	ARG	NE-CZ-NH2	-8.85	111.24	119.20	5	2
1	A	127	ARG	CA-C-N	8.74	131.99	120.28	2	4
1	A	127	ARG	C-N-CA	8.74	131.99	120.28	2	4
1	A	207	SER	CA-C-N	8.73	128.70	122.33	12	2
1	A	207	SER	C-N-CA	8.73	128.70	122.33	12	2
1	A	131	ASP	CA-C-N	8.69	132.26	120.44	11	7
1	A	131	ASP	C-N-CA	8.69	132.26	120.44	11	7
1	A	232	PRO	N-CA-C	8.63	125.07	113.84	12	2
1	A	242	TYR	CA-C-N	8.63	134.95	122.69	13	5
1	A	242	TYR	C-N-CA	8.63	134.95	122.69	13	5
1	A	217	VAL	CA-C-O	-8.62	111.98	120.95	5	3
1	A	120	ASN	CA-CB-CG	8.59	121.19	112.60	2	5
1	A	170	ASP	CA-CB-CG	8.59	121.19	112.60	4	3
1	A	227	GLY	O-C-N	-8.57	117.35	123.95	13	3
1	A	207	SER	N-CA-C	8.55	123.46	112.34	6	5
1	A	204	THR	CA-CB-CG2	8.51	124.96	110.50	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	198	ASP	CA-CB-CG	8.50	121.10	112.60	1	4
1	A	175	ASP	N-CA-C	8.49	122.61	111.75	14	5
1	A	155	GLY	CA-C-N	8.45	134.01	122.77	6	4
1	A	155	GLY	C-N-CA	8.45	134.01	122.77	6	4
1	A	254	ASP	CA-C-N	8.45	131.84	120.77	6	3
1	A	254	ASP	C-N-CA	8.45	131.84	120.77	6	3
1	A	238	PRO	N-CA-CB	8.44	112.61	103.33	2	3
1	A	147	LEU	CA-C-O	-8.41	111.24	120.92	7	2
1	A	162	VAL	CB-CA-C	8.40	121.55	110.12	4	7
1	A	206	HIS	CA-CB-CG	8.40	122.20	113.80	8	1
1	A	249	ARG	NE-CZ-NH1	8.38	129.88	121.50	11	2
1	A	232	PRO	N-CA-CB	8.38	112.05	103.25	1	3
1	A	101	ARG	CA-C-N	8.34	134.51	121.26	14	9
1	A	101	ARG	C-N-CA	8.34	134.51	121.26	14	9
1	A	178	GLY	CA-C-O	-8.33	116.45	122.45	5	3
1	A	110	ARG	CA-C-N	8.26	134.40	123.00	7	2
1	A	110	ARG	C-N-CA	8.26	134.40	123.00	7	2
1	A	209	GLY	O-C-N	-8.24	117.60	123.95	6	1
1	A	183	HIS	ND1-CE1-NE2	8.22	116.62	108.40	8	4
1	A	133	ALA	CA-C-N	8.21	131.06	120.56	7	5
1	A	133	ALA	C-N-CA	8.21	131.06	120.56	7	5
1	A	161	VAL	CA-CB-CG1	8.19	124.31	110.40	14	2
1	A	242	TYR	CA-C-O	8.13	129.93	120.49	8	1
1	A	236	MET	CA-C-N	8.13	132.03	120.49	14	4
1	A	236	MET	C-N-CA	8.13	132.03	120.49	14	4
1	A	231	ASP	CA-CB-CG	8.13	120.73	112.60	12	3
1	A	222	HIS	ND1-CG-CD2	7.99	114.09	106.10	14	4
1	A	108	VAL	CA-C-N	7.98	132.03	120.38	8	5
1	A	108	VAL	C-N-CA	7.98	132.03	120.38	8	5
1	A	192	GLY	CA-C-N	7.97	132.76	122.00	5	4
1	A	192	GLY	C-N-CA	7.97	132.76	122.00	5	4
1	A	143	ASN	CA-CB-CG	7.95	120.55	112.60	3	3
1	A	149	PHE	CA-CB-CG	7.94	121.74	113.80	4	2
1	A	208	GLY	CA-C-N	7.92	130.79	122.63	13	1
1	A	208	GLY	C-N-CA	7.92	130.79	122.63	13	1
1	A	139	GLN	OE1-CD-NE2	-7.90	114.70	122.60	2	2
1	A	145	THR	CB-CA-C	7.83	120.58	110.16	7	1
1	A	139	GLN	CA-C-N	7.82	130.41	120.56	8	5
1	A	139	GLN	C-N-CA	7.82	130.41	120.56	8	5
1	A	101	ARG	CD-NE-CZ	7.80	135.32	124.40	14	1
1	A	115	THR	CA-CB-CG2	7.80	123.76	110.50	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	218	HIS	ND1-CE1-NE2	7.79	116.19	108.40	3	4
1	A	126	ASN	CA-CB-CG	7.78	120.38	112.60	6	3
1	A	253	ASP	CA-C-N	7.77	130.91	120.65	1	4
1	A	253	ASP	C-N-CA	7.77	130.91	120.65	1	4
1	A	228	HIS	CA-CB-CG	7.77	121.57	113.80	1	3
1	A	205	THR	CA-CB-OG1	7.77	121.26	109.60	11	1
1	A	222	HIS	CE1-NE2-CD2	-7.71	101.29	109.00	5	2
1	A	120	ASN	OD1-CG-ND2	-7.69	114.91	122.60	1	1
1	A	231	ASP	CA-C-N	7.68	128.07	119.32	4	7
1	A	231	ASP	C-N-CA	7.68	128.07	119.32	4	7
1	A	228	HIS	ND1-CE1-NE2	7.65	116.05	108.40	3	7
1	A	126	ASN	CA-C-N	7.62	130.82	120.38	9	7
1	A	126	ASN	C-N-CA	7.62	130.82	120.38	9	7
1	A	218	HIS	CA-C-O	-7.56	111.28	119.97	5	1
1	A	206	HIS	ND1-CE1-NE2	7.55	115.95	108.40	5	3
1	A	135	ARG	CA-C-N	7.53	130.36	120.28	5	1
1	A	135	ARG	C-N-CA	7.53	130.36	120.28	5	1
1	A	174	PHE	CA-CB-CG	7.49	121.29	113.80	3	2
1	A	138	PHE	CA-C-N	7.46	131.66	120.31	7	2
1	A	138	PHE	C-N-CA	7.46	131.66	120.31	7	2
1	A	107	PRO	CA-C-N	7.46	135.39	121.97	9	4
1	A	107	PRO	C-N-CA	7.46	135.39	121.97	9	4
1	A	119	ASN	CA-CB-CG	-7.45	105.15	112.60	13	2
1	A	168	HIS	CA-CB-CG	7.45	121.25	113.80	2	5
1	A	130	VAL	CA-C-N	7.43	130.24	120.28	8	3
1	A	130	VAL	C-N-CA	7.43	130.24	120.28	8	3
1	A	115	THR	CB-CA-C	7.41	123.94	109.33	11	5
1	A	218	HIS	CA-C-N	7.41	130.81	120.29	14	3
1	A	218	HIS	C-N-CA	7.41	130.81	120.29	14	3
1	A	125	MET	CA-C-N	7.38	132.53	120.94	10	3
1	A	125	MET	C-N-CA	7.38	132.53	120.94	10	3
1	A	164	ALA	CA-C-N	7.38	133.52	121.86	11	4
1	A	164	ALA	C-N-CA	7.38	133.52	121.86	11	4
1	A	164	ALA	O-C-N	-7.36	114.58	123.19	11	1
1	A	222	HIS	N-CA-C	-7.34	102.45	111.40	5	1
1	A	126	ASN	OD1-CG-ND2	-7.32	115.28	122.60	13	4
1	A	168	HIS	CA-C-N	7.32	135.76	121.41	5	3
1	A	168	HIS	C-N-CA	7.32	135.76	121.41	5	3
1	A	183	HIS	CE1-NE2-CD2	-7.29	101.71	109.00	3	3
1	A	142	SER	N-CA-C	-7.27	103.39	111.82	4	2
1	A	240	TYR	CA-C-N	7.22	134.78	122.37	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	240	TYR	C-N-CA	7.22	134.78	122.37	10	3
1	A	143	ASN	OD1-CG-ND2	-7.22	115.38	122.60	4	2
1	A	125	MET	CA-C-O	-7.19	113.56	121.33	6	2
1	A	129	ASP	CA-C-N	7.19	130.31	120.46	4	3
1	A	129	ASP	C-N-CA	7.19	130.31	120.46	4	3
1	A	161	VAL	CA-CB-CG2	7.19	122.62	110.40	13	2
1	A	110	ARG	NE-CZ-NH1	-7.17	114.33	121.50	12	1
1	A	159	ILE	CA-C-N	7.15	131.73	121.50	6	2
1	A	159	ILE	C-N-CA	7.15	131.73	121.50	6	2
1	A	261	LEU	N-CA-CB	-7.15	101.08	110.59	7	1
1	A	126	ASN	N-CA-C	7.15	120.59	110.23	2	2
1	A	118	ILE	N-CA-C	-7.12	96.73	106.85	4	2
1	A	203	TRP	CG-CD2-CE3	7.12	141.02	133.90	11	1
1	A	256	ARG	CA-C-O	-7.11	112.23	120.20	14	1
1	A	104	PRO	CA-C-N	7.10	129.95	122.63	10	1
1	A	104	PRO	C-N-CA	7.10	129.95	122.63	10	1
1	A	255	ILE	N-CA-CB	7.10	118.36	110.62	3	1
1	A	103	MET	N-CA-CB	-7.09	100.46	110.04	4	1
1	A	206	HIS	CA-C-N	7.08	130.72	120.38	3	6
1	A	206	HIS	C-N-CA	7.08	130.72	120.38	3	6
1	A	106	GLY	O-C-N	-7.08	114.69	121.77	7	2
1	A	254	ASP	CA-C-O	7.08	128.25	120.82	13	2
1	A	223	SER	CA-C-O	-7.06	112.13	120.10	8	1
1	A	163	PHE	CA-C-O	7.04	127.90	120.36	13	1
1	A	253	ASP	N-CA-C	7.04	118.95	111.28	12	1
1	A	110	ARG	NE-CZ-NH2	-7.03	112.87	119.20	13	2
1	A	124	ASP	CA-C-N	7.03	133.60	122.21	4	4
1	A	124	ASP	C-N-CA	7.03	133.60	122.21	4	4
1	A	204	THR	CA-CB-OG1	-7.02	99.06	109.60	8	1
1	A	260	SER	N-CA-C	-7.02	104.53	113.23	3	1
1	A	140	VAL	CA-CB-CG1	7.02	122.33	110.40	4	3
1	A	197	PHE	CA-CB-CG	7.02	120.82	113.80	12	2
1	A	201	GLU	CB-CA-C	-6.99	96.60	109.46	2	1
1	A	170	ASP	OD1-CG-OD2	-6.99	106.13	122.90	8	6
1	A	185	PHE	CA-C-N	6.96	132.80	121.87	9	1
1	A	185	PHE	C-N-CA	6.96	132.80	121.87	9	1
1	A	210	THR	CA-CB-CG2	6.96	122.34	110.50	14	1
1	A	144	VAL	CB-CA-C	6.96	118.58	110.93	5	6
1	A	100	PHE	CA-C-N	6.95	130.87	120.17	9	3
1	A	100	PHE	C-N-CA	6.95	130.87	120.17	9	3
1	A	172	HIS	ND1-CG-CD2	6.92	113.02	106.10	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	165	ARG	CB-CA-C	6.91	120.72	110.62	12	5
1	A	239	THR	CA-C-N	6.90	132.93	122.65	14	2
1	A	239	THR	C-N-CA	6.90	132.93	122.65	14	2
1	A	135	ARG	NE-CZ-NH1	-6.90	114.60	121.50	9	1
1	A	128	GLU	CA-C-N	6.88	130.07	120.29	5	2
1	A	128	GLU	C-N-CA	6.88	130.07	120.29	5	2
1	A	102	GLU	CA-C-N	6.88	130.00	120.65	6	2
1	A	102	GLU	C-N-CA	6.88	130.00	120.65	6	2
1	A	196	HIS	CB-CG-CD2	-6.85	122.29	131.20	3	2
1	A	118	ILE	CA-C-N	6.85	129.34	120.44	5	3
1	A	118	ILE	C-N-CA	6.85	129.34	120.44	5	3
1	A	247	THR	O-C-N	-6.84	112.92	122.37	6	2
1	A	122	THR	CA-CB-CG2	6.84	122.13	110.50	8	1
1	A	184	ALA	N-CA-CB	-6.83	99.75	110.06	12	2
1	A	256	ARG	CD-NE-CZ	6.82	133.95	124.40	9	1
1	A	251	SER	CA-C-N	6.82	129.75	120.54	11	6
1	A	251	SER	C-N-CA	6.82	129.75	120.54	11	6
1	A	257	GLY	O-C-N	6.82	131.57	122.70	8	2
1	A	147	LEU	CA-C-N	6.82	130.55	120.87	4	1
1	A	147	LEU	C-N-CA	6.82	130.55	120.87	4	1
1	A	243	VAL	CA-C-O	-6.81	114.89	121.63	13	1
1	A	122	THR	N-CA-CB	-6.78	100.58	110.14	8	1
1	A	216	ALA	O-C-N	6.78	129.41	122.09	8	1
1	A	262	TYR	CB-CG-CD2	-6.77	110.65	120.80	14	1
1	A	146	PRO	CA-C-N	6.77	132.12	121.56	6	1
1	A	146	PRO	C-N-CA	6.77	132.12	121.56	6	1
1	A	171	PHE	CA-CB-CG	6.75	120.55	113.80	3	2
1	A	160	LEU	CA-C-N	6.75	132.29	123.11	1	2
1	A	160	LEU	C-N-CA	6.75	132.29	123.11	1	2
1	A	176	GLY	CA-C-O	-6.75	115.61	122.56	8	3
1	A	120	ASN	CA-C-N	6.73	132.49	123.00	11	2
1	A	120	ASN	C-N-CA	6.73	132.49	123.00	11	2
1	A	203	TRP	CA-C-N	6.73	132.81	122.11	6	6
1	A	203	TRP	C-N-CA	6.73	132.81	122.11	6	6
1	A	210	THR	CB-CA-C	6.72	120.14	110.79	14	1
1	A	246	ASN	OD1-CG-ND2	-6.72	115.88	122.60	2	1
1	A	166	GLY	CA-C-N	6.71	130.91	121.24	8	1
1	A	166	GLY	C-N-CA	6.71	130.91	121.24	8	1
1	A	128	GLU	O-C-N	-6.71	114.05	122.17	6	1
1	A	130	VAL	N-CA-C	-6.71	104.64	110.74	8	2
1	A	138	PHE	CA-CB-CG	6.70	120.50	113.80	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	135	ARG	CD-NE-CZ	6.68	133.75	124.40	14	2
1	A	145	THR	CA-C-O	-6.68	113.64	119.72	7	4
1	A	215	THR	CA-C-N	6.66	129.20	120.28	3	3
1	A	215	THR	C-N-CA	6.66	129.20	120.28	3	3
1	A	218	HIS	CE1-NE2-CD2	-6.64	102.36	109.00	10	2
1	A	112	HIS	CB-CG-CD2	-6.63	122.58	131.20	12	2
1	A	183	HIS	ND1-CG-CD2	6.63	112.73	106.10	10	3
1	A	102	GLU	N-CA-CB	-6.63	100.24	110.85	13	1
1	A	167	ALA	CA-C-N	6.63	131.95	121.08	14	1
1	A	167	ALA	C-N-CA	6.63	131.95	121.08	14	1
1	A	237	PHE	CA-C-N	6.63	126.57	119.28	7	3
1	A	237	PHE	C-N-CA	6.63	126.57	119.28	7	3
1	A	186	GLY	CA-C-N	6.62	127.07	120.52	9	3
1	A	186	GLY	C-N-CA	6.62	127.07	120.52	9	3
1	A	156	MET	CG-SD-CE	6.60	115.43	100.90	6	1
1	A	216	ALA	CA-C-O	-6.60	113.84	120.90	1	2
1	A	174	PHE	N-CA-C	6.59	119.09	109.07	6	3
1	A	161	VAL	N-CA-CB	-6.57	103.23	111.31	13	2
1	A	172	HIS	CE1-NE2-CD2	-6.56	102.44	109.00	3	1
1	A	161	VAL	CA-C-N	6.55	132.72	122.70	4	1
1	A	161	VAL	C-N-CA	6.55	132.72	122.70	4	1
1	A	101	ARG	NE-CZ-NH2	-6.54	113.31	119.20	12	2
1	A	121	TYR	CA-C-N	6.54	129.99	120.51	1	2
1	A	121	TYR	C-N-CA	6.54	129.99	120.51	1	2
1	A	235	VAL	O-C-N	-6.53	115.49	121.89	5	1
1	A	205	THR	CA-C-N	6.53	133.06	122.81	1	1
1	A	205	THR	C-N-CA	6.53	133.06	122.81	1	1
1	A	109	TRP	N-CA-C	6.53	120.10	111.75	3	1
1	A	212	LEU	CA-C-N	6.52	129.50	120.63	1	2
1	A	212	LEU	C-N-CA	6.52	129.50	120.63	1	2
1	A	185	PHE	CA-C-O	-6.52	113.72	121.60	10	1
1	A	200	ASP	CA-CB-CG	6.50	119.10	112.60	1	2
1	A	109	TRP	O-C-N	6.50	130.26	122.27	12	1
1	A	220	ILE	N-CA-C	-6.49	105.41	111.45	12	2
1	A	239	THR	CA-CB-CG2	6.48	121.52	110.50	10	2
1	A	217	VAL	O-C-N	6.46	128.14	121.87	9	3
1	A	104	PRO	O-C-N	-6.46	115.00	123.13	1	2
1	A	180	ILE	N-CA-C	-6.45	99.14	108.36	2	1
1	A	215	THR	CA-C-O	-6.43	113.73	120.55	6	1
1	A	206	HIS	ND1-CG-CD2	6.43	112.53	106.10	4	3
1	A	211	ASN	CA-C-N	6.41	128.87	120.28	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	211	ASN	C-N-CA	6.41	128.87	120.28	14	4
1	A	241	LYS	CA-C-N	6.41	129.93	120.90	14	1
1	A	241	LYS	C-N-CA	6.41	129.93	120.90	14	1
1	A	202	PHE	CA-CB-CG	-6.40	107.40	113.80	14	3
1	A	172	HIS	CA-C-N	6.38	132.55	122.21	6	2
1	A	172	HIS	C-N-CA	6.38	132.55	122.21	6	2
1	A	212	LEU	O-C-N	-6.38	114.42	122.27	4	1
1	A	122	THR	O-C-N	6.38	130.31	121.64	3	1
1	A	153	ASN	N-CA-C	-6.37	104.56	112.90	10	4
1	A	144	VAL	O-C-N	-6.36	115.23	121.78	11	1
1	A	153	ASN	OD1-CG-ND2	-6.35	116.25	122.60	7	3
1	A	213	PHE	CA-C-O	-6.35	114.14	120.80	6	2
1	A	114	ILE	CA-C-O	-6.34	113.43	121.48	12	1
1	A	108	VAL	O-C-N	-6.33	115.92	122.63	13	2
1	A	128	GLU	N-CA-C	-6.33	103.68	111.40	6	2
1	A	256	ARG	NE-CZ-NH2	6.33	124.90	119.20	10	3
1	A	226	LEU	CA-C-N	6.32	130.50	122.85	7	2
1	A	226	LEU	C-N-CA	6.32	130.50	122.85	7	2
1	A	255	ILE	CA-C-N	6.32	129.60	120.38	14	2
1	A	255	ILE	C-N-CA	6.32	129.60	120.38	14	2
1	A	210	THR	CA-CB-OG1	-6.31	100.14	109.60	7	1
1	A	228	HIS	CE1-NE2-CD2	-6.31	102.69	109.00	6	4
1	A	158	ASP	CA-C-N	6.30	131.18	122.93	6	2
1	A	158	ASP	C-N-CA	6.30	131.18	122.93	6	2
1	A	180	ILE	CA-C-O	6.30	127.31	120.57	2	1
1	A	129	ASP	N-CA-CB	6.29	120.03	110.28	3	1
1	A	196	HIS	CA-CB-CG	6.29	120.09	113.80	3	1
1	A	250	LEU	CA-C-O	-6.28	114.71	121.56	11	1
1	A	141	TRP	CB-CG-CD2	6.27	135.58	126.80	11	1
1	A	214	LEU	CA-C-N	6.27	129.20	120.29	7	3
1	A	214	LEU	C-N-CA	6.27	129.20	120.29	7	3
1	A	235	VAL	CA-CB-CG1	6.27	121.06	110.40	14	2
1	A	220	ILE	CA-C-N	6.27	126.94	119.98	7	3
1	A	220	ILE	C-N-CA	6.27	126.94	119.98	7	3
1	A	215	THR	N-CA-CB	-6.25	100.91	110.16	7	1
1	A	149	PHE	CA-C-O	-6.25	113.84	120.40	6	2
1	A	199	GLU	N-CA-C	-6.24	105.16	112.89	5	2
1	A	215	THR	N-CA-C	-6.23	103.80	111.40	1	1
1	A	141	TRP	NE1-CE2-CD2	-6.22	99.32	107.40	14	1
1	A	244	ASP	CA-C-N	6.22	130.81	120.62	10	3
1	A	244	ASP	C-N-CA	6.22	130.81	120.62	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	108	VAL	N-CA-CB	-6.21	104.82	111.46	8	2
1	A	148	LYS	CA-C-N	6.20	132.54	122.81	14	1
1	A	148	LYS	C-N-CA	6.20	132.54	122.81	14	1
1	A	168	HIS	ND1-CE1-NE2	6.19	114.59	108.40	4	2
1	A	153	ASN	CB-CA-C	6.18	119.77	109.38	2	1
1	A	196	HIS	CG-CD2-NE2	-6.18	101.02	107.20	13	1
1	A	206	HIS	CB-CG-CD2	-6.18	123.17	131.20	4	2
1	A	154	THR	CB-CA-C	6.17	121.91	109.38	14	2
1	A	170	ASP	CA-C-O	-6.17	114.83	121.56	10	1
1	A	216	ALA	N-CA-C	6.14	117.98	111.28	9	2
1	A	242	TYR	N-CA-C	6.13	118.61	109.59	1	1
1	A	219	ALA	CA-C-N	6.13	130.36	120.30	1	3
1	A	219	ALA	C-N-CA	6.13	130.36	120.30	1	3
1	A	222	HIS	CA-C-N	6.12	129.31	120.38	13	3
1	A	222	HIS	C-N-CA	6.12	129.31	120.38	13	3
1	A	136	LYS	CA-C-N	6.11	129.60	120.31	12	2
1	A	136	LYS	C-N-CA	6.11	129.60	120.31	12	2
1	A	150	SER	CA-C-N	6.10	131.12	122.09	4	1
1	A	150	SER	C-N-CA	6.10	131.12	122.09	4	1
1	A	116	TYR	CA-CB-CG	6.10	124.88	113.90	3	1
1	A	170	ASP	CB-CA-C	6.10	119.89	110.14	5	1
1	A	130	VAL	CA-C-O	-6.09	114.29	121.05	5	1
1	A	117	ARG	N-CA-C	-6.09	99.07	109.24	8	1
1	A	213	PHE	O-C-N	-6.08	115.71	122.03	5	1
1	A	179	GLY	CA-C-N	6.08	129.24	120.98	14	2
1	A	179	GLY	C-N-CA	6.08	129.24	120.98	14	2
1	A	115	THR	O-C-N	-6.07	115.78	123.24	13	1
1	A	235	VAL	N-CA-C	-6.06	103.52	111.09	4	3
1	A	135	ARG	N-CA-C	-6.05	104.76	111.36	11	1
1	A	194	ASP	CA-CB-CG	-6.05	106.55	112.60	12	3
1	A	235	VAL	CA-C-N	6.04	133.15	121.18	12	1
1	A	235	VAL	C-N-CA	6.04	133.15	121.18	12	1
1	A	196	HIS	CA-C-N	6.04	131.34	123.00	14	1
1	A	196	HIS	C-N-CA	6.04	131.34	123.00	14	1
1	A	175	ASP	CB-CA-C	6.03	122.42	110.42	4	1
1	A	134	ILE	CA-C-O	-6.03	114.78	121.17	3	2
1	A	180	ILE	O-C-N	-6.02	115.59	122.94	13	1
1	A	176	GLY	CA-C-N	6.01	129.92	121.02	4	2
1	A	176	GLY	C-N-CA	6.01	129.92	121.02	4	2
1	A	229	SER	CA-C-N	6.01	131.81	122.49	2	2
1	A	229	SER	C-N-CA	6.01	131.81	122.49	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	196	HIS	N-CA-C	-6.01	101.63	110.52	7	1
1	A	141	TRP	CA-C-N	6.00	130.21	120.60	11	4
1	A	141	TRP	C-N-CA	6.00	130.21	120.60	11	4
1	A	164	ALA	CB-CA-C	6.00	119.75	110.14	4	1
1	A	222	HIS	CG-ND1-CE1	-6.00	99.10	109.30	12	3
1	A	196	HIS	ND1-CG-CD2	6.00	112.10	106.10	13	2
1	A	246	ASN	CB-CG-ND2	6.00	125.39	116.40	10	1
1	A	201	GLU	CA-C-N	5.99	133.20	123.37	13	3
1	A	201	GLU	C-N-CA	5.99	133.20	123.37	13	3
1	A	119	ASN	OD1-CG-ND2	-5.99	116.61	122.60	13	2
1	A	143	ASN	CA-C-N	5.98	129.30	122.36	12	1
1	A	143	ASN	C-N-CA	5.98	129.30	122.36	12	1
1	A	128	GLU	CA-C-O	-5.98	113.60	120.24	11	4
1	A	256	ARG	CA-C-N	5.97	133.11	121.41	12	2
1	A	256	ARG	C-N-CA	5.97	133.11	121.41	12	2
1	A	112	HIS	ND1-CE1-NE2	5.97	114.37	108.40	9	2
1	A	119	ASN	N-CA-C	-5.97	104.85	111.36	13	2
1	A	118	ILE	CB-CA-C	5.96	118.17	110.96	5	2
1	A	237	PHE	CA-C-O	-5.96	113.82	120.25	8	4
1	A	127	ARG	NH1-CZ-NH2	5.95	127.04	119.30	11	2
1	A	173	ALA	O-C-N	-5.95	115.92	123.24	10	1
1	A	213	PHE	CA-CB-CG	5.95	119.75	113.80	1	2
1	A	192	GLY	CA-C-O	-5.94	118.03	122.37	3	1
1	A	162	VAL	O-C-N	-5.94	117.00	123.18	10	1
1	A	141	TRP	NE1-CE2-CZ2	5.94	139.01	130.10	14	1
1	A	122	THR	CA-C-N	5.94	126.45	120.04	13	2
1	A	122	THR	C-N-CA	5.94	126.45	120.04	13	2
1	A	222	HIS	O-C-N	5.93	128.43	122.08	11	2
1	A	140	VAL	CB-CA-C	5.92	119.80	112.04	10	1
1	A	145	THR	O-C-N	-5.92	116.93	121.55	2	2
1	A	196	HIS	ND1-CE1-NE2	5.91	114.31	108.40	12	3
1	A	147	LEU	N-CA-C	5.91	118.52	110.55	10	1
1	A	169	GLY	CA-C-N	5.90	129.09	120.71	14	3
1	A	169	GLY	C-N-CA	5.90	129.09	120.71	14	3
1	A	141	TRP	CZ3-CH2-CZ2	-5.90	113.83	121.50	6	1
1	A	202	PHE	CA-C-N	5.89	129.92	121.50	3	2
1	A	202	PHE	C-N-CA	5.89	129.92	121.50	3	2
1	A	108	VAL	N-CA-C	5.89	118.11	109.63	13	2
1	A	234	ALA	O-C-N	-5.88	116.08	122.79	3	1
1	A	142	SER	CA-C-N	5.88	130.54	120.72	13	3
1	A	142	SER	C-N-CA	5.88	130.54	120.72	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	168	HIS	CB-CA-C	5.88	121.51	111.46	12	1
1	A	161	VAL	CB-CA-C	5.88	119.54	111.31	12	1
1	A	109	TRP	CA-C-N	5.88	132.76	121.54	13	3
1	A	109	TRP	C-N-CA	5.88	132.76	121.54	13	3
1	A	206	HIS	CE1-NE2-CD2	-5.87	103.13	109.00	14	2
1	A	192	GLY	O-C-N	-5.87	117.28	122.85	13	2
1	A	115	THR	CA-C-N	5.86	131.71	122.21	13	1
1	A	115	THR	C-N-CA	5.86	131.71	122.21	13	1
1	A	172	HIS	CB-CG-CD2	-5.86	123.58	131.20	12	1
1	A	258	ILE	CA-C-N	5.86	130.50	120.72	3	1
1	A	258	ILE	C-N-CA	5.86	130.50	120.72	3	1
1	A	137	ALA	CA-C-N	5.86	128.13	120.28	11	2
1	A	137	ALA	C-N-CA	5.86	128.13	120.28	11	2
1	A	144	VAL	N-CA-C	-5.85	107.58	113.20	11	1
1	A	149	PHE	CA-C-N	5.85	132.43	122.37	3	2
1	A	149	PHE	C-N-CA	5.85	132.43	122.37	3	2
1	A	210	THR	N-CA-C	-5.85	98.88	108.41	13	1
1	A	198	ASP	CA-C-O	-5.84	113.89	120.43	11	2
1	A	145	THR	CA-CB-CG2	5.84	120.43	110.50	5	1
1	A	110	ARG	CD-NE-CZ	5.83	132.57	124.40	12	2
1	A	193	GLY	O-C-N	5.83	128.57	122.51	6	2
1	A	103	MET	CA-C-N	5.83	125.73	119.85	7	4
1	A	103	MET	C-N-CA	5.83	125.73	119.85	7	4
1	A	240	TYR	CB-CG-CD1	-5.83	112.06	120.80	6	1
1	A	255	ILE	CA-C-O	-5.82	115.36	121.41	6	1
1	A	203	TRP	CE2-CD2-CE3	-5.82	112.98	118.80	11	2
1	A	117	ARG	NE-CZ-NH2	-5.81	113.97	119.20	3	1
1	A	223	SER	CA-CB-OG	5.81	122.72	111.10	13	1
1	A	262	TYR	CA-CB-CG	5.81	124.36	113.90	1	1
1	A	165	ARG	NE-CZ-NH1	5.81	127.31	121.50	3	1
1	A	229	SER	N-CA-CB	-5.80	101.63	110.45	14	1
1	A	175	ASP	O-C-N	5.79	128.35	122.09	2	1
1	A	193	GLY	CA-C-N	5.79	131.01	121.86	14	2
1	A	193	GLY	C-N-CA	5.79	131.01	121.86	14	2
1	A	130	VAL	CA-CB-CG1	5.79	120.24	110.40	13	2
1	A	173	ALA	CA-C-N	5.79	132.15	122.20	8	1
1	A	173	ALA	C-N-CA	5.79	132.15	122.20	8	1
1	A	262	TYR	CB-CA-C	5.78	120.42	111.28	2	1
1	A	198	ASP	CA-C-N	5.78	131.74	120.99	1	1
1	A	198	ASP	C-N-CA	5.78	131.74	120.99	1	1
1	A	135	ARG	NE-CZ-NH2	-5.77	114.00	119.20	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	121	TYR	O-C-N	-5.77	116.44	123.19	12	1
1	A	173	ALA	CA-C-O	-5.77	113.67	120.60	4	1
1	A	249	ARG	CA-C-N	5.77	129.06	120.87	7	1
1	A	249	ARG	C-N-CA	5.77	129.06	120.87	7	1
1	A	153	ASN	CA-C-N	5.77	132.36	121.69	10	3
1	A	153	ASN	C-N-CA	5.77	132.36	121.69	10	3
1	A	134	ILE	CA-C-N	5.77	127.94	120.44	10	3
1	A	134	ILE	C-N-CA	5.77	127.94	120.44	10	3
1	A	239	THR	CA-C-O	-5.77	115.31	121.94	7	1
1	A	163	PHE	CA-CB-CG	5.77	119.57	113.80	9	1
1	A	174	PHE	CB-CA-C	5.75	122.84	111.22	14	2
1	A	199	GLU	O-C-N	-5.75	114.78	122.43	1	1
1	A	223	SER	CA-C-N	5.75	132.79	121.58	6	1
1	A	223	SER	C-N-CA	5.75	132.79	121.58	6	1
1	A	183	HIS	CB-CG-ND1	-5.74	114.09	122.70	10	1
1	A	174	PHE	CB-CG-CD1	-5.73	110.95	120.70	8	1
1	A	254	ASP	O-C-N	5.71	127.95	122.07	3	1
1	A	243	VAL	CA-CB-CG2	5.71	120.10	110.40	14	1
1	A	258	ILE	CA-C-O	-5.71	114.09	120.25	1	1
1	A	222	HIS	CB-CG-CD2	-5.71	123.78	131.20	10	2
1	A	162	VAL	CA-CB-CG1	5.70	120.10	110.40	3	2
1	A	159	ILE	N-CA-CB	-5.70	105.16	111.66	14	1
1	A	127	ARG	NE-CZ-NH1	-5.69	115.81	121.50	2	2
1	A	232	PRO	O-C-N	5.68	129.33	122.23	9	1
1	A	112	HIS	CA-CB-CG	5.68	119.48	113.80	1	1
1	A	117	ARG	CD-NE-CZ	5.67	132.34	124.40	6	2
1	A	201	GLU	N-CA-CB	-5.67	102.61	110.38	10	2
1	A	141	TRP	CB-CG-CD1	-5.67	118.40	126.90	11	1
1	A	134	ILE	CB-CA-C	5.66	119.21	111.97	3	1
1	A	168	HIS	ND1-CG-CD2	5.66	111.76	106.10	4	4
1	A	252	ALA	N-CA-C	5.65	117.92	111.02	5	1
1	A	172	HIS	N-CA-C	-5.65	106.51	113.41	8	1
1	A	208	GLY	N-CA-C	-5.65	99.79	113.18	10	1
1	A	220	ILE	CB-CA-C	5.65	119.76	112.14	5	1
1	A	124	ASP	N-CA-C	-5.64	105.89	112.89	7	1
1	A	101	ARG	NH1-CZ-NH2	5.64	126.63	119.30	6	2
1	A	241	LYS	CA-C-O	-5.64	114.17	120.66	11	1
1	A	227	GLY	CA-C-O	-5.64	116.65	121.78	2	1
1	A	258	ILE	CA-CB-CG2	5.63	120.07	110.50	1	2
1	A	221	GLY	CA-C-N	5.63	128.61	120.79	11	2
1	A	221	GLY	C-N-CA	5.63	128.61	120.79	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	201	GLU	N-CA-C	-5.63	102.19	110.52	4	1
1	A	240	TYR	O-C-N	-5.62	116.07	123.21	13	1
1	A	171	PHE	CA-C-N	5.62	129.59	120.60	14	1
1	A	171	PHE	C-N-CA	5.62	129.59	120.60	14	1
1	A	118	ILE	N-CA-CB	5.62	118.74	111.83	4	1
1	A	230	SER	N-CA-CB	-5.60	102.38	110.56	9	2
1	A	248	PHE	CA-C-N	5.60	131.05	121.87	2	2
1	A	248	PHE	C-N-CA	5.60	131.05	121.87	2	2
1	A	215	THR	OG1-CB-CG2	-5.60	98.11	109.30	4	1
1	A	247	THR	CA-C-N	5.58	128.79	120.87	11	2
1	A	247	THR	C-N-CA	5.58	128.79	120.87	11	2
1	A	131	ASP	N-CA-C	5.58	117.17	111.14	4	1
1	A	116	TYR	CB-CA-C	5.58	122.34	110.07	6	1
1	A	212	LEU	N-CA-C	5.57	119.18	112.38	6	1
1	A	182	ALA	CB-CA-C	5.57	118.07	110.94	12	1
1	A	142	SER	O-C-N	-5.57	115.16	122.39	9	1
1	A	246	ASN	CA-C-N	5.55	129.48	120.60	4	1
1	A	246	ASN	C-N-CA	5.55	129.48	120.60	4	1
1	A	218	HIS	N-CA-CB	5.55	118.38	110.16	13	1
1	A	227	GLY	CA-C-N	5.54	129.35	121.42	7	2
1	A	227	GLY	C-N-CA	5.54	129.35	121.42	7	2
1	A	113	TYR	CG-CD1-CE1	-5.54	112.89	121.20	9	1
1	A	245	ILE	CA-CB-CG2	5.54	119.92	110.50	1	1
1	A	230	SER	O-C-N	-5.54	115.42	122.34	14	1
1	A	208	GLY	CA-C-O	-5.53	110.94	120.57	4	2
1	A	178	GLY	CA-C-N	5.53	132.25	121.41	11	1
1	A	178	GLY	C-N-CA	5.53	132.25	121.41	11	1
1	A	107	PRO	N-CD-CG	5.53	111.50	103.20	3	1
1	A	108	VAL	CB-CA-C	-5.53	103.96	111.15	5	1
1	A	145	THR	N-CA-C	5.53	114.66	108.25	8	1
1	A	109	TRP	NE1-CE2-CD2	-5.52	100.23	107.40	11	1
1	A	114	ILE	CB-CA-C	5.52	118.76	110.98	9	1
1	A	219	ALA	N-CA-CB	-5.51	102.02	110.12	11	1
1	A	170	ASP	CA-C-N	5.51	132.06	121.54	10	5
1	A	170	ASP	C-N-CA	5.51	132.06	121.54	10	5
1	A	131	ASP	CA-CB-CG	-5.51	107.09	112.60	11	2
1	A	206	HIS	O-C-N	-5.50	116.04	123.19	1	2
1	A	241	LYS	CB-CA-C	5.50	121.06	109.79	1	2
1	A	135	ARG	CA-C-O	-5.49	114.60	120.42	8	1
1	A	113	TYR	CA-C-N	5.49	130.61	122.71	11	1
1	A	113	TYR	C-N-CA	5.49	130.61	122.71	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	175	ASP	CA-CB-CG	5.49	118.09	112.60	6	2
1	A	187	PRO	CA-C-N	5.48	130.36	122.63	2	1
1	A	187	PRO	C-N-CA	5.48	130.36	122.63	2	1
1	A	113	TYR	CB-CG-CD2	-5.47	112.59	120.80	2	1
1	A	182	ALA	N-CA-C	-5.47	100.75	109.23	1	1
1	A	259	GLN	OE1-CD-NE2	-5.47	117.13	122.60	7	2
1	A	241	LYS	N-CA-C	-5.47	99.76	109.06	13	1
1	A	124	ASP	O-C-N	5.46	127.91	122.12	10	1
1	A	112	HIS	N-CA-CB	-5.46	102.62	110.65	4	1
1	A	139	GLN	N-CA-CB	-5.46	101.89	110.30	1	1
1	A	119	ASN	CA-C-O	5.46	126.73	121.00	3	1
1	A	160	LEU	N-CA-CB	-5.45	101.50	109.95	6	1
1	A	194	ASP	OD1-CG-OD2	-5.45	109.82	122.90	8	1
1	A	146	PRO	N-CA-C	5.45	120.73	114.03	13	1
1	A	151	LYS	CA-C-O	5.43	127.17	120.92	2	1
1	A	195	ALA	CA-C-O	5.43	126.78	120.49	6	1
1	A	150	SER	CB-CA-C	5.42	120.39	109.38	3	1
1	A	203	TRP	CA-CB-CG	5.42	123.90	113.60	6	1
1	A	222	HIS	CG-CD2-NE2	-5.41	101.79	107.20	6	2
1	A	176	GLY	O-C-N	-5.41	118.07	123.48	13	1
1	A	118	ILE	O-C-N	-5.40	116.35	122.94	9	1
1	A	117	ARG	CB-CA-C	5.40	120.05	109.35	8	2
1	A	230	SER	N-CA-C	-5.40	106.74	113.38	1	2
1	A	241	LYS	CB-CG-CD	5.40	123.71	111.30	13	1
1	A	220	ILE	CA-CB-CG2	5.39	119.67	110.50	8	1
1	A	235	VAL	CB-CA-C	5.39	118.77	111.88	8	1
1	A	159	ILE	CA-CB-CG2	5.37	119.63	110.50	10	1
1	A	147	LEU	CB-CA-C	-5.37	101.25	110.22	3	1
1	A	181	LEU	N-CA-C	-5.37	106.41	113.12	1	2
1	A	159	ILE	N-CA-C	-5.36	99.37	107.73	5	1
1	A	199	GLU	CA-C-O	-5.36	112.25	119.11	8	1
1	A	233	LYS	N-CA-C	-5.35	105.98	112.88	11	1
1	A	243	VAL	CB-CA-C	5.34	118.67	110.55	1	1
1	A	114	ILE	N-CA-C	-5.34	100.68	109.12	2	1
1	A	222	HIS	CA-C-O	5.33	125.94	119.38	1	2
1	A	101	ARG	O-C-N	-5.33	115.55	121.84	9	1
1	A	116	TYR	O-C-N	-5.33	115.32	122.94	2	1
1	A	150	SER	N-CA-CB	-5.33	101.56	110.83	6	1
1	A	187	PRO	N-CA-CB	-5.33	97.66	103.25	2	1
1	A	114	ILE	CA-CB-CG1	5.33	119.45	110.40	3	1
1	A	154	THR	CA-CB-CG2	5.32	119.54	110.50	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	232	PRO	N-CD-CG	5.32	111.17	103.20	12	2
1	A	243	VAL	CA-C-N	5.31	132.48	121.32	3	1
1	A	243	VAL	C-N-CA	5.31	132.48	121.32	3	1
1	A	251	SER	N-CA-CB	-5.31	102.68	110.85	9	1
1	A	204	THR	CA-C-N	5.31	131.00	122.14	13	1
1	A	204	THR	C-N-CA	5.31	131.00	122.14	13	1
1	A	226	LEU	N-CA-C	-5.31	102.90	110.59	14	3
1	A	221	GLY	O-C-N	-5.29	117.11	122.19	7	1
1	A	169	GLY	N-CA-C	-5.29	107.38	115.00	2	1
1	A	243	VAL	N-CA-CB	5.29	121.82	111.92	7	1
1	A	163	PHE	N-CA-C	-5.29	99.15	108.20	12	1
1	A	261	LEU	CB-CA-C	-5.29	100.83	109.56	3	2
1	A	238	PRO	CA-C-N	5.29	128.36	120.90	5	1
1	A	238	PRO	C-N-CA	5.29	128.36	120.90	5	1
1	A	131	ASP	CA-C-O	5.29	126.56	120.90	7	1
1	A	174	PHE	CD1-CG-CD2	5.28	126.52	118.60	11	1
1	A	222	HIS	CB-CA-C	5.26	119.80	110.85	3	1
1	A	237	PHE	N-CA-C	5.26	117.16	109.84	9	1
1	A	216	ALA	CA-C-N	5.26	127.66	120.77	6	1
1	A	216	ALA	C-N-CA	5.26	127.66	120.77	6	1
1	A	172	HIS	CG-ND1-CE1	-5.26	100.36	109.30	3	1
1	A	148	LYS	N-CA-CB	-5.25	101.86	110.52	8	1
1	A	205	THR	CB-CA-C	5.25	120.47	111.45	10	1
1	A	158	ASP	CA-C-O	-5.24	114.94	120.71	8	1
1	A	209	GLY	CA-C-N	5.24	130.39	123.00	13	2
1	A	209	GLY	C-N-CA	5.24	130.39	123.00	13	2
1	A	153	ASN	O-C-N	-5.24	116.52	122.23	6	1
1	A	122	THR	CA-CB-OG1	5.24	117.45	109.60	7	1
1	A	199	GLU	CA-CB-CG	5.23	124.57	114.10	13	1
1	A	196	HIS	CA-C-O	-5.23	114.90	120.92	3	1
1	A	141	TRP	CA-C-O	-5.23	113.62	119.79	9	1
1	A	151	LYS	N-CA-CB	-5.23	101.89	110.41	13	1
1	A	180	ILE	CA-CB-CG1	5.22	119.28	110.40	5	1
1	A	197	PHE	CA-C-N	5.22	128.26	120.95	13	2
1	A	197	PHE	C-N-CA	5.22	128.26	120.95	13	2
1	A	231	ASP	N-CA-CB	-5.21	102.40	110.07	7	1
1	A	211	ASN	CA-CB-CG	-5.21	107.39	112.60	6	1
1	A	193	GLY	CA-C-O	-5.21	113.87	118.77	12	1
1	A	129	ASP	O-C-N	-5.21	116.22	122.15	4	1
1	A	108	VAL	CA-CB-CG2	5.20	119.24	110.40	1	2
1	A	122	THR	CB-CA-C	5.20	116.20	108.87	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	251	SER	O-C-N	-5.20	116.59	122.68	5	1
1	A	106	GLY	CA-C-N	5.20	126.33	119.84	11	1
1	A	106	GLY	C-N-CA	5.20	126.33	119.84	11	1
1	A	153	ASN	CA-C-O	-5.19	113.52	119.60	1	1
1	A	237	PHE	CA-CB-CG	5.19	118.99	113.80	14	1
1	A	123	PRO	N-CA-CB	5.18	108.12	103.20	5	1
1	A	248	PHE	CA-CB-CG	5.17	118.97	113.80	5	1
1	A	205	THR	CA-CB-CG2	5.17	119.29	110.50	5	1
1	A	223	SER	N-CA-CB	-5.17	101.34	110.39	7	1
1	A	126	ASN	N-CA-CB	-5.16	102.04	109.83	3	1
1	A	107	PRO	CB-CA-C	-5.15	103.06	111.56	6	2
1	A	154	THR	N-CA-CB	-5.15	101.95	111.53	8	1
1	A	140	VAL	N-CA-C	-5.15	105.52	110.72	12	1
1	A	129	ASP	N-CA-C	-5.15	105.75	111.36	4	1
1	A	183	HIS	CB-CG-CD2	-5.15	124.51	131.20	13	1
1	A	162	VAL	N-CA-C	5.15	115.39	107.77	10	2
1	A	235	VAL	CA-C-O	5.14	126.40	121.05	5	1
1	A	211	ASN	CA-C-O	5.14	126.55	120.69	5	1
1	A	214	LEU	O-C-N	5.13	128.57	122.27	14	1
1	A	256	ARG	O-C-N	-5.12	115.57	122.43	12	1
1	A	139	GLN	CA-C-O	-5.11	114.10	119.97	5	1
1	A	158	ASP	N-CA-C	-5.10	100.66	110.56	8	1
1	A	249	ARG	NE-CZ-NH2	5.10	123.79	119.20	5	1
1	A	198	ASP	N-CA-C	5.10	116.80	108.63	7	1
1	A	222	HIS	N-CA-CB	-5.10	102.36	110.22	2	1
1	A	229	SER	CA-C-O	-5.09	115.45	121.66	8	1
1	A	120	ASN	CB-CA-C	5.09	120.86	109.56	11	1
1	A	134	ILE	N-CA-C	-5.08	105.46	111.00	13	1
1	A	113	TYR	CD1-CE1-CZ	-5.08	110.46	119.60	5	1
1	A	243	VAL	O-C-N	5.07	128.75	123.02	13	1
1	A	135	ARG	NH1-CZ-NH2	5.07	125.89	119.30	12	1
1	A	123	PRO	N-CA-C	-5.06	107.43	114.27	2	1
1	A	230	SER	CB-CA-C	5.06	119.35	110.64	7	1
1	A	206	HIS	N-CA-CB	-5.06	102.67	110.56	13	1
1	A	137	ALA	CA-C-O	-5.06	113.82	119.79	6	1
1	A	228	HIS	CA-C-N	5.06	129.58	122.09	12	1
1	A	228	HIS	C-N-CA	5.06	129.58	122.09	12	1
1	A	146	PRO	N-CA-CB	-5.06	98.40	103.20	2	1
1	A	165	ARG	NH1-CZ-NH2	5.05	125.86	119.30	5	1
1	A	194	ASP	CA-C-O	5.04	126.65	120.60	12	1
1	A	246	ASN	CB-CA-C	-5.04	100.10	110.38	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	175	ASP	CA-C-N	5.04	131.58	122.66	4	1
1	A	175	ASP	C-N-CA	5.04	131.58	122.66	4	1
1	A	223	SER	N-CA-C	5.04	118.68	112.54	10	1
1	A	208	GLY	O-C-N	-5.04	119.17	123.80	11	1
1	A	125	MET	N-CA-CB	5.03	120.45	111.69	9	1
1	A	257	GLY	N-CA-C	-5.03	106.40	112.49	10	1
1	A	113	TYR	CG-CD2-CE2	-5.03	113.66	121.20	13	1
1	A	147	LEU	O-C-N	-5.02	117.35	123.13	3	1
1	A	229	SER	CA-CB-OG	5.02	121.15	111.10	12	1
1	A	132	TYR	N-CA-C	5.02	116.75	111.28	2	1
1	A	128	GLU	N-CA-CB	-5.02	102.57	110.30	4	1
1	A	256	ARG	CB-CG-CD	5.02	122.84	111.30	4	1
1	A	167	ALA	CA-C-O	-5.02	114.93	120.60	5	1
1	A	228	HIS	ND1-CG-CD2	5.01	111.11	106.10	11	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	242	TYR	Sidechain,Peptide	7
1	A	121	TYR	Sidechain	5
1	A	204	THR	Peptide	5
1	A	262	TYR	Sidechain	5
1	A	240	TYR	Sidechain,Peptide	4
1	A	113	TYR	Sidechain	3
1	A	116	TYR	Mainchain,Sidechain	3
1	A	132	TYR	Sidechain	3
1	A	110	ARG	Sidechain	2
1	A	248	PHE	Peptide,Sidechain	2
1	A	185	PHE	Sidechain	2
1	A	135	ARG	Sidechain	2
1	A	197	PHE	Sidechain	2
1	A	159	ILE	Peptide	1
1	A	256	ARG	Sidechain	1
1	A	164	ALA	Peptide	1
1	A	199	GLU	Sidechain	1
1	A	202	PHE	Sidechain	1
1	A	222	HIS	Sidechain	1
1	A	249	ARG	Sidechain	1
1	A	171	PHE	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	206	HIS	Sidechain	1
1	A	172	HIS	Sidechain	1
1	A	117	ARG	Sidechain	1
1	A	163	PHE	Sidechain	1
1	A	252	ALA	Mainchain	1
1	A	101	ARG	Sidechain	1
1	A	151	LYS	Peptide	1
1	A	218	HIS	Sidechain	1
1	A	224	LEU	Mainchain	1
1	A	183	HIS	Sidechain	1
1	A	237	PHE	Sidechain	1
1	A	100	PHE	Sidechain	1
1	A	127	ARG	Mainchain	1
1	A	174	PHE	Peptide	1
1	A	196	HIS	Sidechain	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	1265	1199	1196	2±2
4	A	5750	0	9000	131±13
All	All	98280	16786	142744	1847

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:388:PX4:H39	4:A:411:PX4:H17	0.99	1.35	4	1
4:A:337:PX4:H47	4:A:353:PX4:H15	0.93	1.41	8	2
4:A:413:PX4:H24	4:A:430:PX4:H63	0.92	1.40	10	1
4:A:320:PX4:H20	4:A:359:PX4:H57	0.92	1.42	5	1
4:A:368:PX4:H22	4:A:369:PX4:H51	0.90	1.40	6	1
4:A:342:PX4:H24	4:A:352:PX4:H47	0.88	1.43	11	1
4:A:378:PX4:H16	4:A:417:PX4:H47	0.85	1.46	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:309:PX4:H59	4:A:324:PX4:H57	0.84	1.50	12	1
4:A:355:PX4:H48	4:A:356:PX4:H14	0.83	1.49	4	2
4:A:332:PX4:H61	4:A:349:PX4:H51	0.83	1.51	6	1
4:A:329:PX4:H70	4:A:382:PX4:H26	0.82	1.50	7	1
4:A:316:PX4:H20	4:A:364:PX4:H47	0.82	1.49	9	1
4:A:386:PX4:H28	4:A:394:PX4:H50	0.82	1.50	11	1
4:A:313:PX4:H18	4:A:318:PX4:H46	0.81	1.50	9	2
4:A:416:PX4:H21	4:A:425:PX4:H46	0.81	1.51	11	1
4:A:335:PX4:H21	4:A:343:PX4:H22	0.81	1.52	5	1
4:A:317:PX4:H17	4:A:325:PX4:H52	0.81	1.53	9	1
4:A:384:PX4:H60	4:A:385:PX4:H35	0.80	1.54	2	1
4:A:387:PX4:H47	4:A:411:PX4:H17	0.79	1.54	12	1
4:A:340:PX4:H31	4:A:340:PX4:H66	0.79	1.55	5	1
4:A:387:PX4:H24	4:A:394:PX4:H53	0.78	1.55	1	2
4:A:404:PX4:H34	4:A:419:PX4:H22	0.78	1.55	8	1
4:A:376:PX4:H54	4:A:385:PX4:H17	0.77	1.57	13	1
4:A:317:PX4:H47	4:A:342:PX4:H69	0.77	1.57	12	1
4:A:421:PX4:H31	4:A:422:PX4:H39	0.77	1.55	2	1
4:A:368:PX4:H25	4:A:425:PX4:H42	0.76	1.58	4	1
4:A:310:PX4:H16	4:A:363:PX4:H20	0.76	1.56	9	2
4:A:413:PX4:H50	4:A:422:PX4:H33	0.75	1.58	2	1
4:A:393:PX4:H22	4:A:394:PX4:H19	0.75	1.58	7	1
4:A:321:PX4:H20	4:A:354:PX4:H48	0.75	1.56	10	1
4:A:326:PX4:H50	4:A:351:PX4:H18	0.75	1.58	4	1
4:A:400:PX4:H51	4:A:409:PX4:H20	0.75	1.57	12	1
4:A:321:PX4:H41	4:A:354:PX4:H59	0.75	1.58	10	1
4:A:417:PX4:H31	4:A:426:PX4:H61	0.74	1.58	6	1
4:A:398:PX4:H16	4:A:407:PX4:H49	0.74	1.58	14	1
4:A:330:PX4:H22	4:A:335:PX4:H19	0.74	1.60	2	1
4:A:345:PX4:H48	4:A:353:PX4:H46	0.74	1.59	4	1
4:A:330:PX4:H60	4:A:357:PX4:H24	0.73	1.60	10	2
4:A:306:PX4:H23	4:A:321:PX4:H39	0.73	1.60	5	1
4:A:332:PX4:H31	4:A:332:PX4:H51	0.73	1.58	7	1
4:A:392:PX4:H18	4:A:393:PX4:H50	0.72	1.61	1	1
4:A:395:PX4:H53	4:A:405:PX4:H22	0.72	1.60	4	1
4:A:317:PX4:H17	4:A:325:PX4:H49	0.72	1.60	1	1
4:A:403:PX4:H10	4:A:427:PX4:H49	0.72	1.61	3	2
4:A:325:PX4:H30	4:A:334:PX4:H18	0.72	1.60	4	1
4:A:376:PX4:H50	4:A:385:PX4:H17	0.72	1.60	11	2
4:A:383:PX4:H65	4:A:399:PX4:H31	0.72	1.60	8	1
4:A:317:PX4:H46	4:A:324:PX4:H17	0.72	1.60	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:367:PX4:H28	4:A:424:PX4:H52	0.72	1.62	4	1
4:A:371:PX4:H59	4:A:379:PX4:H33	0.72	1.61	4	1
4:A:323:PX4:H68	4:A:367:PX4:H40	0.72	1.62	3	1
4:A:378:PX4:H63	4:A:417:PX4:H62	0.72	1.62	11	1
4:A:321:PX4:H38	4:A:328:PX4:H57	0.72	1.61	13	1
4:A:385:PX4:H52	4:A:386:PX4:H26	0.71	1.61	14	1
4:A:383:PX4:H61	4:A:399:PX4:H29	0.71	1.60	6	1
4:A:402:PX4:H38	4:A:404:PX4:H62	0.71	1.59	14	1
4:A:376:PX4:H64	4:A:392:PX4:H29	0.71	1.60	5	1
4:A:387:PX4:H65	4:A:411:PX4:H54	0.71	1.63	8	1
4:A:409:PX4:H33	4:A:410:PX4:H46	0.71	1.60	2	1
4:A:332:PX4:H43	4:A:363:PX4:H72	0.71	1.63	12	1
4:A:402:PX4:H60	4:A:413:PX4:H41	0.71	1.63	7	1
4:A:363:PX4:H1	4:A:364:PX4:H20	0.71	1.61	11	1
4:A:391:PX4:H64	4:A:408:PX4:H55	0.71	1.63	7	1
4:A:321:PX4:H38	4:A:412:PX4:H43	0.70	1.62	14	1
4:A:370:PX4:H19	4:A:403:PX4:H17	0.70	1.63	11	2
4:A:419:PX4:H49	4:A:427:PX4:H49	0.70	1.63	13	1
4:A:308:PX4:H62	4:A:311:PX4:H41	0.70	1.64	13	1
4:A:325:PX4:H31	4:A:332:PX4:H25	0.70	1.63	11	1
4:A:306:PX4:H56	4:A:321:PX4:H55	0.69	1.64	13	1
4:A:384:PX4:H42	4:A:385:PX4:H43	0.69	1.62	8	1
4:A:317:PX4:H16	4:A:351:PX4:H24	0.69	1.64	14	1
4:A:408:PX4:H17	4:A:415:PX4:H20	0.69	1.64	8	1
4:A:322:PX4:H50	4:A:336:PX4:H27	0.69	1.63	1	1
4:A:332:PX4:H33	4:A:347:PX4:H62	0.69	1.64	11	1
4:A:374:PX4:H49	4:A:382:PX4:H46	0.69	1.62	8	2
4:A:358:PX4:H23	4:A:363:PX4:H53	0.69	1.64	9	1
4:A:315:PX4:H17	4:A:316:PX4:H49	0.69	1.64	13	1
4:A:360:PX4:H70	4:A:419:PX4:H41	0.69	1.62	4	1
4:A:399:PX4:H63	4:A:399:PX4:H29	0.69	1.64	2	1
4:A:368:PX4:H17	4:A:369:PX4:H53	0.69	1.63	9	1
4:A:331:PX4:H58	4:A:339:PX4:H22	0.69	1.63	4	1
4:A:396:PX4:H38	4:A:402:PX4:H41	0.69	1.64	12	1
4:A:422:PX4:H36	4:A:423:PX4:H23	0.68	1.65	5	1
4:A:388:PX4:H54	4:A:395:PX4:H30	0.68	1.65	12	1
4:A:368:PX4:H47	4:A:369:PX4:H56	0.68	1.63	1	1
4:A:429:PX4:H55	4:A:429:PX4:H30	0.68	1.63	11	1
4:A:337:PX4:H50	4:A:353:PX4:H21	0.68	1.64	4	1
4:A:328:PX4:H70	4:A:412:PX4:H70	0.68	1.65	13	1
4:A:395:PX4:H55	4:A:404:PX4:H46	0.68	1.66	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:416:PX4:H55	4:A:418:PX4:H30	0.68	1.66	12	1
4:A:388:PX4:H38	4:A:411:PX4:H46	0.68	1.65	5	1
4:A:306:PX4:H14	4:A:321:PX4:H28	0.68	1.66	12	1
4:A:316:PX4:H14	4:A:320:PX4:H22	0.68	1.64	10	1
4:A:378:PX4:H51	4:A:418:PX4:H50	0.68	1.65	13	1
4:A:376:PX4:H67	4:A:385:PX4:H30	0.68	1.64	2	1
4:A:391:PX4:H40	4:A:408:PX4:H42	0.67	1.66	2	1
4:A:370:PX4:H22	4:A:403:PX4:H17	0.67	1.65	9	2
4:A:306:PX4:H20	4:A:329:PX4:H52	0.67	1.66	9	1
4:A:346:PX4:H22	4:A:354:PX4:H21	0.67	1.65	9	1
4:A:331:PX4:H63	4:A:340:PX4:H71	0.67	1.67	14	1
4:A:330:PX4:H44	4:A:344:PX4:H45	0.67	1.66	12	1
4:A:312:PX4:H16	4:A:359:PX4:H5	0.67	1.64	14	1
4:A:384:PX4:H2	4:A:385:PX4:H18	0.67	1.66	1	4
4:A:331:PX4:H33	4:A:340:PX4:H69	0.67	1.66	3	1
4:A:315:PX4:H42	4:A:425:PX4:H31	0.67	1.67	4	1
4:A:332:PX4:H25	4:A:390:PX4:H41	0.67	1.67	6	1
4:A:308:PX4:H38	4:A:311:PX4:H69	0.67	1.65	12	1
4:A:417:PX4:H19	4:A:426:PX4:H24	0.67	1.66	12	1
4:A:424:PX4:H53	4:A:425:PX4:H22	0.66	1.67	2	1
4:A:331:PX4:H35	4:A:397:PX4:H44	0.66	1.66	7	1
4:A:395:PX4:H49	4:A:396:PX4:H24	0.66	1.67	14	1
4:A:350:PX4:H56	4:A:364:PX4:H37	0.66	1.66	3	1
4:A:371:PX4:H61	4:A:372:PX4:H27	0.66	1.68	4	1
4:A:306:PX4:H56	4:A:361:PX4:H59	0.66	1.66	5	1
4:A:311:PX4:H53	4:A:316:PX4:H20	0.66	1.68	6	1
4:A:378:PX4:H56	4:A:417:PX4:H58	0.66	1.68	8	2
4:A:313:PX4:H49	4:A:328:PX4:H17	0.65	1.65	4	1
4:A:326:PX4:H28	4:A:350:PX4:H24	0.65	1.68	5	1
4:A:391:PX4:H28	4:A:414:PX4:H46	0.65	1.69	5	1
4:A:311:PX4:H65	4:A:359:PX4:H71	0.65	1.66	7	1
4:A:383:PX4:H50	4:A:399:PX4:H17	0.65	1.67	8	1
4:A:380:PX4:H56	4:A:387:PX4:H50	0.65	1.68	11	1
4:A:311:PX4:H10	4:A:359:PX4:H51	0.65	1.68	2	1
4:A:373:PX4:H26	4:A:381:PX4:H53	0.65	1.68	9	1
4:A:345:PX4:H40	4:A:345:PX4:H64	0.65	1.69	4	1
4:A:321:PX4:H50	4:A:354:PX4:H27	0.65	1.66	6	1
4:A:316:PX4:H51	4:A:320:PX4:H27	0.65	1.69	12	1
4:A:417:PX4:H31	4:A:426:PX4:H37	0.65	1.67	13	1
4:A:387:PX4:H16	4:A:394:PX4:H9	0.65	1.69	2	1
4:A:356:PX4:H10	4:A:356:PX4:H16	0.65	1.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:333:PX4:H56	4:A:341:PX4:H54	0.65	1.68	12	1
4:A:382:PX4:H19	4:A:428:PX4:H23	0.64	1.69	1	1
4:A:388:PX4:H20	4:A:411:PX4:H14	0.64	1.70	3	1
4:A:421:PX4:H22	4:A:422:PX4:H26	0.64	1.68	6	1
4:A:306:PX4:H18	4:A:322:PX4:H51	0.64	1.69	13	1
4:A:317:PX4:H55	4:A:324:PX4:H31	0.64	1.69	14	1
4:A:354:PX4:H50	4:A:360:PX4:H55	0.64	1.69	4	1
4:A:371:PX4:H20	4:A:379:PX4:H21	0.64	1.68	14	1
4:A:385:PX4:H71	4:A:392:PX4:H30	0.64	1.69	5	1
4:A:326:PX4:O8	4:A:351:PX4:H17	0.64	1.91	6	1
4:A:314:PX4:H34	4:A:356:PX4:H33	0.64	1.67	7	1
4:A:403:PX4:H7	4:A:427:PX4:H52	0.64	1.68	9	1
4:A:418:PX4:H42	4:A:422:PX4:H59	0.64	1.68	1	1
4:A:307:PX4:H60	4:A:349:PX4:H45	0.64	1.69	14	1
4:A:360:PX4:H44	4:A:412:PX4:H60	0.64	1.69	4	1
4:A:335:PX4:H48	4:A:343:PX4:H21	0.64	1.67	11	1
4:A:406:PX4:H48	4:A:421:PX4:H53	0.64	1.69	12	1
4:A:311:PX4:H52	4:A:320:PX4:H24	0.64	1.68	5	1
4:A:317:PX4:H48	4:A:342:PX4:H54	0.64	1.69	5	1
4:A:391:PX4:H43	4:A:394:PX4:H34	0.64	1.70	5	1
4:A:371:PX4:H16	4:A:379:PX4:H20	0.64	1.70	14	2
4:A:391:PX4:H48	4:A:408:PX4:H16	0.64	1.69	2	3
4:A:306:PX4:H38	4:A:321:PX4:H43	0.64	1.68	12	1
4:A:403:PX4:H47	4:A:427:PX4:H48	0.64	1.68	12	1
4:A:345:PX4:H37	4:A:353:PX4:H64	0.64	1.68	1	1
4:A:395:PX4:H19	4:A:398:PX4:H54	0.64	1.68	4	1
4:A:387:PX4:H46	4:A:388:PX4:H37	0.64	1.68	6	1
4:A:308:PX4:H34	4:A:314:PX4:H58	0.64	1.70	8	1
4:A:404:PX4:H34	4:A:419:PX4:H48	0.63	1.70	3	1
4:A:409:PX4:H41	4:A:410:PX4:H24	0.63	1.70	4	1
4:A:404:PX4:H39	4:A:419:PX4:H30	0.63	1.68	9	1
4:A:385:PX4:H32	4:A:386:PX4:H32	0.63	1.70	7	1
4:A:350:PX4:H50	4:A:363:PX4:H51	0.63	1.68	11	2
4:A:421:PX4:H39	4:A:423:PX4:H33	0.63	1.68	11	1
4:A:404:PX4:H49	4:A:413:PX4:H21	0.63	1.68	5	1
4:A:424:PX4:H48	4:A:425:PX4:H21	0.63	1.70	9	1
4:A:313:PX4:H22	4:A:318:PX4:H51	0.63	1.70	11	1
4:A:324:PX4:H48	4:A:341:PX4:H3	0.63	1.69	8	1
4:A:322:PX4:H17	4:A:336:PX4:H23	0.63	1.70	11	1
4:A:355:PX4:H72	4:A:356:PX4:H53	0.63	1.70	3	1
4:A:428:PX4:H61	4:A:430:PX4:H29	0.63	1.71	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:410:PX4:H62	4:A:426:PX4:H37	0.63	1.69	4	1
4:A:382:PX4:H22	4:A:428:PX4:H32	0.63	1.68	5	1
4:A:320:PX4:H17	4:A:359:PX4:H56	0.63	1.71	7	1
4:A:408:PX4:H47	4:A:415:PX4:H21	0.63	1.70	9	1
4:A:395:PX4:H47	4:A:396:PX4:H20	0.63	1.71	12	1
4:A:363:PX4:H20	4:A:364:PX4:H33	0.63	1.69	1	1
4:A:372:PX4:H38	4:A:378:PX4:H42	0.63	1.70	13	1
4:A:311:PX4:H50	4:A:316:PX4:H19	0.63	1.71	14	1
4:A:325:PX4:H24	4:A:340:PX4:H53	0.63	1.70	5	1
4:A:362:PX4:O2	4:A:362:PX4:H13	0.62	1.93	11	1
4:A:370:PX4:H54	4:A:411:PX4:H50	0.62	1.71	12	1
4:A:308:PX4:H22	4:A:364:PX4:H14	0.62	1.71	3	1
4:A:320:PX4:H68	4:A:417:PX4:H72	0.62	1.71	1	1
4:A:353:PX4:H39	4:A:366:PX4:H26	0.62	1.70	1	1
4:A:375:PX4:H55	4:A:429:PX4:H41	0.62	1.70	5	1
4:A:377:PX4:H4	4:A:418:PX4:H49	0.62	1.71	6	1
4:A:309:PX4:H40	4:A:372:PX4:H45	0.62	1.69	11	1
4:A:317:PX4:H55	4:A:324:PX4:H20	0.62	1.70	2	1
4:A:331:PX4:H66	4:A:373:PX4:H45	0.62	1.71	13	1
4:A:378:PX4:H21	4:A:417:PX4:H48	0.62	1.72	3	1
4:A:337:PX4:H58	4:A:353:PX4:H27	0.62	1.69	5	1
4:A:330:PX4:H64	4:A:357:PX4:H28	0.62	1.71	10	1
4:A:395:PX4:H63	4:A:421:PX4:H20	0.62	1.70	9	1
4:A:317:PX4:H63	4:A:325:PX4:H59	0.62	1.71	5	1
4:A:326:PX4:H17	4:A:351:PX4:O8	0.62	1.95	14	2
4:A:389:PX4:H69	4:A:397:PX4:H45	0.62	1.71	8	1
4:A:345:PX4:H29	4:A:362:PX4:H65	0.62	1.71	12	1
4:A:354:PX4:H39	4:A:362:PX4:H33	0.62	1.70	8	1
4:A:378:PX4:H22	4:A:417:PX4:H48	0.62	1.69	8	1
4:A:405:PX4:H17	4:A:406:PX4:H54	0.62	1.70	1	2
4:A:331:PX4:H28	4:A:347:PX4:H49	0.62	1.71	4	1
4:A:307:PX4:H28	4:A:349:PX4:H23	0.62	1.71	14	1
4:A:426:PX4:H64	4:A:426:PX4:H38	0.61	1.72	1	1
4:A:317:PX4:H16	4:A:342:PX4:H52	0.61	1.70	5	1
4:A:329:PX4:H18	4:A:336:PX4:H53	0.61	1.69	8	1
4:A:314:PX4:H57	4:A:364:PX4:H53	0.61	1.71	9	1
4:A:417:PX4:O6	4:A:417:PX4:H4	0.61	1.95	5	1
4:A:306:PX4:H15	4:A:321:PX4:H42	0.61	1.70	10	1
4:A:369:PX4:H38	4:A:378:PX4:H68	0.61	1.72	14	1
4:A:380:PX4:H18	4:A:381:PX4:H15	0.61	1.71	4	3
4:A:376:PX4:H46	4:A:385:PX4:H17	0.61	1.71	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:316:PX4:H34	4:A:320:PX4:H37	0.61	1.71	3	1
4:A:391:PX4:H62	4:A:408:PX4:H52	0.61	1.72	4	1
4:A:320:PX4:H54	4:A:359:PX4:H26	0.61	1.70	6	1
4:A:307:PX4:H52	4:A:321:PX4:H59	0.61	1.72	13	1
4:A:403:PX4:H53	4:A:403:PX4:H32	0.61	1.73	12	1
4:A:376:PX4:H40	4:A:399:PX4:H64	0.61	1.73	1	1
4:A:368:PX4:H52	4:A:369:PX4:H64	0.61	1.73	3	1
4:A:386:PX4:O6	4:A:394:PX4:H18	0.61	1.94	7	1
4:A:398:PX4:H16	4:A:407:PX4:H48	0.61	1.72	9	1
4:A:423:PX4:H48	4:A:425:PX4:H18	0.61	1.73	12	1
4:A:369:PX4:H31	4:A:377:PX4:H62	0.61	1.73	13	1
4:A:360:PX4:H2	4:A:366:PX4:H16	0.61	1.71	6	2
4:A:380:PX4:H67	4:A:387:PX4:H65	0.61	1.73	12	1
4:A:306:PX4:H66	4:A:362:PX4:H45	0.61	1.71	10	1
1:A:214:LEU:HD12	1:A:240:TYR:CE1	0.61	2.30	13	1
4:A:347:PX4:H19	4:A:348:PX4:H14	0.61	1.72	13	1
4:A:367:PX4:H49	4:A:428:PX4:H51	0.60	1.73	1	1
4:A:391:PX4:H55	4:A:408:PX4:H55	0.60	1.72	3	1
4:A:317:PX4:H17	4:A:325:PX4:H46	0.60	1.73	7	2
4:A:371:PX4:H20	4:A:372:PX4:H17	0.60	1.71	7	1
4:A:406:PX4:O1	4:A:414:PX4:H9	0.60	1.95	8	1
4:A:363:PX4:H24	4:A:364:PX4:H37	0.60	1.71	1	1
4:A:329:PX4:H24	4:A:336:PX4:H60	0.60	1.73	3	1
4:A:393:PX4:O2	4:A:394:PX4:H17	0.60	1.96	10	2
4:A:347:PX4:H30	4:A:348:PX4:H19	0.60	1.72	14	1
4:A:404:PX4:H70	4:A:430:PX4:H65	0.60	1.73	11	1
4:A:306:PX4:H23	4:A:328:PX4:H54	0.60	1.73	13	1
4:A:325:PX4:H45	4:A:407:PX4:H29	0.60	1.72	7	1
4:A:371:PX4:H14	4:A:379:PX4:H20	0.60	1.71	11	1
4:A:401:PX4:H46	4:A:426:PX4:H56	0.60	1.72	13	1
4:A:398:PX4:H30	4:A:407:PX4:H18	0.60	1.72	10	1
4:A:350:PX4:H67	4:A:358:PX4:H33	0.60	1.71	3	1
4:A:378:PX4:H20	4:A:410:PX4:H52	0.60	1.73	12	2
4:A:395:PX4:H64	4:A:406:PX4:H56	0.60	1.72	1	2
1:A:244:ASP:OD2	4:A:349:PX4:H9	0.60	1.96	7	2
4:A:348:PX4:H11	4:A:355:PX4:O2	0.60	1.95	5	2
4:A:311:PX4:H60	4:A:311:PX4:H29	0.60	1.74	9	1
4:A:321:PX4:H26	4:A:360:PX4:H61	0.60	1.72	12	1
4:A:327:PX4:H20	4:A:328:PX4:H16	0.60	1.72	7	2
4:A:381:PX4:H51	4:A:396:PX4:H46	0.60	1.73	14	1
4:A:380:PX4:H52	4:A:387:PX4:H49	0.60	1.73	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:315:PX4:H55	4:A:323:PX4:H46	0.59	1.74	1	1
4:A:400:PX4:H71	4:A:426:PX4:H43	0.59	1.73	2	1
4:A:328:PX4:H72	4:A:374:PX4:H43	0.59	1.74	5	1
4:A:424:PX4:H47	4:A:429:PX4:H21	0.59	1.74	2	1
4:A:347:PX4:H64	4:A:356:PX4:H56	0.59	1.72	3	1
4:A:422:PX4:H35	4:A:423:PX4:H32	0.59	1.74	3	1
4:A:413:PX4:O2	4:A:430:PX4:H18	0.59	1.96	3	1
4:A:347:PX4:H35	4:A:348:PX4:H24	0.59	1.73	4	1
4:A:403:PX4:H2	4:A:427:PX4:H46	0.59	1.73	14	1
4:A:316:PX4:O6	4:A:364:PX4:H12	0.59	1.98	3	1
4:A:335:PX4:H28	4:A:343:PX4:H56	0.59	1.74	6	1
4:A:331:PX4:H31	4:A:340:PX4:H56	0.59	1.73	8	1
4:A:371:PX4:H54	4:A:379:PX4:H25	0.59	1.73	11	1
4:A:306:PX4:H29	4:A:329:PX4:H51	0.59	1.73	3	1
4:A:350:PX4:H60	4:A:364:PX4:H41	0.59	1.73	3	1
4:A:416:PX4:H58	4:A:423:PX4:H60	0.59	1.74	6	1
4:A:388:PX4:O6	4:A:395:PX4:H5	0.59	1.97	8	2
4:A:351:PX4:H50	4:A:358:PX4:H55	0.59	1.74	10	1
4:A:330:PX4:H25	4:A:343:PX4:H54	0.59	1.75	14	1
4:A:342:PX4:H24	4:A:352:PX4:C24	0.59	2.24	11	1
4:A:345:PX4:H33	4:A:362:PX4:H69	0.59	1.73	12	1
4:A:400:PX4:H46	4:A:408:PX4:H64	0.59	1.74	12	1
4:A:393:PX4:H45	4:A:394:PX4:H37	0.59	1.72	5	1
4:A:369:PX4:H20	4:A:377:PX4:H51	0.59	1.75	14	1
4:A:327:PX4:H57	4:A:327:PX4:H26	0.59	1.73	1	1
4:A:421:PX4:H44	4:A:428:PX4:H58	0.59	1.74	2	1
4:A:371:PX4:H34	4:A:377:PX4:H36	0.59	1.74	5	1
4:A:375:PX4:H65	4:A:412:PX4:H38	0.59	1.74	9	1
4:A:334:PX4:H42	4:A:391:PX4:H43	0.58	1.75	2	1
4:A:416:PX4:H49	4:A:425:PX4:H57	0.58	1.75	9	1
4:A:347:PX4:H34	4:A:348:PX4:H22	0.58	1.73	14	1
4:A:383:PX4:H63	4:A:399:PX4:H67	0.58	1.74	3	1
4:A:312:PX4:H61	4:A:359:PX4:H33	0.58	1.73	6	1
4:A:377:PX4:H72	4:A:425:PX4:H68	0.58	1.74	6	1
4:A:409:PX4:H51	4:A:415:PX4:H21	0.58	1.74	8	1
4:A:350:PX4:H9	4:A:358:PX4:O6	0.58	1.99	12	2
4:A:337:PX4:H71	4:A:353:PX4:H62	0.58	1.75	10	1
4:A:354:PX4:H51	4:A:360:PX4:H18	0.58	1.74	4	1
4:A:360:PX4:H62	4:A:360:PX4:H25	0.58	1.73	4	1
4:A:377:PX4:H34	4:A:379:PX4:H27	0.58	1.76	7	1
4:A:404:PX4:O2	4:A:413:PX4:H17	0.58	1.97	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:428:PX4:H52	4:A:430:PX4:H53	0.58	1.75	7	1
4:A:308:PX4:H24	4:A:364:PX4:H22	0.58	1.74	12	1
4:A:382:PX4:H69	4:A:412:PX4:H71	0.58	1.75	13	1
4:A:375:PX4:H42	4:A:424:PX4:H69	0.58	1.76	2	1
4:A:395:PX4:H67	4:A:406:PX4:H56	0.58	1.75	2	1
4:A:378:PX4:H20	4:A:410:PX4:H48	0.58	1.75	13	1
4:A:307:PX4:H56	4:A:362:PX4:H23	0.58	1.75	14	1
4:A:412:PX4:H55	4:A:427:PX4:H22	0.58	1.75	3	1
4:A:363:PX4:H24	4:A:365:PX4:H22	0.58	1.75	13	2
4:A:350:PX4:H54	4:A:415:PX4:H43	0.58	1.76	7	1
4:A:392:PX4:H66	4:A:415:PX4:H39	0.58	1.75	8	1
4:A:374:PX4:H31	4:A:427:PX4:H20	0.58	1.74	10	1
4:A:314:PX4:H34	4:A:362:PX4:H16	0.58	1.75	3	1
4:A:354:PX4:H60	4:A:360:PX4:H63	0.58	1.76	7	1
4:A:318:PX4:H53	4:A:359:PX4:H25	0.58	1.75	2	1
4:A:316:PX4:H61	4:A:323:PX4:H70	0.58	1.76	12	1
4:A:410:PX4:H51	4:A:426:PX4:H25	0.58	1.74	3	1
4:A:351:PX4:H28	4:A:352:PX4:H26	0.58	1.76	4	1
4:A:329:PX4:H69	4:A:382:PX4:H41	0.58	1.75	8	1
4:A:382:PX4:H21	4:A:428:PX4:H29	0.58	1.76	9	1
4:A:400:PX4:H17	4:A:408:PX4:H61	0.58	1.76	12	1
4:A:395:PX4:H49	4:A:396:PX4:H20	0.58	1.74	13	1
4:A:388:PX4:H20	4:A:411:PX4:H19	0.58	1.74	1	1
4:A:348:PX4:H5	4:A:355:PX4:O3	0.58	1.99	3	1
4:A:370:PX4:H35	4:A:403:PX4:H67	0.58	1.75	3	1
4:A:326:PX4:H16	4:A:351:PX4:H16	0.58	1.76	4	3
4:A:317:PX4:H60	4:A:325:PX4:H68	0.58	1.76	9	1
4:A:323:PX4:H55	4:A:323:PX4:H34	0.58	1.74	9	1
4:A:314:PX4:H49	4:A:364:PX4:H18	0.58	1.75	10	2
4:A:372:PX4:H62	4:A:379:PX4:H61	0.57	1.75	2	1
4:A:403:PX4:H50	4:A:404:PX4:H28	0.57	1.75	8	1
4:A:409:PX4:H29	4:A:425:PX4:H71	0.57	1.76	8	1
4:A:393:PX4:H11	4:A:401:PX4:H16	0.57	1.75	11	1
4:A:332:PX4:H67	4:A:349:PX4:H57	0.57	1.76	12	1
4:A:410:PX4:H58	4:A:426:PX4:H32	0.57	1.76	4	1
4:A:352:PX4:H20	4:A:358:PX4:H15	0.57	1.75	9	1
4:A:340:PX4:H66	4:A:397:PX4:H31	0.57	1.74	11	1
4:A:402:PX4:H15	4:A:404:PX4:H14	0.57	1.75	2	1
4:A:349:PX4:H17	4:A:356:PX4:H21	0.57	1.76	7	2
4:A:337:PX4:H63	4:A:353:PX4:H56	0.57	1.77	8	1
4:A:420:PX4:H72	4:A:426:PX4:H40	0.57	1.76	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:H62	4:A:400:PX4:H32	0.57	1.76	9	1
4:A:378:PX4:H30	4:A:417:PX4:H56	0.57	1.76	10	1
4:A:367:PX4:O2	4:A:424:PX4:H1	0.57	1.99	3	1
4:A:334:PX4:H69	4:A:352:PX4:H32	0.57	1.77	6	1
4:A:400:PX4:H28	4:A:408:PX4:H52	0.57	1.75	7	1
4:A:318:PX4:H27	4:A:327:PX4:H56	0.57	1.75	12	1
4:A:319:PX4:H39	4:A:324:PX4:H37	0.57	1.77	14	1
4:A:333:PX4:H39	4:A:375:PX4:H28	0.57	1.76	1	1
4:A:393:PX4:H46	4:A:401:PX4:H19	0.57	1.75	4	1
4:A:330:PX4:H21	4:A:335:PX4:H22	0.57	1.75	12	1
4:A:352:PX4:H33	4:A:358:PX4:H64	0.57	1.74	4	1
4:A:388:PX4:H17	4:A:396:PX4:H22	0.57	1.75	8	1
4:A:334:PX4:H37	4:A:407:PX4:H43	0.57	1.75	12	1
4:A:351:PX4:H62	4:A:358:PX4:H30	0.57	1.76	13	1
4:A:331:PX4:H11	4:A:340:PX4:O1	0.57	1.99	2	1
4:A:314:PX4:H69	4:A:350:PX4:H55	0.57	1.77	5	1
4:A:326:PX4:H47	4:A:334:PX4:H56	0.57	1.77	8	1
4:A:376:PX4:H52	4:A:385:PX4:H21	0.57	1.77	8	1
4:A:342:PX4:O2	4:A:352:PX4:H4	0.57	1.99	14	1
4:A:345:PX4:H15	4:A:353:PX4:H16	0.57	1.76	2	1
4:A:344:PX4:H28	4:A:348:PX4:H21	0.57	1.76	3	1
4:A:337:PX4:H17	4:A:345:PX4:H46	0.57	1.76	4	2
4:A:320:PX4:H20	4:A:359:PX4:C29	0.57	2.26	5	1
4:A:371:PX4:H56	4:A:378:PX4:H62	0.57	1.75	5	1
4:A:312:PX4:H65	4:A:359:PX4:H37	0.57	1.76	6	1
4:A:311:PX4:H70	4:A:312:PX4:H69	0.56	1.77	3	1
4:A:424:PX4:H17	4:A:429:PX4:O6	0.56	2.00	3	1
4:A:380:PX4:H67	4:A:388:PX4:H62	0.56	1.77	10	1
4:A:367:PX4:H47	4:A:428:PX4:H48	0.56	1.76	11	1
4:A:349:PX4:H56	4:A:350:PX4:H30	0.56	1.77	12	1
4:A:362:PX4:H38	4:A:430:PX4:H69	0.56	1.76	12	1
4:A:375:PX4:H10	4:A:375:PX4:H14	0.56	1.77	14	1
1:A:207:SER:O	4:A:321:PX4:H4	0.56	2.00	2	1
4:A:317:PX4:H31	4:A:326:PX4:H62	0.56	1.76	5	1
4:A:360:PX4:H33	4:A:366:PX4:H64	0.56	1.76	5	1
4:A:391:PX4:H21	4:A:392:PX4:H47	0.56	1.78	5	1
4:A:393:PX4:H20	4:A:401:PX4:H16	0.56	1.77	5	2
4:A:400:PX4:H59	4:A:426:PX4:H40	0.56	1.76	6	1
4:A:336:PX4:H70	4:A:382:PX4:H42	0.56	1.76	8	1
4:A:371:PX4:H68	4:A:379:PX4:H41	0.56	1.76	9	1
4:A:329:PX4:H26	4:A:336:PX4:H60	0.56	1.75	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H31	4:A:381:PX4:H30	0.56	1.77	11	1
4:A:309:PX4:H63	4:A:316:PX4:H65	0.56	1.77	14	1
4:A:318:PX4:H27	4:A:359:PX4:H23	0.56	1.76	2	1
4:A:388:PX4:H23	4:A:402:PX4:H16	0.56	1.75	3	1
4:A:320:PX4:C10	4:A:359:PX4:H57	0.56	2.25	5	1
4:A:315:PX4:H29	4:A:361:PX4:H24	0.56	1.77	4	1
4:A:429:PX4:H33	4:A:429:PX4:H53	0.56	1.77	9	1
4:A:318:PX4:H64	4:A:318:PX4:H43	0.56	1.78	11	1
4:A:379:PX4:H58	4:A:420:PX4:H31	0.56	1.78	11	1
4:A:310:PX4:H20	4:A:365:PX4:H21	0.56	1.76	14	1
4:A:313:PX4:H58	4:A:327:PX4:H23	0.56	1.78	2	1
4:A:320:PX4:H19	4:A:359:PX4:H59	0.56	1.77	14	1
4:A:352:PX4:O8	4:A:365:PX4:H11	0.56	2.00	1	1
4:A:316:PX4:H48	4:A:320:PX4:H26	0.56	1.77	3	1
4:A:332:PX4:H56	4:A:349:PX4:H48	0.56	1.76	3	1
4:A:402:PX4:H3	4:A:404:PX4:O1	0.56	2.01	3	1
4:A:307:PX4:H65	4:A:349:PX4:H28	0.56	1.76	11	1
4:A:369:PX4:H56	4:A:416:PX4:H69	0.56	1.78	9	1
4:A:400:PX4:H53	4:A:410:PX4:H50	0.56	1.78	12	1
4:A:408:PX4:H43	4:A:414:PX4:H64	0.56	1.76	12	1
4:A:338:PX4:H71	4:A:395:PX4:H40	0.56	1.78	13	1
4:A:389:PX4:H30	4:A:397:PX4:H54	0.55	1.79	4	1
4:A:358:PX4:H19	4:A:363:PX4:H49	0.55	1.77	3	1
1:A:177:LYS:O	4:A:354:PX4:H13	0.55	2.01	7	1
4:A:337:PX4:H62	4:A:366:PX4:H53	0.55	1.77	8	1
4:A:377:PX4:H16	4:A:418:PX4:H7	0.55	1.78	8	1
4:A:309:PX4:H55	4:A:324:PX4:H53	0.55	1.77	12	1
4:A:381:PX4:H29	4:A:386:PX4:H58	0.55	1.77	12	1
4:A:330:PX4:H19	4:A:338:PX4:H19	0.55	1.77	1	1
4:A:380:PX4:H66	4:A:411:PX4:H22	0.55	1.77	2	1
4:A:375:PX4:H58	4:A:382:PX4:H71	0.55	1.78	6	1
4:A:395:PX4:H36	4:A:397:PX4:H61	0.55	1.76	6	1
4:A:347:PX4:H69	4:A:407:PX4:H68	0.55	1.77	11	1
4:A:349:PX4:H54	4:A:355:PX4:H34	0.55	1.76	11	1
4:A:412:PX4:H20	4:A:428:PX4:H46	0.55	1.77	11	1
4:A:337:PX4:H55	4:A:353:PX4:H47	0.55	1.77	10	1
4:A:326:PX4:H18	4:A:334:PX4:H72	0.55	1.79	11	1
4:A:360:PX4:H47	4:A:366:PX4:H46	0.55	1.77	11	1
4:A:341:PX4:H34	4:A:399:PX4:H69	0.55	1.78	14	1
4:A:399:PX4:H25	4:A:399:PX4:H59	0.55	1.77	2	1
4:A:392:PX4:H35	4:A:399:PX4:H56	0.55	1.77	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:313:PX4:H64	4:A:328:PX4:H68	0.55	1.77	1	1
4:A:412:PX4:H19	4:A:428:PX4:H54	0.55	1.79	5	1
4:A:354:PX4:H56	4:A:360:PX4:H59	0.55	1.77	7	1
4:A:338:PX4:H34	4:A:357:PX4:H27	0.55	1.78	9	1
4:A:357:PX4:H29	4:A:365:PX4:H62	0.55	1.78	14	1
4:A:416:PX4:H25	4:A:422:PX4:H56	0.55	1.77	6	1
4:A:367:PX4:H2	4:A:428:PX4:O8	0.55	2.02	14	1
4:A:375:PX4:H68	4:A:428:PX4:H54	0.55	1.78	14	1
4:A:329:PX4:H46	4:A:336:PX4:H18	0.55	1.78	2	1
4:A:346:PX4:H70	4:A:357:PX4:H31	0.55	1.77	6	1
4:A:369:PX4:H38	4:A:416:PX4:H63	0.55	1.78	11	1
4:A:306:PX4:H49	4:A:321:PX4:H22	0.55	1.77	1	1
4:A:373:PX4:H20	4:A:381:PX4:H18	0.55	1.78	1	1
4:A:316:PX4:H36	4:A:364:PX4:H55	0.55	1.78	3	1
4:A:360:PX4:H45	4:A:404:PX4:H41	0.55	1.78	9	1
4:A:385:PX4:H45	4:A:386:PX4:H45	0.55	1.78	10	1
4:A:314:PX4:H46	4:A:364:PX4:H18	0.55	1.79	11	1
4:A:317:PX4:H51	4:A:324:PX4:H17	0.55	1.79	11	1
4:A:395:PX4:H19	4:A:396:PX4:H14	0.55	1.79	12	1
4:A:348:PX4:H69	4:A:355:PX4:H27	0.55	1.79	14	1
4:A:416:PX4:H30	4:A:423:PX4:H30	0.55	1.79	2	1
4:A:392:PX4:H60	4:A:408:PX4:H31	0.55	1.78	7	1
4:A:392:PX4:O6	4:A:392:PX4:H2	0.55	2.02	9	1
4:A:307:PX4:H31	4:A:364:PX4:H57	0.54	1.79	1	1
4:A:332:PX4:H17	4:A:356:PX4:H7	0.54	1.78	2	1
4:A:408:PX4:H72	4:A:426:PX4:H69	0.54	1.79	2	1
4:A:382:PX4:H45	4:A:428:PX4:H43	0.54	1.78	8	1
4:A:339:PX4:H32	4:A:339:PX4:H50	0.54	1.78	9	1
4:A:389:PX4:H63	4:A:397:PX4:H35	0.54	1.78	14	1
4:A:355:PX4:H52	4:A:356:PX4:H14	0.54	1.77	1	1
4:A:318:PX4:O2	4:A:359:PX4:H14	0.54	2.03	5	1
4:A:321:PX4:H71	4:A:322:PX4:H33	0.54	1.79	8	1
4:A:383:PX4:H57	4:A:407:PX4:H24	0.54	1.80	9	1
4:A:380:PX4:H32	4:A:381:PX4:H59	0.54	1.77	3	1
4:A:416:PX4:H20	4:A:422:PX4:H48	0.54	1.80	4	1
4:A:330:PX4:H25	4:A:343:PX4:H51	0.54	1.77	6	1
4:A:323:PX4:H55	4:A:424:PX4:H70	0.54	1.77	6	1
4:A:307:PX4:H43	4:A:311:PX4:H43	0.54	1.78	12	1
4:A:372:PX4:H51	4:A:420:PX4:H19	0.54	1.78	3	1
4:A:308:PX4:H54	4:A:364:PX4:H31	0.54	1.79	4	1
4:A:403:PX4:H61	4:A:427:PX4:H62	0.54	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:383:PX4:H54	4:A:407:PX4:H20	0.54	1.78	9	1
4:A:404:PX4:H21	4:A:419:PX4:H10	0.54	1.79	9	1
4:A:317:PX4:H21	4:A:342:PX4:H68	0.54	1.78	10	1
4:A:325:PX4:H53	4:A:334:PX4:H36	0.54	1.78	12	1
4:A:332:PX4:O8	4:A:347:PX4:H52	0.54	2.03	13	1
4:A:428:PX4:H70	4:A:430:PX4:H32	0.54	1.79	1	1
4:A:331:PX4:H56	4:A:339:PX4:H22	0.54	1.80	2	1
4:A:351:PX4:H67	4:A:358:PX4:H36	0.54	1.79	2	1
4:A:354:PX4:H28	4:A:362:PX4:H17	0.54	1.79	5	1
4:A:372:PX4:H58	4:A:379:PX4:H57	0.54	1.80	5	1
4:A:386:PX4:H25	4:A:394:PX4:H20	0.54	1.79	9	1
4:A:338:PX4:H59	4:A:348:PX4:H57	0.54	1.78	12	1
4:A:369:PX4:H21	4:A:377:PX4:H56	0.54	1.78	1	1
4:A:419:PX4:H63	4:A:427:PX4:H60	0.54	1.80	2	1
4:A:327:PX4:H19	4:A:329:PX4:H23	0.54	1.78	5	1
4:A:373:PX4:H25	4:A:397:PX4:H15	0.54	1.79	7	1
4:A:406:PX4:H12	4:A:406:PX4:H15	0.54	1.80	9	1
4:A:423:PX4:H13	4:A:430:PX4:H46	0.54	1.80	10	1
4:A:377:PX4:H51	4:A:418:PX4:H52	0.54	1.79	13	1
4:A:416:PX4:H48	4:A:425:PX4:H49	0.54	1.79	14	1
4:A:307:PX4:H4	4:A:322:PX4:O8	0.54	2.03	3	1
4:A:384:PX4:O2	4:A:385:PX4:H18	0.54	2.03	8	2
4:A:372:PX4:H52	4:A:420:PX4:H21	0.54	1.80	4	1
4:A:370:PX4:H23	4:A:427:PX4:H59	0.54	1.80	9	1
4:A:308:PX4:H43	4:A:425:PX4:H68	0.54	1.79	13	1
1:A:208:GLY:HA3	4:A:307:PX4:H15	0.53	1.80	2	3
4:A:391:PX4:H23	4:A:414:PX4:H51	0.53	1.80	1	1
4:A:409:PX4:H16	4:A:410:PX4:H8	0.53	1.80	4	1
4:A:412:PX4:H48	4:A:419:PX4:H22	0.53	1.80	4	2
4:A:381:PX4:H57	4:A:397:PX4:H46	0.53	1.80	6	1
4:A:412:PX4:H54	4:A:427:PX4:H22	0.53	1.79	6	1
4:A:367:PX4:H22	4:A:424:PX4:H16	0.53	1.79	7	1
4:A:340:PX4:H63	4:A:397:PX4:H30	0.53	1.81	10	1
4:A:381:PX4:H62	4:A:381:PX4:H35	0.53	1.79	11	1
4:A:337:PX4:H64	4:A:345:PX4:H63	0.53	1.78	1	1
4:A:378:PX4:H49	4:A:410:PX4:H23	0.53	1.80	6	1
4:A:307:PX4:H29	4:A:361:PX4:H28	0.53	1.80	8	1
4:A:317:PX4:H26	4:A:334:PX4:H40	0.53	1.80	9	1
4:A:400:PX4:H51	4:A:409:PX4:H21	0.53	1.80	9	1
4:A:393:PX4:H66	4:A:399:PX4:H69	0.53	1.79	12	1
4:A:332:PX4:H44	4:A:389:PX4:H57	0.53	1.79	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:371:PX4:H21	4:A:379:PX4:H20	0.53	1.80	13	1
4:A:328:PX4:H55	4:A:329:PX4:H47	0.53	1.79	1	1
4:A:421:PX4:H4	4:A:422:PX4:O6	0.53	2.03	1	1
4:A:311:PX4:O2	4:A:359:PX4:H13	0.53	2.03	5	1
4:A:406:PX4:H27	4:A:415:PX4:H59	0.53	1.80	7	1
4:A:430:PX4:H71	4:A:430:PX4:H28	0.53	1.79	11	1
4:A:329:PX4:H66	4:A:375:PX4:H35	0.53	1.79	1	1
4:A:352:PX4:H48	4:A:358:PX4:H50	0.53	1.79	3	1
4:A:367:PX4:H59	4:A:424:PX4:H21	0.53	1.81	4	1
4:A:311:PX4:H43	4:A:425:PX4:H68	0.53	1.78	5	1
4:A:311:PX4:H17	4:A:359:PX4:H51	0.53	1.79	6	2
4:A:389:PX4:H48	4:A:390:PX4:H49	0.53	1.79	5	2
4:A:363:PX4:H70	4:A:392:PX4:H66	0.53	1.81	7	1
4:A:388:PX4:H58	4:A:397:PX4:H54	0.53	1.78	9	1
4:A:345:PX4:H37	4:A:403:PX4:H45	0.53	1.80	14	1
4:A:384:PX4:H19	4:A:385:PX4:H23	0.53	1.79	1	1
4:A:386:PX4:H35	4:A:394:PX4:H36	0.53	1.81	3	1
4:A:429:PX4:H15	4:A:429:PX4:H10	0.53	1.80	3	1
4:A:395:PX4:H44	4:A:398:PX4:H69	0.53	1.81	4	1
4:A:345:PX4:H44	4:A:402:PX4:H67	0.53	1.81	6	1
4:A:388:PX4:H18	4:A:411:PX4:O2	0.53	2.04	6	1
4:A:350:PX4:H68	4:A:351:PX4:H58	0.53	1.81	2	1
4:A:308:PX4:H16	4:A:311:PX4:H20	0.53	1.78	5	1
4:A:338:PX4:H32	4:A:348:PX4:H33	0.53	1.81	6	1
4:A:395:PX4:H58	4:A:404:PX4:H48	0.53	1.79	6	1
4:A:398:PX4:H38	4:A:414:PX4:H47	0.53	1.80	6	1
4:A:391:PX4:H49	4:A:408:PX4:H16	0.53	1.80	7	1
4:A:317:PX4:H20	4:A:351:PX4:O6	0.53	2.04	11	1
4:A:351:PX4:H66	4:A:358:PX4:H32	0.53	1.79	3	1
4:A:311:PX4:H48	4:A:320:PX4:H21	0.53	1.79	4	1
4:A:325:PX4:H15	4:A:341:PX4:H17	0.53	1.79	5	1
4:A:358:PX4:H29	4:A:363:PX4:H26	0.53	1.79	10	1
4:A:345:PX4:H42	4:A:388:PX4:H40	0.53	1.79	12	1
4:A:370:PX4:H69	4:A:411:PX4:H65	0.53	1.80	2	1
4:A:307:PX4:H37	4:A:423:PX4:H39	0.53	1.78	4	1
4:A:416:PX4:H51	4:A:418:PX4:H26	0.53	1.79	4	1
4:A:329:PX4:H30	4:A:336:PX4:H68	0.53	1.79	8	1
4:A:310:PX4:H65	4:A:312:PX4:H52	0.53	1.80	9	1
4:A:361:PX4:H34	4:A:423:PX4:H35	0.53	1.80	12	1
4:A:400:PX4:H28	4:A:426:PX4:H59	0.53	1.81	12	1
4:A:410:PX4:H16	4:A:418:PX4:H28	0.53	1.80	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:376:PX4:H26	4:A:399:PX4:H48	0.53	1.81	4	1
4:A:309:PX4:H51	4:A:316:PX4:H48	0.53	1.80	5	1
4:A:335:PX4:H31	4:A:343:PX4:H55	0.53	1.79	11	1
4:A:405:PX4:H22	4:A:406:PX4:H61	0.53	1.79	13	1
4:A:392:PX4:H68	4:A:400:PX4:H45	0.53	1.80	1	1
4:A:311:PX4:H60	4:A:311:PX4:H24	0.53	1.81	6	1
4:A:337:PX4:H40	4:A:338:PX4:H47	0.53	1.79	10	1
4:A:347:PX4:H20	4:A:348:PX4:H14	0.52	1.81	6	1
4:A:367:PX4:H64	4:A:375:PX4:H57	0.52	1.80	7	1
4:A:413:PX4:H61	4:A:430:PX4:H42	0.52	1.81	9	1
4:A:349:PX4:H58	4:A:356:PX4:H42	0.52	1.80	10	1
4:A:398:PX4:H39	4:A:414:PX4:H31	0.52	1.81	10	1
4:A:412:PX4:H12	4:A:419:PX4:O1	0.52	2.04	12	1
4:A:314:PX4:H53	4:A:364:PX4:H18	0.52	1.81	1	1
4:A:337:PX4:H56	4:A:345:PX4:H59	0.52	1.81	5	1
4:A:389:PX4:H32	4:A:397:PX4:H22	0.52	1.82	6	1
4:A:306:PX4:H47	4:A:322:PX4:H50	0.52	1.81	7	1
4:A:398:PX4:H21	4:A:407:PX4:H49	0.52	1.80	10	1
4:A:346:PX4:H19	4:A:354:PX4:H28	0.52	1.80	1	1
4:A:361:PX4:H26	4:A:364:PX4:H54	0.52	1.81	3	1
4:A:315:PX4:H10	4:A:315:PX4:O6	0.52	2.04	4	1
4:A:326:PX4:H48	4:A:334:PX4:H35	0.52	1.79	5	1
4:A:407:PX4:H30	4:A:414:PX4:H61	0.52	1.81	11	1
4:A:311:PX4:H44	4:A:314:PX4:H65	0.52	1.82	13	1
4:A:388:PX4:H49	4:A:396:PX4:H21	0.52	1.81	12	1
4:A:313:PX4:H56	4:A:327:PX4:H27	0.52	1.82	13	1
4:A:415:PX4:H56	4:A:422:PX4:H53	0.52	1.81	13	1
4:A:410:PX4:H67	4:A:417:PX4:H37	0.52	1.81	14	1
4:A:310:PX4:H34	4:A:365:PX4:H34	0.52	1.81	3	1
4:A:329:PX4:H56	4:A:336:PX4:H35	0.52	1.82	6	2
4:A:314:PX4:H33	4:A:362:PX4:O8	0.52	2.04	9	1
4:A:325:PX4:H55	4:A:334:PX4:H40	0.52	1.81	11	1
4:A:400:PX4:H46	4:A:409:PX4:H23	0.52	1.81	1	1
4:A:340:PX4:H22	4:A:341:PX4:H63	0.52	1.81	2	1
4:A:405:PX4:H51	4:A:406:PX4:H51	0.52	1.81	3	1
4:A:308:PX4:H21	4:A:311:PX4:H55	0.52	1.82	7	1
4:A:329:PX4:H60	4:A:336:PX4:H40	0.52	1.82	8	1
4:A:313:PX4:H28	4:A:366:PX4:H21	0.52	1.81	9	1
4:A:404:PX4:H21	4:A:413:PX4:H30	0.52	1.81	10	1
4:A:393:PX4:H71	4:A:414:PX4:H53	0.52	1.81	11	1
4:A:340:PX4:H59	4:A:340:PX4:H36	0.52	1.79	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:307:PX4:H45	4:A:422:PX4:H39	0.52	1.80	13	1
4:A:317:PX4:H21	4:A:326:PX4:H53	0.52	1.81	13	1
4:A:390:PX4:H1	4:A:399:PX4:O6	0.52	2.05	13	1
4:A:354:PX4:H69	4:A:360:PX4:H27	0.52	1.81	2	1
4:A:405:PX4:H55	4:A:406:PX4:H51	0.52	1.82	2	1
4:A:312:PX4:H29	4:A:365:PX4:H24	0.52	1.82	3	1
4:A:348:PX4:H52	4:A:355:PX4:H67	0.52	1.81	5	1
4:A:306:PX4:H61	4:A:362:PX4:H37	0.52	1.82	9	1
4:A:342:PX4:H29	4:A:352:PX4:H60	0.52	1.82	9	1
4:A:331:PX4:H38	4:A:340:PX4:H40	0.52	1.82	10	1
4:A:380:PX4:H6	4:A:381:PX4:O1	0.52	2.04	11	1
4:A:383:PX4:H71	4:A:399:PX4:H67	0.52	1.80	5	1
4:A:419:PX4:H67	4:A:427:PX4:H69	0.52	1.81	5	1
4:A:370:PX4:H19	4:A:427:PX4:H55	0.52	1.82	9	1
4:A:410:PX4:H16	4:A:418:PX4:H31	0.52	1.81	10	1
4:A:310:PX4:H60	4:A:312:PX4:H53	0.52	1.82	4	2
4:A:371:PX4:H56	4:A:372:PX4:H23	0.52	1.82	4	1
4:A:341:PX4:H39	4:A:399:PX4:H72	0.52	1.81	5	1
4:A:306:PX4:H43	4:A:328:PX4:H67	0.52	1.82	8	1
4:A:327:PX4:H14	4:A:328:PX4:O2	0.52	2.05	7	1
4:A:308:PX4:H27	4:A:316:PX4:H27	0.52	1.81	8	1
4:A:361:PX4:H39	4:A:364:PX4:H65	0.52	1.81	9	1
4:A:314:PX4:H26	4:A:356:PX4:H25	0.52	1.82	12	1
4:A:313:PX4:H61	4:A:329:PX4:H25	0.52	1.81	13	1
4:A:354:PX4:H65	4:A:360:PX4:H20	0.51	1.81	1	1
4:A:409:PX4:H67	4:A:415:PX4:H33	0.51	1.81	3	1
4:A:377:PX4:H71	4:A:425:PX4:H19	0.51	1.81	8	1
4:A:324:PX4:H66	4:A:341:PX4:H32	0.51	1.82	9	1
4:A:393:PX4:H23	4:A:401:PX4:H16	0.51	1.81	4	1
4:A:421:PX4:H71	4:A:422:PX4:H32	0.51	1.81	4	1
4:A:321:PX4:H28	4:A:412:PX4:H41	0.51	1.80	5	1
4:A:387:PX4:H47	4:A:411:PX4:H54	0.51	1.80	5	1
4:A:360:PX4:H31	4:A:419:PX4:H42	0.51	1.80	7	1
4:A:338:PX4:H67	4:A:348:PX4:H58	0.51	1.82	10	1
4:A:416:PX4:H45	4:A:422:PX4:H67	0.51	1.81	12	1
4:A:368:PX4:H10	4:A:369:PX4:O2	0.51	2.05	1	1
4:A:360:PX4:H43	4:A:403:PX4:H65	0.51	1.82	3	1
4:A:323:PX4:H38	4:A:361:PX4:H54	0.51	1.82	6	1
4:A:350:PX4:H51	4:A:363:PX4:H62	0.51	1.82	8	1
4:A:380:PX4:H60	4:A:380:PX4:H32	0.51	1.80	12	1
4:A:398:PX4:H44	4:A:415:PX4:H27	0.51	1.82	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H27	4:A:311:PX4:H31	0.51	1.81	4	1
4:A:347:PX4:H56	4:A:356:PX4:H58	0.51	1.83	4	1
4:A:400:PX4:H59	4:A:410:PX4:H62	0.51	1.82	5	1
4:A:417:PX4:H31	4:A:426:PX4:H66	0.51	1.83	7	1
4:A:404:PX4:H15	4:A:413:PX4:H20	0.51	1.81	1	1
4:A:378:PX4:H29	4:A:420:PX4:H57	0.51	1.82	4	1
4:A:322:PX4:H49	4:A:336:PX4:H25	0.51	1.83	9	1
4:A:393:PX4:H18	4:A:401:PX4:H20	0.51	1.83	12	1
4:A:402:PX4:H21	4:A:404:PX4:H67	0.51	1.83	14	1
4:A:345:PX4:H15	4:A:353:PX4:H14	0.51	1.81	4	2
4:A:358:PX4:H23	4:A:363:PX4:H55	0.51	1.83	12	1
4:A:363:PX4:H71	4:A:392:PX4:H66	0.51	1.82	3	1
4:A:349:PX4:H26	4:A:356:PX4:H38	0.51	1.83	11	1
4:A:392:PX4:H57	4:A:401:PX4:H29	0.51	1.81	13	1
4:A:312:PX4:H31	4:A:365:PX4:H46	0.51	1.82	14	1
4:A:314:PX4:H47	4:A:350:PX4:H43	0.51	1.82	14	1
4:A:346:PX4:H68	4:A:362:PX4:H72	0.51	1.82	14	1
4:A:372:PX4:H34	4:A:420:PX4:H29	0.51	1.82	14	1
4:A:346:PX4:H19	4:A:354:PX4:H31	0.51	1.82	3	1
4:A:311:PX4:O1	4:A:359:PX4:H3	0.51	2.06	5	2
4:A:355:PX4:H36	4:A:356:PX4:H41	0.51	1.81	4	1
4:A:372:PX4:H23	4:A:417:PX4:H46	0.51	1.83	8	1
4:A:306:PX4:H22	4:A:321:PX4:H35	0.51	1.82	9	1
4:A:306:PX4:H60	4:A:362:PX4:H38	0.51	1.83	10	1
4:A:321:PX4:H56	4:A:361:PX4:H54	0.51	1.82	10	1
4:A:318:PX4:H53	4:A:328:PX4:H22	0.51	1.81	11	1
4:A:333:PX4:H14	4:A:340:PX4:H1	0.51	1.82	11	1
4:A:316:PX4:H20	4:A:364:PX4:H14	0.51	1.81	12	1
4:A:343:PX4:H33	4:A:344:PX4:H30	0.51	1.83	12	1
4:A:378:PX4:H59	4:A:410:PX4:H26	0.51	1.82	12	1
4:A:309:PX4:H3	4:A:320:PX4:O1	0.51	2.05	13	1
4:A:409:PX4:O6	4:A:410:PX4:H5	0.51	2.06	13	1
4:A:410:PX4:H42	4:A:418:PX4:H42	0.51	1.82	14	1
4:A:354:PX4:H49	4:A:360:PX4:H49	0.51	1.83	4	1
4:A:410:PX4:H16	4:A:418:PX4:H29	0.51	1.81	6	1
4:A:333:PX4:H54	4:A:341:PX4:H54	0.51	1.83	11	1
4:A:319:PX4:H51	4:A:324:PX4:H16	0.51	1.83	1	1
4:A:395:PX4:H24	4:A:396:PX4:H64	0.51	1.83	4	1
4:A:320:PX4:H51	4:A:359:PX4:H25	0.51	1.81	8	1
4:A:388:PX4:H51	4:A:396:PX4:H48	0.51	1.81	10	1
4:A:390:PX4:H57	4:A:429:PX4:H60	0.51	1.82	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H20	4:A:426:PX4:H50	0.51	1.82	12	1
4:A:327:PX4:H16	4:A:328:PX4:O6	0.50	2.05	5	1
4:A:313:PX4:H20	4:A:360:PX4:H15	0.50	1.82	7	1
4:A:344:PX4:H25	4:A:344:PX4:H60	0.50	1.83	14	1
4:A:363:PX4:H47	4:A:364:PX4:H37	0.50	1.81	14	1
1:A:206:HIS:ND1	4:A:314:PX4:H1	0.50	2.21	13	3
4:A:307:PX4:H42	4:A:350:PX4:H45	0.50	1.82	2	1
4:A:402:PX4:H21	4:A:403:PX4:H21	0.50	1.82	3	1
4:A:388:PX4:H29	4:A:411:PX4:H24	0.50	1.83	5	1
4:A:310:PX4:H48	4:A:365:PX4:H20	0.50	1.81	7	1
4:A:413:PX4:H63	4:A:430:PX4:H36	0.50	1.82	7	1
4:A:337:PX4:H39	4:A:338:PX4:H51	0.50	1.83	9	1
4:A:345:PX4:H70	4:A:370:PX4:H39	0.50	1.83	10	1
4:A:369:PX4:H19	4:A:418:PX4:H15	0.50	1.83	10	1
4:A:308:PX4:H18	4:A:311:PX4:O8	0.50	2.06	14	2
4:A:403:PX4:H3	4:A:427:PX4:H48	0.50	1.83	11	1
4:A:412:PX4:H47	4:A:419:PX4:H14	0.50	1.84	12	1
4:A:346:PX4:H12	4:A:360:PX4:H46	0.50	1.82	13	1
4:A:370:PX4:H17	4:A:403:PX4:O1	0.50	2.06	4	1
4:A:352:PX4:H61	4:A:358:PX4:H57	0.50	1.82	9	1
4:A:311:PX4:O4	4:A:359:PX4:H6	0.50	2.05	13	1
4:A:363:PX4:H25	4:A:365:PX4:H26	0.50	1.83	13	1
4:A:378:PX4:H35	4:A:410:PX4:H60	0.50	1.83	13	1
4:A:416:PX4:H53	4:A:418:PX4:H30	0.50	1.84	13	1
4:A:368:PX4:H32	4:A:425:PX4:H42	0.50	1.81	3	1
4:A:347:PX4:H35	4:A:348:PX4:H28	0.50	1.83	13	1
4:A:394:PX4:O8	4:A:394:PX4:H9	0.50	2.07	14	1
4:A:407:PX4:H9	4:A:414:PX4:H48	0.50	1.83	14	1
4:A:421:PX4:H13	4:A:423:PX4:O6	0.50	2.07	1	1
4:A:383:PX4:H46	4:A:399:PX4:H50	0.50	1.83	3	1
4:A:316:PX4:H65	4:A:320:PX4:H40	0.50	1.83	5	1
4:A:378:PX4:H50	4:A:418:PX4:H51	0.50	1.81	9	1
4:A:388:PX4:H24	4:A:402:PX4:O8	0.50	2.05	11	1
4:A:374:PX4:H22	4:A:428:PX4:H20	0.50	1.82	14	1
4:A:307:PX4:H34	4:A:307:PX4:H67	0.50	1.84	2	1
4:A:384:PX4:H56	4:A:385:PX4:H32	0.50	1.82	3	1
4:A:409:PX4:H54	4:A:422:PX4:H62	0.50	1.82	3	1
4:A:408:PX4:H18	4:A:408:PX4:H2	0.50	1.84	6	1
4:A:422:PX4:H38	4:A:423:PX4:H40	0.50	1.83	6	1
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.50	2.42	9	1
4:A:392:PX4:H27	4:A:393:PX4:H61	0.50	1.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:402:PX4:H4	4:A:404:PX4:O2	0.50	2.06	11	2
4:A:395:PX4:H42	4:A:405:PX4:H36	0.50	1.81	13	1
4:A:400:PX4:H30	4:A:401:PX4:H57	0.50	1.83	1	1
4:A:408:PX4:H17	4:A:415:PX4:O6	0.50	2.07	1	1
4:A:369:PX4:H18	4:A:425:PX4:H9	0.50	1.82	4	1
4:A:416:PX4:H24	4:A:422:PX4:H17	0.50	1.83	10	1
4:A:345:PX4:H46	4:A:346:PX4:H56	0.50	1.84	12	1
4:A:371:PX4:H35	4:A:371:PX4:H68	0.50	1.83	12	1
4:A:322:PX4:O2	4:A:333:PX4:H9	0.50	2.07	13	1
4:A:321:PX4:H24	4:A:354:PX4:H53	0.50	1.81	2	2
4:A:306:PX4:H19	4:A:321:PX4:H42	0.50	1.84	6	1
4:A:380:PX4:H49	4:A:381:PX4:H13	0.50	1.83	12	1
4:A:338:PX4:H17	4:A:348:PX4:H17	0.49	1.84	1	1
4:A:356:PX4:H32	4:A:362:PX4:H27	0.49	1.82	1	1
4:A:395:PX4:H58	4:A:404:PX4:H50	0.49	1.83	1	1
4:A:308:PX4:H40	4:A:316:PX4:H41	0.49	1.84	4	1
4:A:428:PX4:H63	4:A:430:PX4:H32	0.49	1.84	8	1
4:A:400:PX4:H68	4:A:410:PX4:H67	0.49	1.84	10	1
4:A:409:PX4:H51	4:A:415:PX4:C11	0.49	2.36	8	1
4:A:306:PX4:H22	4:A:322:PX4:H57	0.49	1.84	1	1
4:A:347:PX4:H22	4:A:348:PX4:H56	0.49	1.83	5	1
4:A:393:PX4:H3	4:A:401:PX4:O2	0.49	2.08	5	1
4:A:374:PX4:H18	4:A:382:PX4:O7	0.49	2.06	8	1
4:A:390:PX4:H62	4:A:397:PX4:H42	0.49	1.84	9	1
4:A:312:PX4:H29	4:A:365:PX4:H22	0.49	1.84	12	1
4:A:421:PX4:H67	4:A:423:PX4:H45	0.49	1.83	3	1
4:A:393:PX4:H37	4:A:401:PX4:H70	0.49	1.84	7	1
4:A:308:PX4:O6	4:A:364:PX4:H3	0.49	2.07	12	1
4:A:372:PX4:H20	4:A:420:PX4:H16	0.49	1.84	13	2
4:A:317:PX4:H14	4:A:351:PX4:H20	0.49	1.85	5	1
4:A:337:PX4:H9	4:A:357:PX4:H2	0.49	1.84	11	1
4:A:316:PX4:H51	4:A:320:PX4:C14	0.49	2.37	12	1
4:A:312:PX4:H35	4:A:365:PX4:H46	0.49	1.83	13	1
4:A:377:PX4:H42	4:A:379:PX4:H56	0.49	1.84	13	1
4:A:313:PX4:H65	4:A:360:PX4:H70	0.49	1.85	1	1
4:A:316:PX4:H29	4:A:361:PX4:H25	0.49	1.85	2	1
4:A:347:PX4:H21	4:A:348:PX4:H55	0.49	1.83	3	1
4:A:369:PX4:H20	4:A:377:PX4:H46	0.49	1.85	4	1
4:A:326:PX4:O6	4:A:363:PX4:H61	0.49	2.07	8	1
4:A:326:PX4:H19	4:A:334:PX4:H55	0.49	1.83	4	1
4:A:335:PX4:O6	4:A:343:PX4:H14	0.49	2.08	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:419:PX4:H42	4:A:427:PX4:H41	0.49	1.83	5	1
4:A:390:PX4:O1	4:A:399:PX4:H12	0.49	2.08	6	1
4:A:348:PX4:H35	4:A:380:PX4:H42	0.49	1.83	7	1
4:A:306:PX4:H59	4:A:361:PX4:H57	0.49	1.84	8	1
4:A:340:PX4:H42	4:A:389:PX4:H27	0.49	1.84	9	1
4:A:345:PX4:O1	4:A:346:PX4:H9	0.49	2.08	9	1
4:A:332:PX4:H53	4:A:356:PX4:H47	0.49	1.84	5	1
4:A:392:PX4:H70	4:A:415:PX4:H33	0.49	1.84	7	1
4:A:344:PX4:H56	4:A:347:PX4:H33	0.49	1.84	10	1
4:A:408:PX4:H4	4:A:414:PX4:O2	0.49	2.07	10	2
4:A:406:PX4:H23	4:A:415:PX4:H22	0.49	1.85	13	1
4:A:312:PX4:H25	4:A:365:PX4:H20	0.49	1.84	3	1
4:A:332:PX4:H52	4:A:347:PX4:H65	0.49	1.85	3	1
4:A:313:PX4:H51	4:A:354:PX4:H66	0.49	1.85	5	1
4:A:337:PX4:H42	4:A:347:PX4:H30	0.49	1.84	7	1
4:A:395:PX4:H19	4:A:396:PX4:H15	0.49	1.85	8	1
4:A:337:PX4:H31	4:A:338:PX4:H28	0.49	1.84	10	1
4:A:337:PX4:H48	4:A:345:PX4:H51	0.49	1.82	12	1
4:A:393:PX4:H32	4:A:401:PX4:H53	0.49	1.83	12	1
4:A:313:PX4:H15	4:A:360:PX4:C9	0.49	2.38	14	1
4:A:405:PX4:H64	4:A:406:PX4:H67	0.49	1.85	3	1
4:A:415:PX4:H56	4:A:421:PX4:H68	0.49	1.83	3	1
4:A:385:PX4:H49	4:A:393:PX4:H52	0.49	1.84	5	1
4:A:400:PX4:H39	4:A:401:PX4:H35	0.49	1.84	5	1
4:A:421:PX4:H26	4:A:423:PX4:H22	0.49	1.85	7	1
4:A:319:PX4:H17	4:A:324:PX4:O4	0.49	2.08	8	1
4:A:400:PX4:H57	4:A:408:PX4:H72	0.49	1.85	8	1
4:A:326:PX4:H69	4:A:393:PX4:H62	0.49	1.83	9	1
4:A:344:PX4:H52	4:A:347:PX4:H27	0.49	1.84	9	1
4:A:361:PX4:H37	4:A:423:PX4:H36	0.49	1.84	9	1
4:A:387:PX4:H47	4:A:411:PX4:C8	0.49	2.34	12	1
4:A:321:PX4:H34	4:A:322:PX4:H58	0.49	1.83	13	1
4:A:335:PX4:H1	4:A:344:PX4:O6	0.48	2.08	4	1
4:A:376:PX4:H59	4:A:385:PX4:H57	0.48	1.84	5	1
4:A:385:PX4:H23	4:A:386:PX4:H28	0.48	1.85	5	1
4:A:355:PX4:H54	4:A:356:PX4:H47	0.48	1.85	8	1
4:A:367:PX4:H18	4:A:424:PX4:O3	0.48	2.08	8	1
4:A:373:PX4:O2	4:A:382:PX4:H9	0.48	2.08	12	1
4:A:316:PX4:H64	4:A:323:PX4:H69	0.48	1.84	14	1
4:A:376:PX4:H61	4:A:392:PX4:H32	0.48	1.85	14	1
4:A:308:PX4:H19	4:A:311:PX4:H52	0.48	1.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H56	4:A:336:PX4:H31	0.48	1.85	3	1
4:A:404:PX4:H48	4:A:413:PX4:O6	0.48	2.08	4	1
4:A:406:PX4:H28	4:A:421:PX4:H63	0.48	1.86	5	1
4:A:385:PX4:H28	4:A:386:PX4:H28	0.48	1.85	7	1
4:A:369:PX4:H32	4:A:410:PX4:H21	0.48	1.83	2	1
4:A:332:PX4:H43	4:A:407:PX4:H61	0.48	1.85	3	1
4:A:372:PX4:H25	4:A:420:PX4:H50	0.48	1.84	4	1
4:A:421:PX4:H40	4:A:423:PX4:H53	0.48	1.85	7	1
4:A:311:PX4:H31	4:A:364:PX4:H27	0.48	1.86	11	1
4:A:307:PX4:H71	4:A:349:PX4:H45	0.48	1.84	1	1
4:A:376:PX4:H60	4:A:392:PX4:H25	0.48	1.84	5	1
4:A:316:PX4:H24	4:A:364:PX4:H47	0.48	1.86	8	1
4:A:320:PX4:H71	4:A:378:PX4:H40	0.48	1.85	8	1
4:A:357:PX4:H71	4:A:357:PX4:H29	0.48	1.84	10	1
4:A:345:PX4:H20	4:A:346:PX4:H15	0.48	1.85	11	1
4:A:307:PX4:H22	4:A:321:PX4:H64	0.48	1.83	13	1
4:A:378:PX4:H2	4:A:410:PX4:O6	0.48	2.09	13	1
4:A:389:PX4:H51	4:A:390:PX4:H24	0.48	1.85	13	1
4:A:400:PX4:H40	4:A:401:PX4:H45	0.48	1.85	1	1
4:A:309:PX4:H65	4:A:320:PX4:H36	0.48	1.85	2	1
4:A:326:PX4:H21	4:A:350:PX4:H17	0.48	1.85	9	1
4:A:349:PX4:H38	4:A:421:PX4:H42	0.48	1.85	10	1
4:A:400:PX4:H46	4:A:409:PX4:H20	0.48	1.85	10	1
4:A:346:PX4:H50	4:A:362:PX4:H56	0.48	1.86	11	1
4:A:354:PX4:H24	4:A:362:PX4:H17	0.48	1.84	11	1
4:A:310:PX4:O6	4:A:365:PX4:H11	0.48	2.08	12	1
4:A:400:PX4:H60	4:A:410:PX4:H54	0.48	1.85	13	1
4:A:331:PX4:O6	4:A:340:PX4:H4	0.48	2.08	1	1
4:A:330:PX4:C11	4:A:335:PX4:H19	0.48	2.36	2	1
4:A:393:PX4:H42	4:A:401:PX4:H40	0.48	1.84	2	1
4:A:353:PX4:H70	4:A:412:PX4:H37	0.48	1.86	5	1
4:A:377:PX4:H60	4:A:416:PX4:H62	0.48	1.85	5	1
4:A:388:PX4:H23	4:A:396:PX4:H30	0.48	1.84	11	1
4:A:392:PX4:H67	4:A:408:PX4:H36	0.48	1.84	12	1
4:A:369:PX4:H18	4:A:425:PX4:H1	0.48	1.86	1	1
4:A:395:PX4:H48	4:A:405:PX4:H19	0.48	1.86	12	2
4:A:358:PX4:H27	4:A:363:PX4:H26	0.48	1.86	2	1
1:A:242:TYR:CD1	4:A:314:PX4:H19	0.48	2.43	4	1
4:A:337:PX4:H30	4:A:338:PX4:H48	0.48	1.86	5	1
4:A:319:PX4:H21	4:A:324:PX4:H19	0.48	1.84	6	1
4:A:374:PX4:H29	4:A:427:PX4:H31	0.48	1.86	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:390:PX4:H62	4:A:397:PX4:C21	0.48	2.38	9	1
4:A:337:PX4:H50	4:A:353:PX4:H25	0.48	1.84	10	1
1:A:145:THR:HB	1:A:146:PRO:HD2	0.48	1.85	2	1
4:A:318:PX4:O2	4:A:359:PX4:H18	0.48	2.07	4	1
4:A:323:PX4:H26	4:A:333:PX4:H17	0.48	1.85	4	1
4:A:331:PX4:H18	4:A:340:PX4:H21	0.48	1.84	5	1
4:A:346:PX4:H51	4:A:355:PX4:H14	0.48	1.85	6	1
4:A:406:PX4:H18	4:A:415:PX4:O1	0.48	2.09	11	1
4:A:326:PX4:H49	4:A:351:PX4:H18	0.48	1.84	1	1
4:A:307:PX4:H49	4:A:321:PX4:H56	0.48	1.86	5	1
4:A:348:PX4:H55	4:A:388:PX4:H71	0.48	1.84	6	1
4:A:315:PX4:H45	4:A:425:PX4:H27	0.48	1.85	7	1
4:A:326:PX4:H20	4:A:350:PX4:H48	0.48	1.86	8	1
4:A:404:PX4:H53	4:A:413:PX4:H24	0.48	1.86	14	1
4:A:416:PX4:H10	4:A:416:PX4:O3	0.48	2.09	1	1
4:A:347:PX4:H13	4:A:348:PX4:O1	0.48	2.08	6	3
4:A:404:PX4:H59	4:A:430:PX4:H40	0.48	1.86	4	1
4:A:351:PX4:C5	4:A:352:PX4:H24	0.48	2.39	9	1
4:A:325:PX4:H62	4:A:334:PX4:H45	0.48	1.86	11	1
4:A:321:PX4:H15	4:A:354:PX4:H15	0.48	1.85	12	1
4:A:337:PX4:H22	4:A:337:PX4:H8	0.48	1.85	12	1
4:A:421:PX4:H30	4:A:423:PX4:H19	0.48	1.86	12	1
4:A:373:PX4:H60	4:A:381:PX4:H25	0.47	1.85	3	1
4:A:357:PX4:H39	4:A:402:PX4:H41	0.47	1.84	4	1
4:A:308:PX4:O1	4:A:311:PX4:H14	0.47	2.10	7	1
4:A:349:PX4:H30	4:A:356:PX4:H38	0.47	1.86	7	1
4:A:424:PX4:H69	4:A:429:PX4:H67	0.47	1.86	7	1
4:A:325:PX4:H17	4:A:341:PX4:H47	0.47	1.85	14	1
4:A:388:PX4:H17	4:A:396:PX4:O6	0.47	2.09	1	2
4:A:331:PX4:H14	4:A:347:PX4:H14	0.47	1.86	5	1
4:A:421:PX4:H30	4:A:430:PX4:H19	0.47	1.84	5	1
4:A:402:PX4:O2	4:A:402:PX4:H10	0.47	2.09	7	1
4:A:413:PX4:H50	4:A:430:PX4:H23	0.47	1.86	7	1
4:A:338:PX4:H68	4:A:396:PX4:H38	0.47	1.85	2	1
4:A:314:PX4:H61	4:A:364:PX4:H71	0.47	1.86	7	1
4:A:351:PX4:H55	4:A:358:PX4:H52	0.47	1.86	7	1
4:A:322:PX4:H25	4:A:361:PX4:H48	0.47	1.86	10	2
4:A:326:PX4:H35	4:A:350:PX4:H52	0.47	1.86	10	1
4:A:335:PX4:H24	4:A:344:PX4:H24	0.47	1.86	11	1
4:A:332:PX4:H3	4:A:356:PX4:O3	0.47	2.08	14	1
4:A:367:PX4:H28	4:A:423:PX4:H50	0.47	1.85	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:376:PX4:H68	4:A:385:PX4:H63	0.47	1.87	14	1
4:A:368:PX4:H1	4:A:369:PX4:O2	0.47	2.09	1	1
4:A:421:PX4:H5	4:A:423:PX4:O1	0.47	2.09	3	2
4:A:372:PX4:H55	4:A:379:PX4:H53	0.47	1.86	2	1
4:A:398:PX4:H40	4:A:414:PX4:H32	0.47	1.86	6	1
4:A:310:PX4:H48	4:A:312:PX4:H21	0.47	1.86	10	1
4:A:311:PX4:H69	4:A:320:PX4:H44	0.47	1.86	10	1
4:A:342:PX4:H54	4:A:351:PX4:H29	0.47	1.86	11	2
4:A:345:PX4:H19	4:A:346:PX4:H19	0.47	1.86	11	1
4:A:405:PX4:H54	4:A:414:PX4:H30	0.47	1.86	11	1
4:A:378:PX4:H52	4:A:410:PX4:H26	0.47	1.87	13	1
4:A:355:PX4:H20	4:A:362:PX4:H51	0.47	1.86	14	1
4:A:325:PX4:H17	4:A:341:PX4:H17	0.47	1.87	1	1
4:A:326:PX4:H51	4:A:334:PX4:H40	0.47	1.87	3	1
4:A:351:PX4:H56	4:A:358:PX4:H56	0.47	1.86	3	1
1:A:205:THR:O	4:A:314:PX4:H9	0.47	2.09	4	1
4:A:317:PX4:O1	4:A:351:PX4:H20	0.47	2.09	4	1
4:A:338:PX4:H70	4:A:362:PX4:H44	0.47	1.86	4	1
4:A:325:PX4:H14	4:A:325:PX4:H12	0.47	1.87	5	1
4:A:412:PX4:H5	4:A:427:PX4:O1	0.47	2.10	7	1
4:A:399:PX4:O1	4:A:407:PX4:H7	0.47	2.10	9	1
4:A:400:PX4:H47	4:A:426:PX4:H26	0.47	1.85	12	1
4:A:361:PX4:H31	4:A:367:PX4:H42	0.47	1.84	1	1
4:A:417:PX4:H64	4:A:420:PX4:H60	0.47	1.86	4	1
4:A:340:PX4:H47	4:A:341:PX4:H61	0.47	1.87	7	1
4:A:405:PX4:O2	4:A:406:PX4:H12	0.47	2.09	7	1
4:A:424:PX4:H48	4:A:425:PX4:H22	0.47	1.86	7	1
4:A:358:PX4:H20	4:A:363:PX4:H18	0.47	1.86	14	2
4:A:316:PX4:H61	4:A:323:PX4:C36	0.47	2.38	12	1
4:A:306:PX4:H29	4:A:336:PX4:H31	0.47	1.87	1	1
4:A:319:PX4:H12	4:A:342:PX4:O2	0.47	2.09	1	1
4:A:359:PX4:H44	4:A:372:PX4:H40	0.47	1.87	2	1
4:A:336:PX4:H36	4:A:361:PX4:H67	0.47	1.86	4	1
4:A:349:PX4:O6	4:A:349:PX4:H12	0.47	2.09	4	1
4:A:306:PX4:H70	4:A:349:PX4:H35	0.47	1.86	5	1
4:A:308:PX4:H54	4:A:364:PX4:H30	0.47	1.85	5	1
4:A:310:PX4:H54	4:A:312:PX4:H22	0.47	1.87	5	1
4:A:322:PX4:H40	4:A:361:PX4:H54	0.47	1.84	5	1
4:A:346:PX4:H29	4:A:354:PX4:H19	0.47	1.86	5	1
4:A:395:PX4:H59	4:A:405:PX4:H42	0.47	1.84	5	1
4:A:345:PX4:O1	4:A:346:PX4:H13	0.47	2.08	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:360:PX4:H3	4:A:366:PX4:O4	0.47	2.10	6	1
4:A:403:PX4:H52	4:A:419:PX4:H55	0.47	1.86	6	1
1:A:214:LEU:H	1:A:214:LEU:HD23	0.47	1.69	7	1
4:A:390:PX4:H60	4:A:390:PX4:H29	0.47	1.86	7	1
4:A:309:PX4:O6	4:A:320:PX4:H4	0.47	2.09	9	1
4:A:358:PX4:H38	4:A:365:PX4:H34	0.47	1.86	9	1
4:A:396:PX4:H63	4:A:398:PX4:H50	0.47	1.86	9	1
4:A:400:PX4:O2	4:A:426:PX4:H14	0.47	2.09	9	1
4:A:346:PX4:H46	4:A:355:PX4:O1	0.47	2.10	10	1
4:A:388:PX4:H52	4:A:411:PX4:H28	0.47	1.87	11	1
4:A:405:PX4:H9	4:A:405:PX4:O6	0.47	2.10	11	1
4:A:335:PX4:H48	4:A:343:PX4:H22	0.47	1.86	12	1
4:A:391:PX4:H64	4:A:409:PX4:H62	0.47	1.87	13	1
4:A:402:PX4:H37	4:A:413:PX4:H36	0.47	1.86	13	1
4:A:331:PX4:H69	4:A:347:PX4:H42	0.47	1.85	14	1
4:A:381:PX4:H52	4:A:388:PX4:H46	0.47	1.86	14	1
4:A:392:PX4:H51	4:A:408:PX4:H24	0.47	1.85	14	1
4:A:323:PX4:H43	4:A:424:PX4:H27	0.47	1.86	1	1
4:A:413:PX4:H66	4:A:422:PX4:H41	0.47	1.87	1	1
4:A:389:PX4:H21	4:A:396:PX4:H71	0.47	1.87	5	1
4:A:315:PX4:H28	4:A:322:PX4:H40	0.47	1.87	9	1
4:A:400:PX4:H48	4:A:410:PX4:H46	0.47	1.87	10	1
4:A:412:PX4:H27	4:A:413:PX4:H38	0.47	1.84	10	1
4:A:376:PX4:H23	4:A:399:PX4:H49	0.47	1.86	11	1
4:A:371:PX4:H71	4:A:378:PX4:H62	0.47	1.87	14	1
4:A:326:PX4:H36	4:A:349:PX4:H71	0.47	1.87	1	1
4:A:307:PX4:H64	4:A:321:PX4:H67	0.47	1.87	4	1
4:A:369:PX4:H32	4:A:377:PX4:H61	0.47	1.86	4	1
4:A:375:PX4:H68	4:A:419:PX4:H32	0.47	1.86	4	1
4:A:334:PX4:H41	4:A:408:PX4:H41	0.47	1.87	5	1
4:A:350:PX4:H49	4:A:363:PX4:H50	0.47	1.87	5	1
4:A:398:PX4:H16	4:A:407:PX4:H46	0.47	1.85	7	1
4:A:400:PX4:H17	4:A:408:PX4:H53	0.47	1.85	7	1
4:A:312:PX4:H28	4:A:365:PX4:H46	0.47	1.85	8	1
4:A:355:PX4:H61	4:A:355:PX4:H17	0.47	1.85	9	1
4:A:408:PX4:H72	4:A:426:PX4:H57	0.47	1.87	9	1
4:A:391:PX4:H41	4:A:408:PX4:H39	0.47	1.85	10	1
4:A:371:PX4:H39	4:A:420:PX4:H36	0.47	1.86	11	1
4:A:332:PX4:H37	4:A:390:PX4:H39	0.47	1.86	14	1
4:A:402:PX4:H51	4:A:404:PX4:H47	0.47	1.87	3	1
4:A:388:PX4:H34	4:A:402:PX4:H24	0.47	1.87	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:416:PX4:H57	4:A:423:PX4:H64	0.47	1.86	9	1
4:A:322:PX4:H25	4:A:361:PX4:H46	0.47	1.85	13	1
4:A:419:PX4:O8	4:A:427:PX4:H17	0.47	2.09	13	1
4:A:308:PX4:H62	4:A:363:PX4:H21	0.46	1.87	1	1
4:A:368:PX4:O2	4:A:369:PX4:H4	0.46	2.09	2	1
4:A:345:PX4:H20	4:A:346:PX4:H47	0.46	1.86	5	1
4:A:349:PX4:H41	4:A:422:PX4:H45	0.46	1.87	7	1
4:A:372:PX4:H26	4:A:378:PX4:H34	0.46	1.87	9	1
4:A:342:PX4:H19	4:A:352:PX4:H23	0.46	1.87	10	1
4:A:404:PX4:H41	4:A:412:PX4:H64	0.46	1.88	10	1
4:A:370:PX4:H68	4:A:403:PX4:H23	0.46	1.88	13	1
4:A:358:PX4:H31	4:A:364:PX4:H43	0.46	1.85	14	1
4:A:325:PX4:H47	4:A:341:PX4:H22	0.46	1.87	2	1
4:A:393:PX4:H38	4:A:401:PX4:H36	0.46	1.86	2	1
4:A:382:PX4:H59	4:A:428:PX4:H21	0.46	1.88	3	1
4:A:310:PX4:H71	4:A:311:PX4:H20	0.46	1.85	7	1
4:A:400:PX4:H31	4:A:426:PX4:H58	0.46	1.87	8	1
4:A:392:PX4:H18	4:A:393:PX4:H47	0.46	1.87	11	2
4:A:353:PX4:H27	4:A:366:PX4:H14	0.46	1.86	10	1
4:A:380:PX4:H52	4:A:387:PX4:H46	0.46	1.87	11	1
4:A:386:PX4:H29	4:A:387:PX4:H26	0.46	1.86	12	1
4:A:400:PX4:H29	4:A:401:PX4:H31	0.46	1.87	13	1
4:A:322:PX4:H38	4:A:413:PX4:H68	0.46	1.88	2	1
4:A:355:PX4:H40	4:A:356:PX4:H35	0.46	1.87	3	1
4:A:395:PX4:H35	4:A:397:PX4:H64	0.46	1.86	3	1
4:A:310:PX4:H72	4:A:311:PX4:H67	0.46	1.87	6	1
4:A:424:PX4:H40	4:A:429:PX4:H68	0.46	1.88	6	1
4:A:404:PX4:H15	4:A:413:PX4:O6	0.46	2.11	9	1
4:A:310:PX4:H63	4:A:311:PX4:H21	0.46	1.87	10	1
4:A:378:PX4:H19	4:A:410:PX4:H27	0.46	1.87	12	1
4:A:315:PX4:H5	4:A:361:PX4:O6	0.46	2.11	14	1
4:A:392:PX4:H49	4:A:393:PX4:H50	0.46	1.88	14	1
4:A:404:PX4:H69	4:A:412:PX4:H45	0.46	1.87	1	1
4:A:371:PX4:H60	4:A:378:PX4:H66	0.46	1.87	5	1
4:A:331:PX4:H42	4:A:397:PX4:H30	0.46	1.88	6	1
4:A:315:PX4:H17	4:A:316:PX4:H54	0.46	1.87	7	1
4:A:353:PX4:O6	4:A:366:PX4:H3	0.46	2.10	8	1
4:A:383:PX4:H59	4:A:399:PX4:H17	0.46	1.87	9	1
4:A:398:PX4:H19	4:A:407:PX4:H19	0.46	1.86	9	1
4:A:330:PX4:H30	4:A:338:PX4:H29	0.46	1.87	10	1
4:A:390:PX4:H61	4:A:397:PX4:H36	0.46	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:315:PX4:H21	4:A:316:PX4:H32	0.46	1.88	12	1
4:A:407:PX4:H18	4:A:414:PX4:H49	0.46	1.85	12	1
4:A:410:PX4:H60	4:A:417:PX4:H62	0.46	1.87	14	1
4:A:322:PX4:H24	4:A:361:PX4:H48	0.46	1.85	2	1
4:A:347:PX4:H43	4:A:348:PX4:H31	0.46	1.86	3	1
4:A:378:PX4:H17	4:A:410:PX4:H22	0.46	1.86	3	1
4:A:378:PX4:H42	4:A:410:PX4:H71	0.46	1.85	5	1
4:A:321:PX4:H68	4:A:361:PX4:H49	0.46	1.88	7	1
4:A:417:PX4:H20	4:A:426:PX4:H23	0.46	1.87	7	1
4:A:349:PX4:H56	4:A:350:PX4:H28	0.46	1.86	10	1
4:A:321:PX4:H70	4:A:423:PX4:H41	0.46	1.88	12	1
4:A:307:PX4:H39	4:A:349:PX4:H69	0.46	1.86	13	1
4:A:391:PX4:H29	4:A:414:PX4:H46	0.46	1.87	13	1
4:A:367:PX4:H25	4:A:424:PX4:H26	0.46	1.87	1	1
4:A:350:PX4:H69	4:A:351:PX4:H69	0.46	1.87	3	1
4:A:331:PX4:H28	4:A:347:PX4:C25	0.46	2.40	4	1
4:A:387:PX4:H14	4:A:387:PX4:H6	0.46	1.86	6	1
4:A:402:PX4:H18	4:A:404:PX4:H20	0.46	1.85	6	1
4:A:347:PX4:H72	4:A:356:PX4:H65	0.46	1.87	9	1
4:A:307:PX4:H55	4:A:362:PX4:H27	0.46	1.86	11	1
4:A:349:PX4:H64	4:A:405:PX4:H70	0.46	1.87	11	1
4:A:369:PX4:H25	4:A:418:PX4:H25	0.46	1.87	11	1
4:A:346:PX4:H30	4:A:353:PX4:H65	0.46	1.86	13	1
4:A:421:PX4:H43	4:A:423:PX4:H41	0.46	1.87	7	1
4:A:331:PX4:H29	4:A:347:PX4:H52	0.46	1.87	8	1
4:A:337:PX4:H47	4:A:353:PX4:C6	0.46	2.29	8	1
4:A:340:PX4:H36	4:A:397:PX4:H65	0.46	1.85	9	1
4:A:313:PX4:C19	4:A:337:PX4:H64	0.46	2.41	10	1
4:A:423:PX4:H55	4:A:425:PX4:H28	0.46	1.88	10	1
4:A:308:PX4:H52	4:A:363:PX4:H24	0.46	1.86	12	1
4:A:321:PX4:H61	4:A:361:PX4:H46	0.46	1.88	12	1
4:A:340:PX4:H65	4:A:340:PX4:H28	0.46	1.86	13	1
4:A:407:PX4:O6	4:A:407:PX4:H7	0.46	2.11	1	1
4:A:396:PX4:H63	4:A:398:PX4:H51	0.46	1.88	11	1
4:A:337:PX4:H65	4:A:353:PX4:H40	0.46	1.86	12	1
4:A:383:PX4:H20	4:A:392:PX4:H27	0.46	1.85	12	1
4:A:313:PX4:H60	4:A:327:PX4:H31	0.46	1.87	13	1
4:A:390:PX4:H57	4:A:397:PX4:H35	0.46	1.86	13	1
4:A:330:PX4:H13	4:A:338:PX4:O6	0.46	2.11	5	1
4:A:317:PX4:H42	4:A:342:PX4:H72	0.46	1.88	6	1
4:A:391:PX4:H17	4:A:408:PX4:H2	0.46	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:344:PX4:H31	4:A:348:PX4:H25	0.46	1.88	8	1
4:A:392:PX4:H68	4:A:408:PX4:H35	0.46	1.88	8	1
4:A:367:PX4:H48	4:A:428:PX4:H50	0.46	1.86	9	1
4:A:392:PX4:H29	4:A:393:PX4:H61	0.46	1.88	11	1
4:A:357:PX4:H43	4:A:358:PX4:H44	0.46	1.86	13	1
4:A:325:PX4:H42	4:A:334:PX4:H59	0.46	1.87	14	1
4:A:340:PX4:H37	4:A:397:PX4:H29	0.46	1.88	1	1
4:A:370:PX4:H42	4:A:403:PX4:H38	0.46	1.86	1	1
4:A:402:PX4:H20	4:A:411:PX4:O8	0.46	2.11	1	1
4:A:332:PX4:H29	4:A:347:PX4:H66	0.46	1.87	5	1
4:A:311:PX4:H51	4:A:359:PX4:H59	0.46	1.86	7	1
4:A:362:PX4:H26	4:A:413:PX4:H72	0.46	1.88	7	1
4:A:388:PX4:H14	4:A:396:PX4:H18	0.46	1.88	7	1
4:A:338:PX4:H47	4:A:348:PX4:C23	0.46	2.41	8	1
4:A:382:PX4:H60	4:A:412:PX4:H64	0.46	1.88	8	1
4:A:398:PX4:H32	4:A:414:PX4:H55	0.46	1.86	8	1
4:A:311:PX4:H20	4:A:311:PX4:H55	0.46	1.88	10	1
4:A:398:PX4:H48	4:A:407:PX4:H57	0.46	1.86	12	1
4:A:404:PX4:H26	4:A:419:PX4:H9	0.45	1.87	3	1
4:A:409:PX4:H64	4:A:415:PX4:H60	0.45	1.88	4	1
4:A:334:PX4:H33	4:A:407:PX4:H38	0.45	1.88	9	1
4:A:330:PX4:C4	4:A:330:PX4:H19	0.45	2.41	10	1
4:A:410:PX4:O2	4:A:416:PX4:H3	0.45	2.10	14	2
4:A:326:PX4:H55	4:A:408:PX4:H44	0.45	1.87	11	1
4:A:391:PX4:H16	4:A:392:PX4:H46	0.45	1.88	12	1
4:A:312:PX4:H32	4:A:357:PX4:H55	0.45	1.88	14	1
4:A:361:PX4:H19	4:A:364:PX4:H46	0.45	1.87	14	1
4:A:323:PX4:H4	4:A:333:PX4:O2	0.45	2.11	3	1
4:A:308:PX4:H21	4:A:311:PX4:H49	0.45	1.88	7	1
4:A:308:PX4:H16	4:A:311:PX4:C9	0.45	2.41	7	1
4:A:316:PX4:H48	4:A:320:PX4:H21	0.45	1.87	7	1
4:A:317:PX4:H51	4:A:341:PX4:H19	0.45	1.87	8	1
4:A:360:PX4:H43	4:A:382:PX4:H64	0.45	1.88	8	1
4:A:380:PX4:H62	4:A:388:PX4:H42	0.45	1.88	9	1
4:A:421:PX4:H7	4:A:422:PX4:O6	0.45	2.11	9	1
4:A:413:PX4:H35	4:A:419:PX4:H27	0.45	1.87	10	1
4:A:333:PX4:H33	4:A:389:PX4:H45	0.45	1.88	11	1
4:A:367:PX4:H16	4:A:424:PX4:H14	0.45	1.87	14	1
4:A:403:PX4:H46	4:A:419:PX4:H51	0.45	1.88	1	1
4:A:383:PX4:O4	4:A:392:PX4:H1	0.45	2.10	3	1
4:A:393:PX4:H31	4:A:394:PX4:C11	0.45	2.41	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:354:PX4:H63	4:A:360:PX4:H63	0.45	1.88	4	1
4:A:422:PX4:H3	4:A:423:PX4:O2	0.45	2.10	4	1
4:A:331:PX4:C21	4:A:397:PX4:H30	0.45	2.41	6	1
4:A:391:PX4:H48	4:A:392:PX4:H46	0.45	1.87	8	1
4:A:351:PX4:H12	4:A:352:PX4:H24	0.45	1.88	9	1
4:A:345:PX4:C36	4:A:370:PX4:H39	0.45	2.41	10	1
4:A:390:PX4:H1	4:A:399:PX4:H18	0.45	1.88	12	1
4:A:317:PX4:H59	4:A:319:PX4:H56	0.45	1.88	14	1
4:A:348:PX4:H55	4:A:388:PX4:H70	0.45	1.88	1	1
4:A:405:PX4:H47	4:A:406:PX4:H48	0.45	1.88	4	1
4:A:307:PX4:H37	4:A:416:PX4:H42	0.45	1.88	5	1
4:A:310:PX4:H70	4:A:359:PX4:H59	0.45	1.88	5	1
4:A:313:PX4:H21	4:A:366:PX4:H18	0.45	1.88	5	1
4:A:331:PX4:H40	4:A:340:PX4:H63	0.45	1.88	5	1
4:A:337:PX4:H48	4:A:345:PX4:H49	0.45	1.88	6	1
4:A:328:PX4:H47	4:A:329:PX4:H28	0.45	1.89	9	1
4:A:380:PX4:H20	4:A:381:PX4:H48	0.45	1.89	9	1
4:A:348:PX4:H59	4:A:362:PX4:H54	0.45	1.89	13	1
4:A:338:PX4:H66	4:A:395:PX4:H38	0.45	1.89	4	1
4:A:381:PX4:H59	4:A:397:PX4:H47	0.45	1.87	7	1
4:A:369:PX4:H21	4:A:377:PX4:H71	0.45	1.87	10	1
4:A:323:PX4:H36	4:A:424:PX4:H67	0.45	1.87	4	1
4:A:313:PX4:H42	4:A:403:PX4:H62	0.45	1.87	5	1
4:A:421:PX4:H24	4:A:423:PX4:H19	0.45	1.87	5	1
4:A:307:PX4:H5	4:A:321:PX4:H48	0.45	1.87	8	1
4:A:412:PX4:O8	4:A:428:PX4:H17	0.45	2.11	8	1
4:A:349:PX4:O1	4:A:350:PX4:H14	0.45	2.11	10	1
4:A:391:PX4:H46	4:A:401:PX4:O6	0.45	2.12	11	1
4:A:378:PX4:H19	4:A:410:PX4:C14	0.45	2.42	12	1
4:A:371:PX4:H58	4:A:379:PX4:H32	0.45	1.89	13	1
4:A:375:PX4:H50	4:A:428:PX4:H14	0.45	1.88	13	1
4:A:322:PX4:H22	4:A:323:PX4:H19	0.45	1.89	1	1
4:A:393:PX4:H56	4:A:401:PX4:H35	0.45	1.89	1	1
4:A:313:PX4:H42	4:A:403:PX4:H66	0.45	1.89	2	1
4:A:368:PX4:H37	4:A:418:PX4:H72	0.45	1.89	4	1
4:A:416:PX4:H27	4:A:423:PX4:H24	0.45	1.87	7	1
4:A:312:PX4:H62	4:A:320:PX4:H67	0.45	1.87	11	1
4:A:373:PX4:O6	4:A:397:PX4:H12	0.45	2.12	11	1
4:A:419:PX4:H18	4:A:419:PX4:H12	0.45	1.87	11	1
4:A:391:PX4:H40	4:A:392:PX4:H56	0.45	1.88	13	1
1:A:214:LEU:HD11	1:A:243:VAL:H	0.45	1.71	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H36	4:A:381:PX4:H45	0.45	1.88	2	1
4:A:316:PX4:H25	4:A:320:PX4:H33	0.45	1.88	3	1
4:A:394:PX4:H34	4:A:401:PX4:H39	0.45	1.89	3	1
4:A:331:PX4:H53	4:A:340:PX4:H34	0.45	1.87	4	1
4:A:402:PX4:H57	4:A:404:PX4:H60	0.45	1.88	4	1
4:A:342:PX4:H27	4:A:358:PX4:H58	0.45	1.89	5	1
1:A:243:VAL:HG12	4:A:356:PX4:H23	0.45	1.88	6	1
4:A:331:PX4:H43	4:A:389:PX4:H29	0.45	1.88	6	1
4:A:367:PX4:H17	4:A:428:PX4:H54	0.45	1.88	9	1
4:A:330:PX4:H21	4:A:338:PX4:H22	0.45	1.87	10	1
4:A:370:PX4:H28	4:A:403:PX4:H57	0.45	1.89	1	1
4:A:306:PX4:H14	4:A:321:PX4:O6	0.45	2.12	3	1
4:A:337:PX4:H53	4:A:353:PX4:H25	0.45	1.89	4	1
4:A:398:PX4:H67	4:A:405:PX4:H57	0.45	1.88	6	1
1:A:125:MET:HE2	1:A:130:VAL:CG2	0.45	2.42	7	1
4:A:378:PX4:H16	4:A:417:PX4:C24	0.45	2.33	7	1
4:A:330:PX4:H7	4:A:330:PX4:H19	0.45	1.87	11	1
4:A:310:PX4:H17	4:A:365:PX4:O5	0.45	2.11	13	1
4:A:392:PX4:H25	4:A:393:PX4:H66	0.45	1.87	13	1
4:A:417:PX4:H24	4:A:426:PX4:H26	0.45	1.89	4	1
4:A:383:PX4:H31	4:A:383:PX4:H24	0.45	1.89	5	1
4:A:384:PX4:H61	4:A:384:PX4:H34	0.45	1.89	5	1
4:A:369:PX4:H52	4:A:425:PX4:H21	0.45	1.89	11	1
4:A:350:PX4:H1	4:A:358:PX4:O2	0.45	2.12	12	1
4:A:389:PX4:O2	4:A:398:PX4:H4	0.45	2.12	14	1
4:A:383:PX4:H66	4:A:399:PX4:H69	0.44	1.89	1	1
4:A:380:PX4:H26	4:A:381:PX4:H36	0.44	1.87	8	1
4:A:412:PX4:H23	4:A:413:PX4:H31	0.44	1.89	9	1
4:A:347:PX4:H10	4:A:348:PX4:O1	0.44	2.13	10	1
4:A:352:PX4:H52	4:A:358:PX4:H50	0.44	1.89	10	1
4:A:322:PX4:H62	4:A:412:PX4:H42	0.44	1.88	11	1
4:A:369:PX4:H44	4:A:418:PX4:H68	0.44	1.87	11	1
4:A:398:PX4:H15	4:A:398:PX4:H13	0.44	1.90	11	1
4:A:306:PX4:H59	4:A:361:PX4:H54	0.44	1.89	13	1
4:A:406:PX4:H25	4:A:415:PX4:H22	0.44	1.88	14	1
4:A:311:PX4:H53	4:A:359:PX4:H56	0.44	1.89	5	1
4:A:319:PX4:H26	4:A:324:PX4:H24	0.44	1.88	5	1
4:A:347:PX4:H9	4:A:347:PX4:H19	0.44	1.89	6	1
4:A:367:PX4:H48	4:A:424:PX4:H19	0.44	1.88	6	1
4:A:317:PX4:O2	4:A:325:PX4:H10	0.44	2.12	7	1
4:A:334:PX4:O6	4:A:334:PX4:H3	0.44	2.12	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H30	4:A:396:PX4:H60	0.44	1.89	8	1
4:A:398:PX4:H45	4:A:414:PX4:H21	0.44	1.89	9	1
4:A:353:PX4:H20	4:A:366:PX4:H2	0.44	1.88	10	1
4:A:313:PX4:H47	4:A:328:PX4:H17	0.44	1.90	11	1
4:A:410:PX4:H66	4:A:426:PX4:H41	0.44	1.89	12	1
4:A:375:PX4:H21	4:A:429:PX4:H45	0.44	1.88	1	1
4:A:307:PX4:H51	4:A:362:PX4:H22	0.44	1.90	6	1
4:A:396:PX4:H31	4:A:411:PX4:H34	0.44	1.90	8	1
4:A:318:PX4:H18	4:A:328:PX4:H19	0.44	1.88	11	1
4:A:419:PX4:H60	4:A:427:PX4:H58	0.44	1.89	11	1
4:A:423:PX4:H16	4:A:425:PX4:O8	0.44	2.12	13	1
4:A:337:PX4:H15	4:A:353:PX4:O1	0.44	2.13	1	2
4:A:311:PX4:H6	4:A:311:PX4:O3	0.44	2.10	2	1
4:A:377:PX4:H10	4:A:418:PX4:O8	0.44	2.13	2	1
4:A:400:PX4:H47	4:A:409:PX4:H23	0.44	1.89	3	1
4:A:422:PX4:H34	4:A:423:PX4:H45	0.44	1.88	6	1
4:A:321:PX4:H68	4:A:322:PX4:H30	0.44	1.90	9	1
4:A:387:PX4:H54	4:A:388:PX4:H38	0.44	1.89	10	1
4:A:370:PX4:H26	4:A:427:PX4:H57	0.44	1.89	11	1
4:A:402:PX4:H54	4:A:404:PX4:H59	0.44	1.89	11	1
4:A:329:PX4:H67	4:A:424:PX4:H40	0.44	1.90	14	1
4:A:369:PX4:O1	4:A:425:PX4:H4	0.44	2.13	12	3
4:A:342:PX4:H29	4:A:351:PX4:H30	0.44	1.89	3	1
4:A:337:PX4:H52	4:A:345:PX4:H55	0.44	1.88	7	2
4:A:319:PX4:H66	4:A:324:PX4:H58	0.44	1.88	9	1
4:A:405:PX4:H53	4:A:414:PX4:H33	0.44	1.89	9	1
4:A:326:PX4:H66	4:A:399:PX4:H65	0.44	1.88	11	1
4:A:380:PX4:H46	4:A:387:PX4:H20	0.44	1.89	11	1
4:A:345:PX4:H35	4:A:346:PX4:H37	0.44	1.89	12	1
4:A:389:PX4:H48	4:A:398:PX4:H17	0.44	1.89	12	1
4:A:320:PX4:H54	4:A:359:PX4:H30	0.44	1.90	13	1
4:A:338:PX4:H55	4:A:348:PX4:H53	0.44	1.90	14	1
4:A:412:PX4:H27	4:A:430:PX4:H60	0.44	1.89	14	1
4:A:310:PX4:O6	4:A:365:PX4:H4	0.44	2.12	1	1
4:A:391:PX4:H25	4:A:393:PX4:H64	0.44	1.89	1	1
4:A:400:PX4:C24	4:A:409:PX4:H23	0.44	2.42	2	1
4:A:315:PX4:H5	4:A:364:PX4:O8	0.44	2.11	7	1
4:A:355:PX4:H38	4:A:356:PX4:H44	0.44	1.88	7	1
4:A:389:PX4:H30	4:A:396:PX4:C31	0.44	2.42	8	1
4:A:390:PX4:H30	4:A:398:PX4:H19	0.44	1.89	8	1
4:A:321:PX4:H37	4:A:354:PX4:H59	0.44	1.90	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:207:SER:O	4:A:321:PX4:H6	0.44	2.13	10	1
4:A:331:PX4:H44	4:A:340:PX4:H71	0.44	1.89	3	1
4:A:315:PX4:H20	4:A:320:PX4:H28	0.44	1.89	4	1
4:A:333:PX4:H61	4:A:368:PX4:H72	0.44	1.90	4	1
4:A:338:PX4:H64	4:A:411:PX4:H36	0.44	1.89	4	1
4:A:346:PX4:H39	4:A:354:PX4:H31	0.44	1.89	5	1
4:A:393:PX4:H14	4:A:394:PX4:C9	0.44	2.43	8	1
4:A:391:PX4:H58	4:A:401:PX4:H36	0.44	1.89	13	1
4:A:402:PX4:H36	4:A:403:PX4:H35	0.44	1.89	1	1
4:A:318:PX4:H24	4:A:320:PX4:H46	0.44	1.90	2	1
4:A:393:PX4:O6	4:A:394:PX4:H15	0.44	2.13	2	1
4:A:406:PX4:H35	4:A:414:PX4:H32	0.44	1.90	3	1
4:A:392:PX4:H35	4:A:399:PX4:H61	0.44	1.89	4	1
4:A:322:PX4:H34	4:A:361:PX4:H22	0.44	1.88	6	1
4:A:400:PX4:H38	4:A:401:PX4:H38	0.44	1.87	7	1
4:A:344:PX4:H37	4:A:347:PX4:H45	0.44	1.90	8	1
4:A:377:PX4:H16	4:A:418:PX4:C3	0.44	2.42	8	1
4:A:403:PX4:H9	4:A:427:PX4:O8	0.44	2.13	8	1
4:A:312:PX4:H25	4:A:363:PX4:H32	0.44	1.90	9	1
4:A:393:PX4:H41	4:A:394:PX4:H40	0.44	1.89	10	1
4:A:338:PX4:H17	4:A:348:PX4:O6	0.44	2.13	13	1
4:A:358:PX4:H22	4:A:363:PX4:H53	0.44	1.89	13	1
4:A:310:PX4:H23	4:A:358:PX4:H49	0.44	1.89	14	1
4:A:313:PX4:H57	4:A:327:PX4:H21	0.44	1.87	14	1
4:A:323:PX4:H16	4:A:333:PX4:H51	0.44	1.90	1	1
4:A:382:PX4:H52	4:A:428:PX4:H28	0.44	1.88	3	1
4:A:413:PX4:H69	4:A:428:PX4:H70	0.44	1.88	4	1
4:A:367:PX4:H46	4:A:428:PX4:H47	0.44	1.90	7	1
4:A:314:PX4:H69	4:A:364:PX4:H45	0.44	1.89	10	1
4:A:326:PX4:H57	4:A:334:PX4:H34	0.44	1.90	11	1
4:A:352:PX4:H32	4:A:358:PX4:H62	0.44	1.90	14	1
4:A:370:PX4:H34	4:A:403:PX4:H67	0.44	1.90	14	1
4:A:340:PX4:H62	4:A:341:PX4:H66	0.43	1.90	1	1
4:A:351:PX4:O7	4:A:352:PX4:H23	0.43	2.13	2	1
4:A:416:PX4:O1	4:A:422:PX4:H10	0.43	2.13	2	1
4:A:351:PX4:H8	4:A:352:PX4:O1	0.43	2.13	4	1
4:A:308:PX4:H44	4:A:311:PX4:H70	0.43	1.90	12	1
4:A:318:PX4:H35	4:A:327:PX4:H65	0.43	1.89	12	1
4:A:330:PX4:H52	4:A:338:PX4:H24	0.43	1.90	12	1
4:A:417:PX4:H28	4:A:426:PX4:H32	0.43	1.90	12	1
4:A:312:PX4:H69	4:A:359:PX4:H37	0.43	1.89	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:321:PX4:H67	4:A:361:PX4:H24	0.43	1.90	13	1
4:A:376:PX4:H66	4:A:385:PX4:H30	0.43	1.90	13	1
4:A:374:PX4:H32	4:A:427:PX4:H23	0.43	1.90	14	1
4:A:330:PX4:H63	4:A:338:PX4:H42	0.43	1.88	2	1
4:A:361:PX4:H40	4:A:423:PX4:H66	0.43	1.90	3	1
4:A:312:PX4:H44	4:A:365:PX4:H68	0.43	1.89	5	1
4:A:393:PX4:H45	4:A:401:PX4:H45	0.43	1.90	6	1
4:A:310:PX4:H43	4:A:365:PX4:H37	0.43	1.90	7	1
4:A:328:PX4:H20	4:A:328:PX4:H25	0.43	1.38	8	1
4:A:416:PX4:O8	4:A:418:PX4:H40	0.43	2.13	8	1
4:A:346:PX4:H46	4:A:362:PX4:H46	0.43	1.90	12	1
4:A:311:PX4:H5	4:A:320:PX4:O4	0.43	2.13	13	1
4:A:326:PX4:H37	4:A:350:PX4:H32	0.43	1.89	1	1
1:A:244:ASP:OD2	4:A:349:PX4:H3	0.43	2.14	2	1
4:A:378:PX4:H23	4:A:378:PX4:H29	0.43	1.63	2	1
4:A:418:PX4:O1	4:A:425:PX4:H5	0.43	2.13	3	1
4:A:347:PX4:O4	4:A:348:PX4:H6	0.43	2.13	5	1
4:A:386:PX4:H38	4:A:394:PX4:H67	0.43	1.89	10	1
4:A:430:PX4:H44	4:A:430:PX4:H38	0.43	1.51	11	1
4:A:395:PX4:H43	4:A:405:PX4:H40	0.43	1.89	13	1
4:A:315:PX4:H10	4:A:316:PX4:O6	0.43	2.13	2	1
4:A:334:PX4:H69	4:A:352:PX4:H37	0.43	1.89	2	1
4:A:389:PX4:H33	4:A:397:PX4:H21	0.43	1.90	2	1
4:A:418:PX4:H36	4:A:418:PX4:H41	0.43	1.56	5	1
4:A:341:PX4:H58	4:A:390:PX4:H72	0.43	1.89	7	1
4:A:320:PX4:H32	4:A:359:PX4:H63	0.43	1.90	8	1
4:A:307:PX4:H61	4:A:362:PX4:H27	0.43	1.91	10	1
4:A:378:PX4:O1	4:A:417:PX4:H17	0.43	2.12	10	1
4:A:314:PX4:H31	4:A:356:PX4:H28	0.43	1.90	11	1
4:A:363:PX4:H30	4:A:363:PX4:H35	0.43	1.61	6	1
4:A:306:PX4:H56	4:A:306:PX4:H51	0.43	1.58	7	1
4:A:331:PX4:H51	4:A:347:PX4:H22	0.43	1.91	8	1
4:A:410:PX4:O2	4:A:416:PX4:H10	0.43	2.14	9	1
4:A:387:PX4:H5	4:A:411:PX4:O3	0.43	2.13	12	1
4:A:314:PX4:H71	4:A:409:PX4:H31	0.43	1.90	13	1
4:A:341:PX4:H72	4:A:397:PX4:H35	0.43	1.89	1	1
4:A:369:PX4:H29	4:A:378:PX4:H51	0.43	1.89	1	1
4:A:314:PX4:H37	4:A:362:PX4:H16	0.43	1.90	4	1
4:A:333:PX4:H53	4:A:341:PX4:H57	0.43	1.89	5	1
1:A:178:GLY:HA3	4:A:354:PX4:H1	0.43	1.89	7	1
4:A:376:PX4:H19	4:A:383:PX4:H19	0.43	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H8	4:A:427:PX4:H20	0.43	1.91	8	1
4:A:338:PX4:H70	4:A:395:PX4:H38	0.43	1.90	10	1
4:A:352:PX4:O8	4:A:365:PX4:H3	0.43	2.13	10	1
4:A:407:PX4:O6	4:A:414:PX4:H49	0.43	2.13	10	1
4:A:342:PX4:C12	4:A:352:PX4:H47	0.43	2.31	11	1
4:A:374:PX4:H58	4:A:382:PX4:H50	0.43	1.91	11	1
4:A:410:PX4:H51	4:A:426:PX4:H33	0.43	1.90	11	1
4:A:423:PX4:H55	4:A:425:PX4:H27	0.43	1.90	11	1
4:A:316:PX4:H47	4:A:320:PX4:H23	0.43	1.90	12	1
4:A:393:PX4:H30	4:A:400:PX4:H31	0.43	1.91	13	1
4:A:412:PX4:H36	4:A:419:PX4:H28	0.43	1.90	2	1
4:A:309:PX4:H28	4:A:309:PX4:H62	0.43	1.89	3	1
4:A:331:PX4:H17	4:A:340:PX4:H5	0.43	1.89	3	1
4:A:346:PX4:O6	4:A:362:PX4:H15	0.43	2.14	3	1
4:A:384:PX4:O1	4:A:385:PX4:H10	0.43	2.13	4	1
4:A:349:PX4:H65	4:A:406:PX4:H68	0.43	1.88	5	1
4:A:412:PX4:H58	4:A:427:PX4:H30	0.43	1.90	5	1
4:A:325:PX4:H49	4:A:341:PX4:H19	0.43	1.89	6	1
4:A:345:PX4:H19	4:A:346:PX4:H22	0.43	1.90	6	1
4:A:387:PX4:H56	4:A:387:PX4:H50	0.43	1.43	6	1
4:A:391:PX4:H26	4:A:392:PX4:H46	0.43	1.89	6	1
4:A:395:PX4:O1	4:A:396:PX4:H17	0.43	2.14	7	1
4:A:333:PX4:H14	4:A:340:PX4:O2	0.43	2.14	9	1
4:A:353:PX4:H35	4:A:366:PX4:H22	0.43	1.91	10	1
4:A:334:PX4:H56	4:A:334:PX4:H51	0.43	1.42	11	1
4:A:356:PX4:H62	4:A:397:PX4:H71	0.43	1.90	11	1
4:A:330:PX4:H31	4:A:348:PX4:H30	0.43	1.89	13	1
4:A:333:PX4:H30	4:A:339:PX4:H28	0.43	1.90	14	1
4:A:398:PX4:H21	4:A:407:PX4:H46	0.43	1.91	14	1
4:A:326:PX4:H47	4:A:334:PX4:H60	0.43	1.90	1	1
4:A:373:PX4:H28	4:A:381:PX4:H57	0.43	1.91	1	1
4:A:381:PX4:H16	4:A:388:PX4:H12	0.43	1.90	2	1
4:A:308:PX4:H14	4:A:311:PX4:O8	0.43	2.14	3	1
4:A:350:PX4:H61	4:A:363:PX4:H23	0.43	1.89	3	1
4:A:330:PX4:H5	4:A:344:PX4:H16	0.43	1.91	4	1
4:A:314:PX4:H33	4:A:362:PX4:H16	0.43	1.89	7	1
4:A:403:PX4:H3	4:A:427:PX4:H49	0.43	1.90	7	1
1:A:116:TYR:CD1	1:A:138:PHE:CE2	0.43	3.06	8	1
4:A:326:PX4:H61	4:A:334:PX4:H35	0.43	1.89	10	1
4:A:345:PX4:H71	4:A:403:PX4:H36	0.43	1.91	10	1
4:A:391:PX4:H23	4:A:392:PX4:H14	0.43	1.89	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:H44	4:A:355:PX4:H46	0.43	1.90	11	1
4:A:339:PX4:H68	4:A:339:PX4:H62	0.43	1.44	13	1
4:A:391:PX4:H37	4:A:393:PX4:H72	0.43	1.89	13	1
4:A:395:PX4:H9	4:A:411:PX4:O2	0.43	2.14	14	1
4:A:325:PX4:H28	4:A:407:PX4:H41	0.43	1.90	1	1
4:A:379:PX4:H65	4:A:379:PX4:H71	0.43	1.55	2	1
4:A:371:PX4:H46	4:A:371:PX4:H16	0.43	1.75	3	2
4:A:378:PX4:H19	4:A:426:PX4:H28	0.43	1.90	3	1
4:A:354:PX4:H65	4:A:360:PX4:H24	0.43	1.89	5	1
4:A:327:PX4:O3	4:A:327:PX4:H10	0.43	2.14	6	1
4:A:376:PX4:H36	4:A:376:PX4:H42	0.43	1.68	6	1
4:A:386:PX4:H17	4:A:394:PX4:O8	0.43	2.13	6	1
4:A:403:PX4:H32	4:A:404:PX4:H21	0.43	1.91	7	1
4:A:337:PX4:H45	4:A:338:PX4:H52	0.43	1.91	8	1
4:A:325:PX4:H32	4:A:332:PX4:H28	0.43	1.90	9	1
4:A:335:PX4:H42	4:A:343:PX4:H64	0.43	1.89	10	1
4:A:412:PX4:H51	4:A:419:PX4:H16	0.43	1.91	12	1
4:A:404:PX4:H71	4:A:404:PX4:H19	0.43	1.89	13	1
4:A:403:PX4:H47	4:A:427:PX4:H47	0.43	1.90	1	1
4:A:314:PX4:H71	4:A:364:PX4:H39	0.43	1.91	2	1
4:A:314:PX4:H38	4:A:355:PX4:H57	0.43	1.91	3	1
4:A:372:PX4:H54	4:A:379:PX4:H53	0.43	1.90	5	1
1:A:207:SER:O	4:A:321:PX4:H9	0.43	2.13	6	1
4:A:328:PX4:H56	4:A:354:PX4:H72	0.43	1.90	7	1
4:A:314:PX4:H47	4:A:349:PX4:H19	0.43	1.91	8	1
4:A:377:PX4:H72	4:A:425:PX4:O2	0.43	2.13	8	1
4:A:367:PX4:H20	4:A:424:PX4:H16	0.43	1.91	10	1
4:A:353:PX4:H58	4:A:360:PX4:H61	0.43	1.91	11	1
4:A:393:PX4:H17	4:A:401:PX4:H22	0.43	1.91	11	1
4:A:419:PX4:H60	4:A:427:PX4:H25	0.42	1.91	1	1
4:A:395:PX4:H62	4:A:413:PX4:O8	0.42	2.14	2	1
4:A:418:PX4:H40	4:A:418:PX4:H33	0.42	1.61	3	1
4:A:378:PX4:H23	4:A:378:PX4:H30	0.42	1.54	4	1
4:A:388:PX4:H63	4:A:397:PX4:H63	0.42	1.89	4	1
4:A:320:PX4:H17	4:A:359:PX4:C29	0.42	2.43	7	1
4:A:335:PX4:H41	4:A:335:PX4:H36	0.42	1.61	7	1
4:A:348:PX4:H67	4:A:348:PX4:H60	0.42	1.52	9	1
4:A:316:PX4:O2	4:A:364:PX4:H12	0.42	2.13	12	1
4:A:398:PX4:H41	4:A:415:PX4:H20	0.42	1.90	1	1
4:A:317:PX4:H55	4:A:324:PX4:C10	0.42	2.42	2	1
4:A:344:PX4:H45	4:A:344:PX4:H37	0.42	1.62	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:412:PX4:H17	4:A:419:PX4:H20	0.42	1.89	5	1
4:A:315:PX4:H3	4:A:361:PX4:O1	0.42	2.14	6	1
4:A:342:PX4:H52	4:A:351:PX4:H27	0.42	1.91	8	1
4:A:349:PX4:H16	4:A:350:PX4:H30	0.42	1.90	9	1
4:A:331:PX4:H28	4:A:347:PX4:H51	0.42	1.91	11	1
4:A:308:PX4:H66	4:A:308:PX4:H61	0.42	1.59	12	1
4:A:308:PX4:H34	4:A:311:PX4:H65	0.42	1.89	12	1
4:A:330:PX4:C22	4:A:344:PX4:H45	0.42	2.40	12	1
4:A:376:PX4:H62	4:A:385:PX4:H30	0.42	1.90	12	1
4:A:354:PX4:H22	4:A:362:PX4:H21	0.42	1.90	13	1
4:A:392:PX4:H10	4:A:392:PX4:O6	0.42	2.13	13	1
4:A:369:PX4:H58	4:A:424:PX4:H50	0.42	1.91	1	1
4:A:380:PX4:O4	4:A:381:PX4:H15	0.42	2.14	4	1
4:A:310:PX4:H16	4:A:363:PX4:O6	0.42	2.14	5	1
4:A:314:PX4:H15	4:A:314:PX4:O8	0.42	2.13	5	1
4:A:429:PX4:H27	4:A:429:PX4:H54	0.42	1.91	7	1
4:A:378:PX4:H60	4:A:410:PX4:H70	0.42	1.90	8	1
4:A:333:PX4:H16	4:A:340:PX4:H15	0.42	1.90	9	1
4:A:351:PX4:H54	4:A:358:PX4:H22	0.42	1.90	9	1
4:A:314:PX4:H26	4:A:314:PX4:H19	0.42	1.66	10	1
4:A:361:PX4:C33	4:A:412:PX4:H40	0.42	2.44	11	1
4:A:423:PX4:H57	4:A:423:PX4:H26	0.42	1.91	11	1
4:A:317:PX4:H1	4:A:317:PX4:O6	0.42	2.14	13	1
4:A:310:PX4:H36	4:A:351:PX4:H65	0.42	1.91	14	1
4:A:332:PX4:H28	4:A:334:PX4:H53	0.42	1.90	14	1
4:A:316:PX4:H71	4:A:333:PX4:H67	0.42	1.92	2	1
4:A:381:PX4:H40	4:A:381:PX4:H61	0.42	1.91	3	1
4:A:355:PX4:H55	4:A:355:PX4:H49	0.42	1.69	4	1
4:A:357:PX4:H66	4:A:357:PX4:H61	0.42	1.65	5	1
4:A:382:PX4:H22	4:A:428:PX4:C16	0.42	2.42	5	1
4:A:416:PX4:H48	4:A:425:PX4:H48	0.42	1.91	5	1
4:A:332:PX4:H66	4:A:349:PX4:H67	0.42	1.91	8	1
4:A:320:PX4:H21	4:A:359:PX4:H60	0.42	1.91	9	1
4:A:361:PX4:H29	4:A:361:PX4:H24	0.42	1.61	9	1
4:A:391:PX4:H67	4:A:401:PX4:H33	0.42	1.91	9	1
4:A:358:PX4:H70	4:A:401:PX4:H37	0.42	1.91	10	1
4:A:356:PX4:H35	4:A:356:PX4:H42	0.42	1.71	11	1
4:A:346:PX4:H25	4:A:354:PX4:H31	0.42	1.90	12	1
4:A:412:PX4:H20	4:A:428:PX4:H49	0.42	1.90	14	1
4:A:415:PX4:H11	4:A:422:PX4:H16	0.42	1.91	1	1
4:A:418:PX4:H34	4:A:425:PX4:H56	0.42	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:335:PX4:H6	4:A:344:PX4:O6	0.42	2.13	2	1
4:A:356:PX4:H42	4:A:405:PX4:H60	0.42	1.91	3	1
4:A:381:PX4:H54	4:A:388:PX4:H57	0.42	1.90	3	1
4:A:307:PX4:H16	4:A:307:PX4:H46	0.42	1.64	4	1
4:A:406:PX4:O1	4:A:414:PX4:H3	0.42	2.15	4	1
4:A:308:PX4:H16	4:A:311:PX4:C10	0.42	2.44	5	1
4:A:356:PX4:O3	4:A:356:PX4:H16	0.42	2.15	5	1
4:A:424:PX4:H17	4:A:429:PX4:H21	0.42	1.92	6	1
4:A:312:PX4:H59	4:A:359:PX4:H30	0.42	1.91	7	1
4:A:325:PX4:H64	4:A:341:PX4:H35	0.42	1.90	7	1
4:A:412:PX4:H24	4:A:430:PX4:H58	0.42	1.92	9	1
4:A:315:PX4:O3	4:A:361:PX4:H4	0.42	2.15	10	1
4:A:369:PX4:H48	4:A:377:PX4:H67	0.42	1.91	10	1
4:A:387:PX4:H17	4:A:411:PX4:H61	0.42	1.90	10	1
4:A:334:PX4:H27	4:A:334:PX4:H22	0.42	1.65	11	1
4:A:387:PX4:H17	4:A:411:PX4:H57	0.42	1.91	12	1
4:A:395:PX4:H27	4:A:405:PX4:H28	0.42	1.91	13	1
4:A:330:PX4:H49	4:A:343:PX4:H46	0.42	1.91	14	1
4:A:317:PX4:H66	4:A:342:PX4:H66	0.42	1.91	2	1
4:A:406:PX4:H33	4:A:414:PX4:H34	0.42	1.91	2	1
4:A:372:PX4:H29	4:A:420:PX4:H55	0.42	1.92	4	1
4:A:404:PX4:H54	4:A:405:PX4:H39	0.42	1.91	5	1
4:A:367:PX4:O6	4:A:423:PX4:H11	0.42	2.15	6	1
4:A:326:PX4:H44	4:A:416:PX4:H41	0.42	1.91	8	1
4:A:350:PX4:O2	4:A:363:PX4:H7	0.42	2.14	8	1
4:A:354:PX4:H50	4:A:360:PX4:H18	0.42	1.90	11	1
4:A:337:PX4:H20	4:A:346:PX4:H63	0.42	1.92	12	1
4:A:384:PX4:H3	4:A:385:PX4:H18	0.42	1.91	14	1
4:A:326:PX4:O6	4:A:350:PX4:H5	0.42	2.14	6	1
4:A:342:PX4:H37	4:A:352:PX4:H33	0.42	1.90	9	1
4:A:346:PX4:O4	4:A:362:PX4:H11	0.42	2.15	10	1
4:A:381:PX4:H53	4:A:397:PX4:H46	0.42	1.90	10	1
4:A:382:PX4:H22	4:A:428:PX4:H34	0.42	1.92	10	1
4:A:391:PX4:H71	4:A:415:PX4:H45	0.42	1.92	10	1
4:A:406:PX4:H17	4:A:414:PX4:H22	0.42	1.92	10	1
4:A:334:PX4:H29	4:A:414:PX4:H69	0.42	1.91	11	1
4:A:338:PX4:H68	4:A:348:PX4:H58	0.42	1.90	11	1
4:A:349:PX4:O6	4:A:349:PX4:H7	0.42	2.15	11	1
4:A:332:PX4:H25	4:A:334:PX4:H49	0.42	1.90	14	1
4:A:321:PX4:H47	4:A:354:PX4:H20	0.42	1.91	2	1
4:A:371:PX4:H36	4:A:379:PX4:H60	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:H19	4:A:429:PX4:H45	0.42	1.90	3	1
4:A:391:PX4:H66	4:A:408:PX4:H57	0.42	1.92	4	1
4:A:402:PX4:H33	4:A:402:PX4:H28	0.42	1.57	4	1
4:A:307:PX4:H58	4:A:314:PX4:H17	0.42	1.92	5	1
4:A:337:PX4:O6	4:A:345:PX4:H49	0.42	2.15	5	1
4:A:347:PX4:H56	4:A:356:PX4:H56	0.42	1.92	5	1
4:A:416:PX4:H17	4:A:425:PX4:O8	0.42	2.14	5	1
4:A:344:PX4:H27	4:A:348:PX4:H21	0.42	1.92	6	1
4:A:398:PX4:H40	4:A:414:PX4:C16	0.42	2.45	6	1
4:A:384:PX4:H30	4:A:384:PX4:H57	0.42	1.91	7	1
4:A:370:PX4:H36	4:A:402:PX4:H40	0.42	1.92	8	1
4:A:331:PX4:H62	4:A:397:PX4:H59	0.42	1.92	10	1
4:A:333:PX4:O8	4:A:340:PX4:H15	0.42	2.15	11	1
4:A:338:PX4:H65	4:A:338:PX4:H58	0.42	1.68	13	1
4:A:367:PX4:O1	4:A:423:PX4:H3	0.42	2.15	2	1
4:A:354:PX4:H30	4:A:362:PX4:H17	0.42	1.90	3	1
4:A:372:PX4:H61	4:A:379:PX4:H59	0.42	1.91	3	1
4:A:353:PX4:H35	4:A:353:PX4:H41	0.42	1.58	4	1
4:A:375:PX4:H3	4:A:429:PX4:H17	0.42	1.91	4	1
4:A:382:PX4:H14	4:A:382:PX4:O6	0.42	2.14	4	1
4:A:337:PX4:H43	4:A:380:PX4:H39	0.42	1.91	6	1
4:A:324:PX4:H23	4:A:342:PX4:H55	0.42	1.91	7	1
4:A:388:PX4:H28	4:A:411:PX4:H16	0.42	1.91	7	1
4:A:363:PX4:H47	4:A:364:PX4:H33	0.42	1.91	9	1
4:A:395:PX4:H70	4:A:421:PX4:H58	0.42	1.91	10	1
4:A:403:PX4:H52	4:A:403:PX4:H47	0.42	1.50	11	1
4:A:408:PX4:H50	4:A:409:PX4:H19	0.42	1.92	11	1
4:A:308:PX4:H7	4:A:308:PX4:O3	0.42	2.15	12	1
4:A:318:PX4:H56	4:A:328:PX4:H33	0.42	1.90	12	1
4:A:335:PX4:H17	4:A:343:PX4:O1	0.42	2.15	12	1
4:A:317:PX4:H41	4:A:385:PX4:H65	0.42	1.92	13	1
4:A:325:PX4:H62	4:A:342:PX4:H70	0.42	1.90	13	1
4:A:332:PX4:H54	4:A:407:PX4:H70	0.42	1.90	13	1
4:A:391:PX4:H17	4:A:408:PX4:O5	0.42	2.15	13	1
4:A:424:PX4:H47	4:A:429:PX4:H19	0.42	1.91	1	1
4:A:372:PX4:H29	4:A:420:PX4:H26	0.42	1.91	2	1
4:A:306:PX4:H40	4:A:329:PX4:H40	0.42	1.91	3	1
4:A:316:PX4:H34	4:A:320:PX4:C19	0.42	2.43	3	1
4:A:376:PX4:H26	4:A:399:PX4:C25	0.42	2.45	4	1
4:A:333:PX4:H23	4:A:340:PX4:H24	0.42	1.91	5	1
4:A:364:PX4:H69	4:A:364:PX4:H62	0.42	1.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:334:PX4:C35	4:A:352:PX4:H32	0.42	2.45	6	1
4:A:350:PX4:H36	4:A:415:PX4:H71	0.42	1.92	6	1
4:A:383:PX4:H13	4:A:399:PX4:O1	0.42	2.15	6	1
4:A:395:PX4:H40	4:A:397:PX4:H65	0.42	1.92	6	1
4:A:398:PX4:H48	4:A:405:PX4:H49	0.42	1.92	6	1
4:A:373:PX4:H22	4:A:397:PX4:O3	0.42	2.14	7	1
4:A:322:PX4:C27	4:A:336:PX4:H32	0.42	2.45	10	1
4:A:354:PX4:H32	4:A:354:PX4:H25	0.42	1.63	10	1
4:A:388:PX4:H6	4:A:396:PX4:O8	0.42	2.15	12	1
4:A:413:PX4:H17	4:A:430:PX4:C8	0.42	2.45	12	1
4:A:424:PX4:H55	4:A:424:PX4:H48	0.42	1.64	13	1
4:A:308:PX4:H69	4:A:426:PX4:H70	0.42	1.91	14	1
4:A:371:PX4:O8	4:A:377:PX4:H3	0.41	2.15	1	1
4:A:378:PX4:H28	4:A:420:PX4:H57	0.41	1.92	1	1
4:A:398:PX4:H51	4:A:405:PX4:C23	0.41	2.45	4	1
4:A:405:PX4:H58	4:A:414:PX4:H26	0.41	1.91	4	1
4:A:318:PX4:H39	4:A:359:PX4:H36	0.41	1.92	5	1
4:A:393:PX4:H10	4:A:393:PX4:O6	0.41	2.14	9	1
4:A:340:PX4:H35	4:A:397:PX4:H60	0.41	1.91	10	1
4:A:363:PX4:H57	4:A:363:PX4:H62	0.41	1.56	10	1
4:A:389:PX4:H68	4:A:390:PX4:H38	0.41	1.92	10	1
4:A:369:PX4:C19	4:A:416:PX4:H63	0.41	2.45	11	1
4:A:410:PX4:H57	4:A:417:PX4:H69	0.41	1.91	11	1
4:A:308:PX4:H41	4:A:410:PX4:H45	0.41	1.91	12	1
4:A:423:PX4:H40	4:A:430:PX4:H36	0.41	1.92	12	1
4:A:322:PX4:H37	4:A:361:PX4:H25	0.41	1.91	13	1
4:A:346:PX4:H24	4:A:360:PX4:H55	0.41	1.92	14	1
4:A:403:PX4:H48	4:A:419:PX4:H9	0.41	1.91	14	1
4:A:309:PX4:H23	4:A:320:PX4:H49	0.41	1.92	1	1
4:A:410:PX4:H14	4:A:418:PX4:H40	0.41	1.92	1	1
4:A:349:PX4:H27	4:A:356:PX4:H30	0.41	1.92	3	1
4:A:308:PX4:H32	4:A:364:PX4:H52	0.41	1.91	4	1
4:A:345:PX4:H68	4:A:345:PX4:H45	0.41	1.91	4	1
4:A:403:PX4:H49	4:A:404:PX4:H28	0.41	1.90	5	1
4:A:347:PX4:H20	4:A:348:PX4:O3	0.41	2.14	6	1
4:A:416:PX4:H22	4:A:425:PX4:H50	0.41	1.92	6	1
4:A:421:PX4:H35	4:A:430:PX4:H48	0.41	1.92	6	1
4:A:378:PX4:H47	4:A:410:PX4:H19	0.41	1.93	7	1
4:A:308:PX4:H68	4:A:308:PX4:H63	0.41	1.64	11	1
4:A:335:PX4:H39	4:A:344:PX4:H39	0.41	1.92	11	1
4:A:337:PX4:H5	4:A:337:PX4:H25	0.41	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:H39	4:A:420:PX4:H34	0.41	1.92	12	1
4:A:308:PX4:H67	4:A:359:PX4:H70	0.41	1.91	13	1
4:A:352:PX4:H38	4:A:352:PX4:H31	0.41	1.60	14	1
4:A:398:PX4:H63	4:A:398:PX4:H68	0.41	1.73	14	1
4:A:313:PX4:H62	4:A:329:PX4:H32	0.41	1.90	1	1
4:A:383:PX4:O6	4:A:392:PX4:H3	0.41	2.14	1	1
4:A:314:PX4:H34	4:A:356:PX4:H41	0.41	1.91	8	1
4:A:373:PX4:H66	4:A:381:PX4:H44	0.41	1.92	10	1
4:A:421:PX4:H34	4:A:423:PX4:H23	0.41	1.93	12	1
4:A:322:PX4:H17	4:A:361:PX4:H56	0.41	1.92	13	1
4:A:376:PX4:H65	4:A:392:PX4:H35	0.41	1.92	14	1
4:A:368:PX4:H46	4:A:429:PX4:H20	0.41	1.90	1	1
4:A:367:PX4:H20	4:A:424:PX4:H22	0.41	1.93	2	1
4:A:331:PX4:H8	4:A:340:PX4:O1	0.41	2.14	3	1
4:A:378:PX4:H35	4:A:378:PX4:H42	0.41	1.61	3	1
4:A:389:PX4:H60	4:A:398:PX4:H17	0.41	1.93	5	1
4:A:393:PX4:H16	4:A:401:PX4:H18	0.41	1.91	5	1
4:A:337:PX4:H24	4:A:346:PX4:H69	0.41	1.91	6	1
4:A:346:PX4:H27	4:A:353:PX4:H58	0.41	1.93	6	1
4:A:347:PX4:H68	4:A:390:PX4:H39	0.41	1.92	6	1
4:A:352:PX4:H13	4:A:352:PX4:H2	0.41	1.76	6	1
4:A:348:PX4:H37	4:A:357:PX4:H36	0.41	1.92	7	1
4:A:421:PX4:H41	4:A:423:PX4:H35	0.41	1.91	7	1
4:A:316:PX4:O2	4:A:364:PX4:H11	0.41	2.15	8	1
4:A:380:PX4:H25	4:A:380:PX4:H59	0.41	1.91	8	1
4:A:403:PX4:H26	4:A:404:PX4:H21	0.41	1.92	8	1
4:A:366:PX4:H55	4:A:366:PX4:H60	0.41	1.70	9	1
4:A:372:PX4:O2	4:A:420:PX4:H9	0.41	2.15	9	1
4:A:420:PX4:H50	4:A:420:PX4:H57	0.41	1.68	9	1
4:A:341:PX4:H29	4:A:341:PX4:H24	0.41	1.63	10	1
4:A:367:PX4:H63	4:A:367:PX4:H68	0.41	1.51	14	1
4:A:407:PX4:H29	4:A:408:PX4:H41	0.41	1.90	14	1
4:A:413:PX4:H9	4:A:430:PX4:O1	0.41	2.16	2	1
4:A:314:PX4:H41	4:A:314:PX4:H35	0.41	1.64	3	1
4:A:359:PX4:H53	4:A:359:PX4:H47	0.41	1.64	3	1
4:A:369:PX4:O1	4:A:425:PX4:H1	0.41	2.15	4	1
4:A:405:PX4:H48	4:A:406:PX4:H52	0.41	1.92	4	1
1:A:244:ASP:OD1	4:A:349:PX4:H3	0.41	2.15	5	1
4:A:325:PX4:H27	4:A:334:PX4:H21	0.41	1.93	5	1
4:A:406:PX4:H34	4:A:406:PX4:H39	0.41	1.55	7	1
1:A:214:LEU:HD22	1:A:243:VAL:CG2	0.41	2.45	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:347:PX4:O1	4:A:348:PX4:H3	0.41	2.15	8	1
4:A:362:PX4:H21	4:A:362:PX4:H28	0.41	1.65	8	1
4:A:337:PX4:H61	4:A:353:PX4:H48	0.41	1.93	9	1
4:A:340:PX4:H43	4:A:389:PX4:H27	0.41	1.93	12	1
4:A:423:PX4:H36	4:A:423:PX4:H42	0.41	1.54	12	1
4:A:306:PX4:H37	4:A:367:PX4:H72	0.41	1.92	14	1
4:A:332:PX4:H38	4:A:407:PX4:H61	0.41	1.93	14	1
4:A:392:PX4:H56	4:A:392:PX4:H63	0.41	1.65	14	1
4:A:321:PX4:H61	4:A:361:PX4:H57	0.41	1.93	1	1
4:A:308:PX4:H14	4:A:311:PX4:H16	0.41	1.92	2	1
4:A:408:PX4:H32	4:A:415:PX4:H42	0.41	1.92	2	1
4:A:345:PX4:O4	4:A:346:PX4:H10	0.41	2.15	3	1
4:A:308:PX4:H72	4:A:308:PX4:H65	0.41	1.59	4	1
4:A:369:PX4:O1	4:A:425:PX4:H13	0.41	2.16	4	1
1:A:138:PHE:CD1	1:A:149:PHE:CD1	0.41	3.08	6	2
4:A:385:PX4:H67	4:A:392:PX4:H26	0.41	1.90	5	1
4:A:383:PX4:H65	4:A:407:PX4:H27	0.41	1.92	6	1
4:A:367:PX4:H60	4:A:429:PX4:H41	0.41	1.91	8	1
4:A:420:PX4:H67	4:A:426:PX4:H38	0.41	1.92	8	1
4:A:360:PX4:H30	4:A:366:PX4:H61	0.41	1.91	9	1
4:A:398:PX4:H42	4:A:408:PX4:H26	0.41	1.92	9	1
4:A:355:PX4:H30	4:A:356:PX4:H51	0.41	1.91	10	1
4:A:350:PX4:H60	4:A:400:PX4:H44	0.41	1.93	11	1
4:A:418:PX4:H72	4:A:418:PX4:H64	0.41	1.59	12	1
4:A:388:PX4:H3	4:A:395:PX4:O1	0.41	2.15	13	1
4:A:337:PX4:H65	4:A:345:PX4:H71	0.41	1.92	14	1
4:A:338:PX4:H63	4:A:338:PX4:H68	0.41	1.58	14	1
4:A:344:PX4:H49	4:A:344:PX4:H54	0.41	1.71	14	1
4:A:308:PX4:H23	4:A:311:PX4:H54	0.41	1.92	1	1
4:A:311:PX4:H17	4:A:359:PX4:H50	0.41	1.93	2	1
4:A:382:PX4:H29	4:A:382:PX4:H36	0.41	1.73	2	1
4:A:409:PX4:H37	4:A:410:PX4:H53	0.41	1.93	3	1
4:A:323:PX4:H19	4:A:333:PX4:H47	0.41	1.92	4	1
4:A:363:PX4:H38	4:A:365:PX4:H30	0.41	1.92	4	1
4:A:391:PX4:H54	4:A:391:PX4:H48	0.41	1.60	4	1
4:A:416:PX4:H40	4:A:421:PX4:H70	0.41	1.92	5	1
4:A:377:PX4:H44	4:A:377:PX4:H38	0.41	1.75	6	1
4:A:395:PX4:H56	4:A:402:PX4:H50	0.41	1.91	6	1
4:A:319:PX4:H60	4:A:324:PX4:H59	0.41	1.92	7	1
4:A:380:PX4:H59	4:A:388:PX4:H40	0.41	1.91	7	1
4:A:381:PX4:H42	4:A:381:PX4:H60	0.41	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H45	4:A:338:PX4:H38	0.41	1.58	11	1
4:A:392:PX4:H72	4:A:392:PX4:H65	0.41	1.73	14	1
4:A:415:PX4:H55	4:A:421:PX4:H56	0.41	1.93	2	1
4:A:307:PX4:H10	4:A:322:PX4:O8	0.41	2.16	4	1
4:A:428:PX4:H44	4:A:428:PX4:H38	0.41	1.78	4	1
4:A:395:PX4:H54	4:A:395:PX4:H61	0.41	1.72	5	1
4:A:388:PX4:H39	4:A:388:PX4:H34	0.41	1.63	6	1
4:A:421:PX4:H59	4:A:421:PX4:H52	0.41	1.65	6	1
4:A:332:PX4:H14	4:A:356:PX4:H9	0.41	1.92	7	1
4:A:352:PX4:H16	4:A:358:PX4:H47	0.41	1.93	8	1
4:A:407:PX4:H17	4:A:414:PX4:O8	0.41	2.16	10	1
4:A:309:PX4:O8	4:A:316:PX4:H46	0.41	2.16	11	1
4:A:367:PX4:H42	4:A:423:PX4:H36	0.41	1.90	11	1
4:A:307:PX4:H46	4:A:307:PX4:H16	0.41	1.69	12	1
4:A:349:PX4:H45	4:A:355:PX4:H45	0.41	1.93	13	1
4:A:378:PX4:H63	4:A:418:PX4:H62	0.41	1.93	13	1
4:A:398:PX4:H21	4:A:407:PX4:H22	0.41	1.93	13	1
4:A:400:PX4:H56	4:A:409:PX4:H34	0.41	1.93	13	1
4:A:328:PX4:H25	4:A:328:PX4:H20	0.41	1.67	14	1
4:A:306:PX4:H56	4:A:354:PX4:C13	0.41	2.46	1	1
4:A:330:PX4:H16	4:A:343:PX4:H2	0.41	1.93	1	1
4:A:345:PX4:H69	4:A:388:PX4:H35	0.41	1.92	1	1
4:A:348:PX4:H63	4:A:348:PX4:H68	0.41	1.63	1	1
4:A:314:PX4:H47	4:A:350:PX4:H37	0.41	1.91	2	1
4:A:337:PX4:H45	4:A:338:PX4:H56	0.41	1.93	2	1
4:A:375:PX4:H60	4:A:375:PX4:H67	0.41	1.66	2	1
4:A:376:PX4:H46	4:A:384:PX4:H3	0.41	1.93	2	1
4:A:404:PX4:H59	4:A:404:PX4:H52	0.41	1.53	2	1
4:A:312:PX4:H39	4:A:365:PX4:H37	0.41	1.93	3	1
4:A:358:PX4:H35	4:A:365:PX4:H31	0.41	1.91	3	1
4:A:363:PX4:H60	4:A:363:PX4:H55	0.41	1.65	3	1
4:A:375:PX4:H18	4:A:382:PX4:O6	0.41	2.16	3	1
4:A:306:PX4:O2	4:A:329:PX4:H12	0.41	2.15	4	1
4:A:314:PX4:H42	4:A:362:PX4:H21	0.41	1.91	4	1
4:A:316:PX4:H26	4:A:364:PX4:H47	0.41	1.92	5	1
4:A:326:PX4:H29	4:A:350:PX4:H51	0.41	1.92	5	1
4:A:345:PX4:H17	4:A:346:PX4:H6	0.41	1.93	5	1
4:A:415:PX4:H5	4:A:421:PX4:H14	0.41	1.92	5	1
4:A:375:PX4:H47	4:A:429:PX4:H40	0.41	1.92	6	1
4:A:404:PX4:H63	4:A:404:PX4:H68	0.41	1.65	7	1
4:A:372:PX4:H47	4:A:372:PX4:H52	0.41	1.71	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:423:PX4:H4	4:A:430:PX4:O8	0.41	2.16	8	1
4:A:315:PX4:H24	4:A:322:PX4:H36	0.41	1.92	9	1
4:A:363:PX4:H28	4:A:365:PX4:H21	0.41	1.92	9	1
4:A:391:PX4:H47	4:A:408:PX4:H16	0.41	1.93	9	1
4:A:416:PX4:H48	4:A:425:PX4:H53	0.41	1.92	9	1
4:A:429:PX4:H33	4:A:429:PX4:C27	0.41	2.46	9	1
4:A:366:PX4:H68	4:A:419:PX4:H38	0.41	1.93	10	1
4:A:335:PX4:H23	4:A:343:PX4:H53	0.41	1.91	12	1
4:A:383:PX4:H20	4:A:392:PX4:C14	0.41	2.46	12	1
4:A:390:PX4:H63	4:A:397:PX4:H40	0.41	1.92	12	1
4:A:307:PX4:H41	4:A:361:PX4:H42	0.41	1.92	13	1
4:A:325:PX4:H9	4:A:341:PX4:O6	0.41	2.15	13	1
4:A:338:PX4:H62	4:A:362:PX4:H62	0.41	1.93	13	1
4:A:331:PX4:H7	4:A:331:PX4:O6	0.41	2.16	14	1
4:A:424:PX4:H25	4:A:424:PX4:H32	0.41	1.37	14	1
4:A:326:PX4:H27	4:A:350:PX4:H21	0.41	1.92	3	1
4:A:325:PX4:H45	4:A:334:PX4:H40	0.41	1.93	4	1
4:A:341:PX4:H32	4:A:383:PX4:H70	0.41	1.93	6	1
4:A:330:PX4:C3	4:A:330:PX4:H19	0.41	2.46	7	1
4:A:332:PX4:O3	4:A:356:PX4:H4	0.41	2.16	7	1
4:A:354:PX4:H21	4:A:362:PX4:C5	0.41	2.46	7	1
4:A:309:PX4:H27	4:A:318:PX4:H28	0.41	1.93	8	1
4:A:382:PX4:H67	4:A:428:PX4:H20	0.41	1.93	9	1
4:A:388:PX4:H15	4:A:396:PX4:H18	0.41	1.92	9	1
4:A:424:PX4:H56	4:A:425:PX4:H31	0.41	1.93	9	1
4:A:349:PX4:H66	4:A:349:PX4:H60	0.41	1.58	10	1
4:A:388:PX4:H51	4:A:396:PX4:C25	0.41	2.45	10	1
4:A:353:PX4:H31	4:A:366:PX4:H25	0.41	1.93	11	1
4:A:311:PX4:H71	4:A:316:PX4:H38	0.41	1.93	12	1
4:A:369:PX4:H71	4:A:369:PX4:H65	0.41	1.47	12	1
4:A:319:PX4:H19	4:A:342:PX4:H50	0.41	1.92	14	1
4:A:326:PX4:H64	4:A:391:PX4:H43	0.41	1.92	14	1
4:A:345:PX4:H4	4:A:353:PX4:O4	0.41	2.16	14	1
4:A:405:PX4:H45	4:A:405:PX4:H37	0.41	1.61	14	1
4:A:387:PX4:H31	4:A:387:PX4:H38	0.40	1.72	1	1
4:A:403:PX4:O8	4:A:419:PX4:H8	0.40	2.15	1	1
4:A:316:PX4:O4	4:A:364:PX4:H5	0.40	2.16	2	1
4:A:314:PX4:H59	4:A:314:PX4:H64	0.40	1.39	4	1
4:A:334:PX4:H65	4:A:363:PX4:H69	0.40	1.93	4	1
4:A:350:PX4:H56	4:A:363:PX4:H52	0.40	1.92	4	1
4:A:371:PX4:H65	4:A:417:PX4:H65	0.40	1.92	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:214:LEU:HD23	1:A:214:LEU:H	0.40	1.75	6	1
4:A:358:PX4:H27	4:A:364:PX4:H42	0.40	1.92	6	1
4:A:366:PX4:H41	4:A:366:PX4:H36	0.40	1.64	7	1
4:A:416:PX4:H35	4:A:421:PX4:H66	0.40	1.92	8	1
4:A:313:PX4:H18	4:A:318:PX4:C24	0.40	2.36	9	1
4:A:389:PX4:H61	4:A:389:PX4:H66	0.40	1.60	10	1
4:A:384:PX4:H46	4:A:386:PX4:H49	0.40	1.93	11	1
4:A:326:PX4:H55	4:A:326:PX4:H60	0.40	1.78	12	1
4:A:380:PX4:H31	4:A:381:PX4:H60	0.40	1.92	12	1
4:A:427:PX4:H37	4:A:427:PX4:H32	0.40	1.63	12	1
4:A:322:PX4:H69	4:A:322:PX4:H62	0.40	1.62	13	1
4:A:378:PX4:H17	4:A:410:PX4:O6	0.40	2.15	13	1
4:A:384:PX4:H17	4:A:385:PX4:H20	0.40	1.93	13	1
4:A:313:PX4:H15	4:A:360:PX4:O6	0.40	2.16	14	1
4:A:404:PX4:H8	4:A:412:PX4:O6	0.40	2.17	14	1
4:A:315:PX4:H43	4:A:425:PX4:H32	0.40	1.92	2	1
4:A:308:PX4:H41	4:A:316:PX4:H39	0.40	1.92	3	1
4:A:419:PX4:H71	4:A:427:PX4:H64	0.40	1.93	3	1
4:A:323:PX4:H58	4:A:323:PX4:H65	0.40	1.68	5	1
4:A:377:PX4:H62	4:A:416:PX4:H55	0.40	1.92	6	1
4:A:330:PX4:H14	4:A:338:PX4:H19	0.40	1.91	7	1
4:A:334:PX4:H59	4:A:334:PX4:H64	0.40	1.36	8	1
4:A:308:PX4:H51	4:A:363:PX4:H19	0.40	1.92	10	1
4:A:308:PX4:H25	4:A:311:PX4:H23	0.40	1.93	10	1
4:A:368:PX4:H20	4:A:377:PX4:H57	0.40	1.92	11	1
4:A:428:PX4:H65	4:A:430:PX4:H48	0.40	1.93	11	1
4:A:327:PX4:H43	4:A:374:PX4:H66	0.40	1.93	12	1
4:A:332:PX4:H45	4:A:407:PX4:H53	0.40	1.93	13	1
4:A:389:PX4:H52	4:A:389:PX4:H59	0.40	1.59	13	1
4:A:391:PX4:H31	4:A:408:PX4:H23	0.40	1.91	13	1
4:A:352:PX4:H15	4:A:352:PX4:H7	0.40	1.93	14	1
4:A:321:PX4:H45	4:A:360:PX4:H69	0.40	1.93	1	1
4:A:323:PX4:H14	4:A:323:PX4:H9	0.40	1.92	4	1
4:A:372:PX4:H38	4:A:372:PX4:H32	0.40	1.63	5	1
4:A:401:PX4:H44	4:A:401:PX4:H38	0.40	1.72	6	1
4:A:319:PX4:O2	4:A:324:PX4:H4	0.40	2.16	7	1
4:A:317:PX4:O5	4:A:351:PX4:H23	0.40	2.17	8	1
4:A:405:PX4:H58	4:A:414:PX4:H30	0.40	1.93	8	1
1:A:109:TRP:CH2	1:A:158:ASP:HB3	0.40	2.51	11	1
4:A:348:PX4:H56	4:A:355:PX4:H72	0.40	1.93	11	1
4:A:383:PX4:H55	4:A:399:PX4:H17	0.40	1.92	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:404:PX4:H2	4:A:412:PX4:O1	0.40	2.16	13	1
4:A:417:PX4:H65	4:A:417:PX4:H58	0.40	1.62	14	1
4:A:410:PX4:H61	4:A:410:PX4:H40	0.40	1.92	2	1
4:A:326:PX4:H34	4:A:406:PX4:H36	0.40	1.93	3	1
4:A:345:PX4:H33	4:A:353:PX4:H61	0.40	1.94	5	1
4:A:416:PX4:H47	4:A:416:PX4:H52	0.40	1.75	5	1
4:A:410:PX4:O2	4:A:416:PX4:H4	0.40	2.17	8	1
4:A:388:PX4:H25	4:A:388:PX4:H32	0.40	1.65	9	1
4:A:375:PX4:H32	4:A:375:PX4:H37	0.40	1.68	10	1
4:A:412:PX4:H16	4:A:428:PX4:H16	0.40	1.93	10	1
4:A:307:PX4:C12	4:A:314:PX4:H16	0.40	2.47	11	1
4:A:362:PX4:H54	4:A:362:PX4:H60	0.40	1.39	11	1
4:A:381:PX4:H10	4:A:381:PX4:H14	0.40	1.93	11	1
4:A:321:PX4:H68	4:A:321:PX4:H63	0.40	1.68	12	1
4:A:402:PX4:H34	4:A:402:PX4:H39	0.40	1.45	12	1
4:A:336:PX4:H28	4:A:361:PX4:H63	0.40	1.93	13	1
4:A:378:PX4:H67	4:A:418:PX4:H66	0.40	1.93	13	1
4:A:378:PX4:H47	4:A:418:PX4:H46	0.40	1.92	13	1
4:A:380:PX4:H20	4:A:381:PX4:H6	0.40	1.93	13	1
4:A:395:PX4:H15	4:A:396:PX4:H15	0.40	1.93	13	1
4:A:394:PX4:H65	4:A:394:PX4:H71	0.40	1.66	14	1
4:A:364:PX4:H32	4:A:364:PX4:H25	0.40	1.68	1	1
4:A:380:PX4:H28	4:A:380:PX4:H33	0.40	1.75	1	1
4:A:345:PX4:H17	4:A:346:PX4:H10	0.40	1.91	2	1
4:A:374:PX4:H34	4:A:374:PX4:H27	0.40	1.72	3	1
4:A:320:PX4:H20	4:A:359:PX4:H58	0.40	1.94	4	1
4:A:316:PX4:H60	4:A:320:PX4:H36	0.40	1.93	5	1
4:A:344:PX4:H38	4:A:347:PX4:H38	0.40	1.93	5	1
4:A:429:PX4:H29	4:A:429:PX4:H53	0.40	1.93	5	1
4:A:319:PX4:H44	4:A:319:PX4:H38	0.40	1.70	6	1
4:A:353:PX4:H35	4:A:353:PX4:H30	0.40	1.62	7	1
4:A:385:PX4:O1	4:A:392:PX4:H8	0.40	2.17	8	1
4:A:319:PX4:H58	4:A:324:PX4:H30	0.40	1.94	11	1
4:A:332:PX4:H39	4:A:334:PX4:H57	0.40	1.92	11	1
4:A:398:PX4:H60	4:A:405:PX4:H29	0.40	1.94	13	1
4:A:355:PX4:C10	4:A:362:PX4:H51	0.40	2.47	14	1
4:A:374:PX4:H20	4:A:374:PX4:H25	0.40	1.49	14	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	158/164 (96%)	145±3 (92±2%)	12±3 (8±2%)	1±1 (1±0%)	24	72
All	All	2212/2296 (96%)	2030 (92%)	168 (8%)	14 (1%)	24	72

All 7 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	171	PHE	5
1	A	175	ASP	3
1	A	107	PRO	2
1	A	183	HIS	1
1	A	146	PRO	1
1	A	179	GLY	1
1	A	213	PHE	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/131 (98%)	123±2 (95±2%)	6±2 (5±2%)	24	77
All	All	1806/1834 (98%)	1720 (95%)	86 (5%)	24	77

All 27 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	101	ARG	14
1	A	244	ASP	14
1	A	199	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	243	VAL	5
1	A	214	LEU	4
1	A	222	HIS	4
1	A	175	ASP	4
1	A	115	THR	3
1	A	162	VAL	3
1	A	142	SER	3
1	A	103	MET	3
1	A	249	ARG	2
1	A	170	ASP	2
1	A	258	ILE	2
1	A	140	VAL	2
1	A	198	ASP	2
1	A	134	ILE	1
1	A	205	THR	1
1	A	122	THR	1
1	A	146	PRO	1
1	A	127	ARG	1
1	A	128	GLU	1
1	A	161	VAL	1
1	A	168	HIS	1
1	A	108	VAL	1
1	A	143	ASN	1
1	A	156	MET	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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	337	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.65±0.02	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	378	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	323	-	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	349	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.65±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	341	-	45,45,45	0.65±0.03	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.65±0.03	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	398	-	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	384	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	328	-	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	429	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.64±0.03	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	331	-	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	411	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.65±0.02	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	337	-	51,53,53	1.46±0.18	8±2 (16±3%)
4	PX4	A	385	-	51,53,53	1.53±0.16	8±2 (16±4%)
4	PX4	A	418	-	51,53,53	1.50±0.15	8±2 (16±3%)
4	PX4	A	395	-	51,53,53	1.51±0.13	9±2 (18±4%)
4	PX4	A	312	-	51,53,53	1.48±0.16	8±2 (16±4%)
4	PX4	A	419	-	51,53,53	1.53±0.11	10±3 (19±5%)
4	PX4	A	393	-	51,53,53	1.56±0.12	9±2 (17±4%)
4	PX4	A	347	-	51,53,53	1.50±0.19	9±3 (18±6%)
4	PX4	A	402	-	51,53,53	1.45±0.13	8±2 (15±4%)
4	PX4	A	378	-	51,53,53	1.45±0.16	8±2 (15±4%)
4	PX4	A	309	-	51,53,53	1.52±0.14	9±2 (18±3%)
4	PX4	A	327	-	51,53,53	1.55±0.11	9±2 (18±3%)
4	PX4	A	356	-	51,53,53	1.49±0.19	8±2 (15±4%)
4	PX4	A	369	-	51,53,53	1.41±0.14	8±2 (15±4%)
4	PX4	A	396	-	51,53,53	1.54±0.17	9±2 (17±3%)
4	PX4	A	374	-	51,53,53	1.48±0.15	9±3 (17±5%)
4	PX4	A	389	-	51,53,53	1.54±0.15	9±2 (17±4%)
4	PX4	A	416	-	51,53,53	1.49±0.16	9±3 (17±6%)
4	PX4	A	388	-	51,53,53	1.45±0.12	8±2 (16±3%)
4	PX4	A	361	-	51,53,53	1.54±0.11	9±2 (17±4%)
4	PX4	A	348	-	51,53,53	1.49±0.15	9±2 (17±4%)
4	PX4	A	428	-	51,53,53	1.55±0.10	9±2 (17±4%)
4	PX4	A	371	-	51,53,53	1.70±0.16	11±2 (22±3%)
4	PX4	A	310	-	51,53,53	1.49±0.15	9±2 (16±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	417	-	51,53,53	1.54±0.16	9±2 (18±3%)
4	PX4	A	405	-	51,53,53	1.52±0.14	10±2 (19±4%)
4	PX4	A	311	-	51,53,53	1.54±0.20	9±2 (18±4%)
4	PX4	A	387	-	51,53,53	1.54±0.16	10±3 (18±5%)
4	PX4	A	315	-	51,53,53	1.44±0.12	8±2 (16±4%)
4	PX4	A	317	-	51,53,53	1.44±0.14	8±3 (16±5%)
4	PX4	A	403	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	427	-	51,53,53	1.63±0.19	10±3 (19±6%)
4	PX4	A	323	-	51,53,53	1.45±0.17	9±2 (16±3%)
4	PX4	A	423	-	51,53,53	1.48±0.13	8±2 (15±3%)
4	PX4	A	349	-	51,53,53	1.54±0.11	9±2 (18±3%)
4	PX4	A	425	-	51,53,53	1.47±0.11	9±3 (17±4%)
4	PX4	A	341	-	51,53,53	1.50±0.14	10±2 (18±3%)
4	PX4	A	424	-	51,53,53	1.44±0.17	8±2 (16±4%)
4	PX4	A	340	-	51,53,53	1.57±0.09	11±1 (20±2%)
4	PX4	A	394	-	51,53,53	1.50±0.15	9±2 (17±4%)
4	PX4	A	321	-	51,53,53	1.44±0.14	9±2 (17±4%)
4	PX4	A	306	-	51,53,53	1.48±0.07	10±2 (19±3%)
4	PX4	A	322	-	51,53,53	1.51±0.17	10±3 (19±6%)
4	PX4	A	380	-	51,53,53	1.47±0.14	8±2 (16±3%)
4	PX4	A	399	-	51,53,53	1.47±0.16	9±2 (18±4%)
4	PX4	A	407	-	51,53,53	1.46±0.17	8±3 (16±5%)
4	PX4	A	351	-	51,53,53	1.50±0.14	8±2 (16±4%)
4	PX4	A	343	-	51,53,53	1.49±0.17	8±3 (16±5%)
4	PX4	A	358	-	51,53,53	1.48±0.14	9±2 (16±4%)
4	PX4	A	415	-	51,53,53	1.57±0.16	10±2 (19±3%)
4	PX4	A	334	-	51,53,53	1.51±0.12	9±2 (17±4%)
4	PX4	A	354	-	51,53,53	1.57±0.15	10±3 (18±5%)
4	PX4	A	391	-	51,53,53	1.52±0.16	9±2 (16±3%)
4	PX4	A	318	-	51,53,53	1.47±0.15	8±2 (16±3%)
4	PX4	A	335	-	51,53,53	1.47±0.14	9±2 (17±4%)
4	PX4	A	345	-	51,53,53	1.46±0.17	8±2 (16±4%)
4	PX4	A	372	-	51,53,53	1.47±0.17	9±2 (17±3%)
4	PX4	A	377	-	51,53,53	1.53±0.19	8±2 (15±4%)
4	PX4	A	422	-	51,53,53	1.50±0.13	9±2 (16±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	401	-	51,53,53	1.58±0.15	10±2 (20±3%)
4	PX4	A	373	-	51,53,53	1.60±0.17	11±3 (20±5%)
4	PX4	A	357	-	51,53,53	1.50±0.14	9±3 (18±5%)
4	PX4	A	316	-	51,53,53	1.44±0.10	8±2 (14±4%)
4	PX4	A	365	-	51,53,53	1.49±0.12	8±2 (16±4%)
4	PX4	A	397	-	51,53,53	1.53±0.18	9±3 (17±5%)
4	PX4	A	382	-	51,53,53	1.47±0.16	8±2 (16±3%)
4	PX4	A	413	-	51,53,53	1.51±0.12	9±2 (16±4%)
4	PX4	A	326	-	51,53,53	1.48±0.17	8±2 (16±4%)
4	PX4	A	379	-	51,53,53	1.56±0.13	10±2 (19±4%)
4	PX4	A	430	-	51,53,53	1.57±0.13	10±1 (19±2%)
4	PX4	A	367	-	51,53,53	1.50±0.18	8±3 (15±6%)
4	PX4	A	308	-	51,53,53	1.52±0.14	9±2 (18±4%)
4	PX4	A	410	-	51,53,53	1.50±0.17	9±2 (17±3%)
4	PX4	A	320	-	51,53,53	1.47±0.14	8±2 (16±3%)
4	PX4	A	421	-	51,53,53	1.47±0.13	9±1 (17±2%)
4	PX4	A	370	-	51,53,53	1.48±0.13	9±2 (17±3%)
4	PX4	A	352	-	51,53,53	1.49±0.13	9±3 (17±4%)
4	PX4	A	333	-	51,53,53	1.50±0.15	8±2 (16±4%)
4	PX4	A	398	-	51,53,53	1.48±0.16	9±2 (17±3%)
4	PX4	A	384	-	51,53,53	1.50±0.20	9±2 (16±4%)
4	PX4	A	355	-	51,53,53	1.50±0.12	9±2 (18±3%)
4	PX4	A	420	-	51,53,53	1.50±0.12	9±2 (18±3%)
4	PX4	A	330	-	51,53,53	1.49±0.12	9±2 (17±3%)
4	PX4	A	342	-	51,53,53	1.53±0.12	9±3 (18±5%)
4	PX4	A	412	-	51,53,53	1.42±0.13	8±3 (15±5%)
4	PX4	A	364	-	51,53,53	1.54±0.19	10±3 (18±5%)
4	PX4	A	404	-	51,53,53	1.55±0.14	9±2 (18±3%)
4	PX4	A	353	-	51,53,53	1.51±0.11	8±3 (15±5%)
4	PX4	A	313	-	51,53,53	1.52±0.14	9±3 (17±5%)
4	PX4	A	363	-	51,53,53	1.47±0.14	8±1 (15±2%)
4	PX4	A	414	-	51,53,53	1.55±0.14	9±2 (18±4%)
4	PX4	A	325	-	51,53,53	1.52±0.14	10±2 (19±3%)
4	PX4	A	383	-	51,53,53	1.43±0.10	8±2 (15±3%)
4	PX4	A	366	-	51,53,53	1.53±0.12	10±2 (19±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	375	-	51,53,53	1.52±0.14	9±2 (18±2%)
4	PX4	A	314	-	51,53,53	1.48±0.17	9±3 (17±5%)
4	PX4	A	324	-	51,53,53	1.46±0.15	8±3 (15±4%)
4	PX4	A	350	-	51,53,53	1.42±0.10	8±2 (14±3%)
4	PX4	A	406	-	51,53,53	1.46±0.13	8±2 (16±4%)
4	PX4	A	376	-	51,53,53	1.50±0.17	10±3 (18±6%)
4	PX4	A	329	-	51,53,53	1.51±0.12	10±3 (18±5%)
4	PX4	A	339	-	51,53,53	1.46±0.21	8±3 (15±6%)
4	PX4	A	338	-	51,53,53	1.55±0.14	10±3 (19±5%)
4	PX4	A	400	-	51,53,53	1.50±0.19	9±2 (17±4%)
4	PX4	A	408	-	51,53,53	1.51±0.14	9±2 (18±3%)
4	PX4	A	426	-	51,53,53	1.47±0.14	8±2 (16±3%)
4	PX4	A	346	-	51,53,53	1.49±0.15	9±2 (16±4%)
4	PX4	A	319	-	51,53,53	1.52±0.14	9±2 (17±3%)
4	PX4	A	328	-	51,53,53	1.52±0.14	9±2 (18±4%)
4	PX4	A	368	-	51,53,53	1.50±0.13	9±3 (17±5%)
4	PX4	A	429	-	51,53,53	1.49±0.18	8±3 (16±5%)
4	PX4	A	332	-	51,53,53	1.48±0.13	9±2 (17±4%)
4	PX4	A	359	-	51,53,53	1.53±0.14	9±2 (17±4%)
4	PX4	A	390	-	51,53,53	1.48±0.13	9±2 (17±3%)
4	PX4	A	381	-	51,53,53	1.58±0.13	10±2 (19±4%)
4	PX4	A	344	-	51,53,53	1.53±0.14	9±2 (18±4%)
4	PX4	A	307	-	51,53,53	1.58±0.19	9±3 (18±6%)
4	PX4	A	409	-	51,53,53	1.52±0.10	10±2 (19±3%)
4	PX4	A	386	-	51,53,53	1.49±0.15	9±2 (17±4%)
4	PX4	A	336	-	51,53,53	1.50±0.17	10±3 (18±5%)
4	PX4	A	362	-	51,53,53	1.49±0.07	9±2 (17±4%)
4	PX4	A	331	-	51,53,53	1.53±0.11	9±2 (18±4%)
4	PX4	A	411	-	51,53,53	1.49±0.08	9±2 (17±3%)
4	PX4	A	360	-	51,53,53	1.51±0.10	9±2 (18±2%)
4	PX4	A	392	-	51,53,53	1.53±0.12	9±3 (17±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	347	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	371	-	-	1±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	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	340	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	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	417	PX4	O7-C23-C24	7.54	127.78	111.48	6	10
4	A	413	PX4	C8-C7-C6	7.07	95.29	111.78	8	12
4	A	396	PX4	C8-C7-C6	7.01	95.44	111.78	3	11
4	A	427	PX4	C8-C7-C6	6.86	95.79	111.78	14	12
4	A	426	PX4	O7-C23-C24	6.84	126.28	111.48	7	8
4	A	385	PX4	O7-C23-C24	6.83	126.27	111.48	6	5
4	A	353	PX4	C8-C7-C6	6.73	96.10	111.78	11	11
4	A	376	PX4	C8-C7-C6	6.70	96.16	111.78	2	10
4	A	389	PX4	C8-C7-C6	6.67	96.24	111.78	10	7
4	A	349	PX4	O7-C23-C24	6.66	125.89	111.48	8	6
4	A	424	PX4	O7-C23-C24	6.63	125.82	111.48	7	8
4	A	397	PX4	O7-C23-C24	6.62	125.81	111.48	13	9
4	A	371	PX4	O7-C23-C24	6.56	125.67	111.48	3	14
4	A	427	PX4	O5-C8-C7	6.54	127.26	108.40	6	11
4	A	310	PX4	C8-C7-C6	6.51	96.60	111.78	3	9
4	A	367	PX4	O7-C23-C24	6.51	125.56	111.48	5	7
4	A	337	PX4	C7-O7-C23	6.47	133.29	117.80	12	5
4	A	428	PX4	C8-C7-C6	6.45	96.74	111.78	6	8
4	A	331	PX4	C8-C7-C6	6.42	96.81	111.78	12	12
4	A	401	PX4	C8-C7-C6	6.41	96.84	111.78	13	13
4	A	380	PX4	C8-C7-C6	6.37	96.92	111.78	14	6
4	A	397	PX4	C8-C7-C6	6.29	97.12	111.78	3	6
4	A	403	PX4	O3-P1-O2	6.26	84.12	108.94	2	6
4	A	317	PX4	C7-O7-C23	6.21	132.66	117.80	5	3
4	A	370	PX4	O5-C8-C7	6.18	126.20	108.40	1	10
4	A	361	PX4	C8-C7-C6	6.17	97.41	111.78	3	6
4	A	320	PX4	O5-C8-C7	6.14	126.09	108.40	7	12
4	A	388	PX4	O5-C8-C7	6.14	126.09	108.40	7	7
4	A	321	PX4	C8-C7-C6	6.14	97.48	111.78	13	9
4	A	312	PX4	O5-C8-C7	6.10	126.00	108.40	5	8
4	A	348	PX4	O7-C7-C8	6.09	130.20	108.34	6	7
4	A	359	PX4	O7-C23-C24	6.09	124.65	111.48	7	8
4	A	334	PX4	O5-C8-C7	6.08	125.92	108.40	4	10
4	A	382	PX4	C8-C7-C6	6.08	97.61	111.78	8	7
4	A	377	PX4	C8-C7-C6	6.07	97.62	111.78	14	8
4	A	345	PX4	C8-C7-C6	6.07	97.63	111.78	6	9
4	A	399	PX4	O7-C23-C24	6.03	124.53	111.48	10	9
4	A	389	PX4	O7-C23-C24	6.03	124.53	111.48	11	6
4	A	339	PX4	O7-C23-C24	6.02	124.50	111.48	3	8
4	A	427	PX4	O7-C23-C24	6.01	124.47	111.48	1	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	387	PX4	P1-O3-C1	6.00	92.70	121.26	5	11
4	A	403	PX4	C5-N1-C3	5.99	93.24	108.98	7	4
4	A	425	PX4	C8-C7-C6	5.97	97.86	111.78	14	8
4	A	414	PX4	C8-C7-C6	5.96	97.88	111.78	6	9
4	A	345	PX4	O5-C8-C7	5.94	125.52	108.40	7	5
4	A	380	PX4	O5-C8-C7	5.93	125.48	108.40	11	9
4	A	426	PX4	O7-C23-O8	5.91	109.89	123.70	7	4
4	A	318	PX4	C8-C7-C6	5.90	98.02	111.78	3	12
4	A	377	PX4	C7-O7-C23	5.87	131.83	117.80	4	2
4	A	415	PX4	C4-N1-C3	5.86	93.59	108.98	14	4
4	A	429	PX4	O5-C8-C7	5.85	125.26	108.40	5	6
4	A	401	PX4	C5-N1-C3	5.85	93.61	108.98	13	2
4	A	311	PX4	C8-C7-C6	5.84	98.17	111.78	8	8
4	A	326	PX4	O5-C8-C7	5.82	125.18	108.40	6	7
4	A	331	PX4	O7-C23-O8	5.82	110.10	123.70	8	7
4	A	430	PX4	C8-C7-C6	5.81	98.24	111.78	10	12
4	A	386	PX4	O7-C23-C24	5.81	124.04	111.48	8	8
4	A	341	PX4	O7-C23-C24	5.80	124.03	111.48	5	12
4	A	405	PX4	O5-C8-C7	5.79	125.09	108.40	11	9
4	A	335	PX4	O5-C8-C7	5.79	125.09	108.40	8	12
4	A	375	PX4	C8-C7-C6	5.77	98.33	111.78	1	9
4	A	418	PX4	O7-C23-C24	5.76	123.95	111.48	4	8
4	A	423	PX4	O5-C9-O6	5.76	109.23	123.63	4	4
4	A	390	PX4	O7-C23-C24	5.75	123.91	111.48	7	7
4	A	378	PX4	O3-P1-O2	5.74	86.18	108.94	4	3
4	A	327	PX4	O7-C23-C24	5.74	123.89	111.48	11	9
4	A	323	PX4	O7-C23-C24	5.73	123.88	111.48	8	8
4	A	379	PX4	C7-O7-C23	5.73	131.51	117.80	2	7
4	A	333	PX4	O5-C8-C7	5.71	124.85	108.40	13	9
4	A	356	PX4	O7-C23-C24	5.71	123.83	111.48	3	8
4	A	415	PX4	C8-C7-C6	5.71	98.48	111.78	3	10
4	A	311	PX4	C5-N1-C3	5.71	93.99	108.98	10	4
4	A	365	PX4	O5-C8-C7	5.69	124.81	108.40	6	11
4	A	363	PX4	O5-C8-C7	5.69	124.80	108.40	9	10
4	A	348	PX4	O7-C23-O8	5.68	110.43	123.70	5	6
4	A	363	PX4	C8-C7-C6	5.64	98.63	111.78	11	9
4	A	413	PX4	O5-C8-C7	5.64	124.65	108.40	10	10
4	A	339	PX4	O5-C8-C7	5.63	124.64	108.40	5	5
4	A	327	PX4	C7-O7-C23	5.63	131.26	117.80	6	5
4	A	390	PX4	O5-C8-C7	5.63	124.61	108.40	6	6
4	A	307	PX4	O7-C23-C24	5.62	123.64	111.48	9	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PX4	P1-O3-C1	5.61	94.57	121.26	10	13
4	A	307	PX4	C7-O7-C23	5.59	131.16	117.80	3	10
4	A	370	PX4	C8-C7-C6	5.56	98.82	111.78	7	10
4	A	381	PX4	C7-O7-C23	5.56	104.49	117.80	8	3
4	A	360	PX4	O5-C8-C7	5.56	124.41	108.40	12	9
4	A	359	PX4	C8-C7-C6	5.55	98.83	111.78	5	8
4	A	319	PX4	C8-C7-C6	5.55	98.85	111.78	6	11
4	A	394	PX4	P1-O3-C1	5.54	94.87	121.26	12	11
4	A	408	PX4	C4-N1-C3	5.54	123.53	108.98	14	4
4	A	306	PX4	O7-C23-C24	5.54	123.46	111.48	5	7
4	A	331	PX4	O7-C23-C24	5.54	123.46	111.48	8	11
4	A	350	PX4	C8-C7-C6	5.54	98.88	111.78	10	8
4	A	327	PX4	C8-C7-C6	5.53	98.89	111.78	4	9
4	A	406	PX4	O7-C23-C24	5.53	123.44	111.48	6	7
4	A	342	PX4	O7-C23-C24	5.52	123.43	111.48	14	10
4	A	389	PX4	P1-O3-C1	5.52	94.98	121.26	6	9
4	A	400	PX4	C8-C7-C6	5.50	98.95	111.78	8	10
4	A	416	PX4	O7-C23-C24	5.50	123.38	111.48	13	5
4	A	351	PX4	C8-C7-C6	5.50	98.96	111.78	4	9
4	A	401	PX4	O5-C8-C7	5.50	124.25	108.40	7	9
4	A	407	PX4	C8-C7-C6	5.49	98.97	111.78	11	8
4	A	312	PX4	C8-C7-C6	5.48	99.00	111.78	5	6
4	A	385	PX4	C8-C7-C6	5.47	99.03	111.78	8	10
4	A	314	PX4	O5-C8-C7	5.47	124.16	108.40	11	10
4	A	353	PX4	O5-C8-C7	5.47	124.15	108.40	14	9
4	A	377	PX4	O5-C8-C7	5.46	124.14	108.40	11	10
4	A	330	PX4	C8-C7-C6	5.46	99.06	111.78	13	7
4	A	334	PX4	C8-C7-C6	5.46	99.06	111.78	9	11
4	A	367	PX4	C8-C7-C6	5.45	99.08	111.78	13	8
4	A	422	PX4	O7-C23-C24	5.45	123.27	111.48	10	9
4	A	375	PX4	O7-C23-C24	5.43	123.23	111.48	3	8
4	A	394	PX4	C8-C7-C6	5.43	99.13	111.78	10	8
4	A	328	PX4	P1-O3-C1	5.42	95.47	121.26	10	12
4	A	371	PX4	C8-C7-C6	5.42	99.15	111.78	9	9
4	A	381	PX4	P1-O3-C1	5.41	95.49	121.26	10	11
4	A	421	PX4	O5-C8-C7	5.41	123.98	108.40	9	6
4	A	429	PX4	C8-C7-C6	5.40	99.18	111.78	14	8
4	A	343	PX4	O7-C23-C24	5.40	123.15	111.48	14	8
4	A	320	PX4	C8-C7-C6	5.39	99.21	111.78	7	11
4	A	362	PX4	C8-C7-C6	5.38	99.23	111.78	10	13
4	A	333	PX4	C8-C7-C6	5.38	99.25	111.78	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	422	PX4	C4-N1-C3	5.37	94.87	108.98	9	5
4	A	428	PX4	O5-C8-C7	5.37	123.88	108.40	1	10
4	A	368	PX4	C8-C7-C6	5.36	99.28	111.78	11	10
4	A	390	PX4	O7-C23-O8	5.35	111.20	123.70	13	6
4	A	369	PX4	P1-O3-C1	5.33	95.87	121.26	5	10
4	A	346	PX4	C8-C7-C6	5.33	99.35	111.78	9	9
4	A	338	PX4	C8-C7-C6	5.33	99.36	111.78	14	7
4	A	346	PX4	O7-C23-C24	5.32	122.99	111.48	6	8
4	A	387	PX4	C8-C7-C6	5.32	99.38	111.78	4	11
4	A	430	PX4	O5-C8-C7	5.31	123.71	108.40	8	7
4	A	415	PX4	P1-O3-C1	5.30	96.02	121.26	3	13
4	A	380	PX4	O7-C23-C24	5.30	122.95	111.48	6	6
4	A	324	PX4	C8-C7-C6	5.30	99.43	111.78	9	8
4	A	378	PX4	P1-O3-C1	5.29	96.07	121.26	7	11
4	A	340	PX4	C8-C7-C6	5.28	99.47	111.78	11	9
4	A	398	PX4	O5-C8-C7	5.28	123.62	108.40	11	4
4	A	339	PX4	C8-C7-C6	5.27	99.49	111.78	11	9
4	A	313	PX4	O7-C23-C24	5.25	122.83	111.48	7	6
4	A	348	PX4	C8-C7-C6	5.24	99.57	111.78	6	9
4	A	368	PX4	O5-C8-C7	5.23	123.49	108.40	13	8
4	A	374	PX4	O5-C8-C7	5.23	123.49	108.40	10	7
4	A	317	PX4	C8-C7-C6	5.23	99.59	111.78	11	7
4	A	311	PX4	O5-C8-C7	5.22	123.44	108.40	8	8
4	A	313	PX4	O3-P1-O2	5.22	88.25	108.94	13	5
4	A	341	PX4	O7-C7-C8	5.22	127.06	108.34	7	5
4	A	355	PX4	O5-C8-C7	5.22	123.44	108.40	7	6
4	A	410	PX4	O3-P1-O2	5.21	88.28	108.94	13	4
4	A	393	PX4	C8-C7-C6	5.21	99.64	111.78	2	8
4	A	364	PX4	C7-O7-C23	5.20	130.25	117.80	9	7
4	A	328	PX4	O7-C23-C24	5.19	122.72	111.48	10	8
4	A	397	PX4	O5-C8-C7	5.19	123.35	108.40	11	10
4	A	360	PX4	C8-C7-C6	5.18	99.70	111.78	12	7
4	A	373	PX4	O5-C8-C7	5.18	123.33	108.40	4	9
4	A	408	PX4	C8-C7-C6	5.18	99.70	111.78	11	11
4	A	418	PX4	O5-C8-C7	5.18	123.33	108.40	13	8
4	A	422	PX4	O5-C8-C7	5.17	123.29	108.40	6	12
4	A	388	PX4	C5-N1-C4	5.16	95.42	108.98	3	3
4	A	330	PX4	O7-C23-O8	5.15	111.66	123.70	11	7
4	A	381	PX4	O7-C23-C24	5.15	122.63	111.48	12	7
4	A	329	PX4	O5-C8-C7	5.13	123.17	108.40	1	9
4	A	394	PX4	O5-C8-C7	5.13	123.17	108.40	6	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	C8-C7-C6	5.12	99.84	111.78	6	9
4	A	309	PX4	O7-C23-C24	5.12	122.56	111.48	13	8
4	A	361	PX4	C7-O7-C23	5.12	130.04	117.80	1	13
4	A	379	PX4	P1-O3-C1	5.11	96.94	121.26	13	12
4	A	412	PX4	P1-O3-C1	5.11	96.95	121.26	12	6
4	A	352	PX4	C8-C7-C6	5.10	99.89	111.78	6	9
4	A	335	PX4	C8-C7-C6	5.10	99.90	111.78	11	11
4	A	385	PX4	O7-C23-O8	5.10	111.78	123.70	6	5
4	A	371	PX4	C7-O7-C23	5.10	129.99	117.80	14	8
4	A	411	PX4	C4-N1-C3	5.09	122.35	108.98	1	6
4	A	372	PX4	O5-C9-O6	5.09	110.89	123.63	8	4
4	A	417	PX4	C8-C7-C6	5.09	99.91	111.78	1	9
4	A	349	PX4	C7-O7-C23	5.09	129.97	117.80	5	13
4	A	392	PX4	C8-C7-C6	5.09	99.93	111.78	12	11
4	A	417	PX4	O5-C8-C7	5.09	123.06	108.40	14	9
4	A	420	PX4	O7-C23-C24	5.08	122.46	111.48	13	8
4	A	410	PX4	C8-C7-C6	5.07	99.95	111.78	8	10
4	A	322	PX4	C7-O7-C23	5.07	129.92	117.80	6	5
4	A	424	PX4	C7-O7-C23	5.06	129.91	117.80	13	4
4	A	353	PX4	O1-P1-O2	5.06	135.99	112.44	2	9
4	A	365	PX4	C8-C7-C6	5.05	100.00	111.78	5	8
4	A	354	PX4	O5-C8-C7	5.05	122.96	108.40	1	10
4	A	328	PX4	C5-N1-C4	5.05	95.72	108.98	5	8
4	A	344	PX4	C5-N1-C4	5.04	95.72	108.98	6	2
4	A	392	PX4	O5-C8-C7	5.04	122.93	108.40	2	9
4	A	412	PX4	O7-C23-C24	5.04	122.39	111.48	7	7
4	A	344	PX4	C8-C7-C6	5.04	100.03	111.78	7	10
4	A	383	PX4	P1-O3-C1	5.04	97.27	121.26	9	7
4	A	428	PX4	P1-O3-C1	5.04	97.27	121.26	10	13
4	A	364	PX4	O7-C23-O8	5.04	111.93	123.70	8	8
4	A	371	PX4	O7-C23-O8	5.03	111.95	123.70	3	10
4	A	411	PX4	O5-C8-C7	5.03	122.89	108.40	12	8
4	A	396	PX4	O7-C7-C6	5.03	126.38	108.34	10	9
4	A	391	PX4	C8-C7-C6	5.03	100.07	111.78	14	9
4	A	410	PX4	C7-O7-C23	5.02	129.82	117.80	7	10
4	A	387	PX4	O7-C23-C24	5.02	122.33	111.48	12	6
4	A	421	PX4	C8-C7-C6	5.02	100.09	111.78	8	6
4	A	427	PX4	O7-C23-O8	5.01	112.00	123.70	3	6
4	A	329	PX4	P1-O3-C1	5.01	97.43	121.26	13	11
4	A	425	PX4	O7-C23-C24	5.01	122.31	111.48	13	7
4	A	384	PX4	O5-C8-C7	5.00	122.81	108.40	13	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	356	PX4	C7-O7-C23	4.99	129.74	117.80	10	3
4	A	365	PX4	C7-O7-C23	4.98	129.71	117.80	7	4
4	A	415	PX4	O5-C8-C7	4.98	122.75	108.40	14	11
4	A	338	PX4	O5-C9-C10	4.97	126.98	111.83	12	3
4	A	316	PX4	C8-C7-C6	4.97	100.21	111.78	9	9
4	A	366	PX4	C7-O7-C23	4.96	129.66	117.80	13	5
4	A	373	PX4	P1-O3-C1	4.96	97.67	121.26	8	11
4	A	388	PX4	C8-C7-C6	4.95	100.23	111.78	1	9
4	A	393	PX4	P1-O3-C1	4.95	97.69	121.26	12	10
4	A	384	PX4	O7-C23-C24	4.95	122.19	111.48	3	7
4	A	391	PX4	O3-P1-O2	4.95	89.33	108.94	2	3
4	A	419	PX4	C7-O7-C23	4.95	129.64	117.80	1	5
4	A	313	PX4	O5-C8-C7	4.93	122.62	108.40	14	11
4	A	421	PX4	O7-C23-C24	4.94	122.16	111.48	9	7
4	A	400	PX4	O5-C8-C7	4.93	122.61	108.40	7	4
4	A	386	PX4	O5-C8-C7	4.92	122.58	108.40	10	8
4	A	423	PX4	O5-C8-C7	4.92	122.57	108.40	5	7
4	A	400	PX4	O7-C23-C24	4.92	122.12	111.48	8	8
4	A	310	PX4	O7-C23-C24	4.91	122.10	111.48	14	10
4	A	391	PX4	O7-C23-O8	4.91	112.24	123.70	6	6
4	A	311	PX4	O7-C23-C24	4.90	122.09	111.48	7	9
4	A	316	PX4	O5-C8-C7	4.90	122.53	108.40	12	11
4	A	378	PX4	O5-C8-C7	4.90	122.53	108.40	12	8
4	A	395	PX4	C8-C7-C6	4.90	100.35	111.78	8	8
4	A	377	PX4	C5-N1-C4	4.90	96.10	108.98	10	3
4	A	377	PX4	O5-C9-O6	4.90	111.37	123.63	14	2
4	A	322	PX4	O7-C23-C24	4.90	122.07	111.48	1	9
4	A	381	PX4	C8-C7-C6	4.90	100.37	111.78	12	10
4	A	308	PX4	O3-P1-O2	4.89	89.56	108.94	8	5
4	A	404	PX4	O5-C9-C10	4.88	126.72	111.83	3	4
4	A	347	PX4	P1-O3-C1	4.88	98.03	121.26	14	7
4	A	307	PX4	O7-C23-O8	4.88	112.30	123.70	8	4
4	A	402	PX4	O5-C9-O6	4.87	111.44	123.63	13	3
4	A	404	PX4	C8-C7-C6	4.87	100.42	111.78	10	10
4	A	310	PX4	O7-C23-O8	4.86	112.33	123.70	14	6
4	A	307	PX4	C8-C7-C6	4.86	100.46	111.78	12	8
4	A	403	PX4	O7-C23-C24	4.86	121.99	111.48	2	8
4	A	405	PX4	O7-C23-O8	4.85	112.36	123.70	4	7
4	A	416	PX4	O1-P1-O2	4.85	135.01	112.44	4	6
4	A	413	PX4	P1-O3-C1	4.84	98.24	121.26	13	13
4	A	430	PX4	O7-C23-O8	4.84	112.40	123.70	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	P1-O3-C1	4.83	98.26	121.26	11	11
4	A	423	PX4	O7-C7-C6	4.83	125.67	108.34	10	6
4	A	353	PX4	O7-C23-C24	4.82	121.92	111.48	7	5
4	A	359	PX4	O5-C8-C7	4.82	122.30	108.40	5	11
4	A	308	PX4	O7-C23-C24	4.82	121.91	111.48	3	8
4	A	410	PX4	P1-O3-C1	4.82	98.31	121.26	3	8
4	A	347	PX4	O5-C8-C7	4.82	122.28	108.40	1	9
4	A	322	PX4	C8-C7-C6	4.81	100.56	111.78	10	12
4	A	308	PX4	O5-C8-C7	4.81	122.26	108.40	10	9
4	A	358	PX4	P1-O3-C1	4.80	98.39	121.26	14	12
4	A	404	PX4	O5-C8-C7	4.80	122.24	108.40	13	8
4	A	347	PX4	O7-C23-C24	4.80	121.86	111.48	2	10
4	A	402	PX4	O7-C23-C24	4.80	121.86	111.48	7	3
4	A	365	PX4	O7-C23-C24	4.79	121.85	111.48	14	7
4	A	395	PX4	C7-O7-C23	4.79	129.26	117.80	13	4
4	A	430	PX4	P1-O3-C1	4.79	98.47	121.26	1	10
4	A	334	PX4	C5-N1-C3	4.78	96.41	108.98	9	7
4	A	338	PX4	O7-C23-C24	4.78	121.83	111.48	12	10
4	A	379	PX4	O5-C8-C7	4.78	122.19	108.40	12	9
4	A	354	PX4	O7-C23-C24	4.78	121.82	111.48	10	5
4	A	330	PX4	O7-C23-C24	4.76	121.79	111.48	10	8
4	A	329	PX4	C7-O7-C23	4.76	129.19	117.80	7	5
4	A	345	PX4	O7-C23-O8	4.76	112.58	123.70	2	6
4	A	383	PX4	C8-C7-C6	4.76	100.69	111.78	3	11
4	A	375	PX4	O5-C8-C7	4.76	122.11	108.40	4	7
4	A	351	PX4	O5-C8-C7	4.75	122.09	108.40	14	11
4	A	384	PX4	O1-P1-O2	4.75	134.54	112.44	13	8
4	A	372	PX4	O3-P1-O2	4.75	90.12	108.94	8	4
4	A	395	PX4	O7-C23-C24	4.75	121.75	111.48	12	7
4	A	341	PX4	O7-C23-O8	4.75	112.61	123.70	5	5
4	A	315	PX4	O5-C9-C10	4.74	126.29	111.83	3	3
4	A	413	PX4	O7-C7-C8	4.74	125.35	108.34	13	6
4	A	309	PX4	O3-P1-O2	4.74	90.16	108.94	12	7
4	A	360	PX4	P1-O3-C1	4.73	98.73	121.26	12	14
4	A	312	PX4	O1-P1-O4	4.73	129.01	107.57	11	1
4	A	411	PX4	C8-C7-C6	4.73	100.75	111.78	4	7
4	A	391	PX4	P1-O3-C1	4.73	98.74	121.26	14	9
4	A	385	PX4	C7-O7-C23	4.73	106.48	117.80	14	4
4	A	372	PX4	O7-C7-C8	4.73	125.30	108.34	10	5
4	A	407	PX4	C7-O7-C23	4.73	129.11	117.80	11	5
4	A	340	PX4	O7-C23-C24	4.72	121.70	111.48	10	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	381	PX4	O3-P1-O2	4.72	90.21	108.94	8	3
4	A	404	PX4	C5-N1-C4	4.72	96.57	108.98	9	1
4	A	320	PX4	O7-C7-C8	4.72	125.27	108.34	13	3
4	A	366	PX4	C8-C7-C6	4.72	100.78	111.78	2	11
4	A	323	PX4	C8-C7-C6	4.72	100.79	111.78	8	6
4	A	386	PX4	O7-C7-C8	4.72	125.27	108.34	9	4
4	A	354	PX4	O5-C9-O6	4.71	111.84	123.63	11	4
4	A	429	PX4	O7-C23-C24	4.71	121.68	111.48	12	6
4	A	332	PX4	C7-O7-C23	4.70	129.05	117.80	14	6
4	A	408	PX4	O7-C23-C24	4.70	121.65	111.48	14	10
4	A	419	PX4	C5-N1-C3	4.70	96.63	108.98	4	4
4	A	312	PX4	O7-C23-C24	4.68	121.62	111.48	11	7
4	A	379	PX4	O7-C23-C24	4.68	121.61	111.48	14	8
4	A	362	PX4	P1-O3-C1	4.68	98.98	121.26	9	13
4	A	409	PX4	O5-C8-C7	4.68	121.88	108.40	6	11
4	A	414	PX4	O5-C9-O6	4.68	111.93	123.63	8	5
4	A	329	PX4	C8-C7-C6	4.67	100.89	111.78	4	13
4	A	424	PX4	C8-C7-C6	4.68	100.88	111.78	14	8
4	A	326	PX4	C8-C7-C6	4.67	100.90	111.78	13	8
4	A	337	PX4	C8-C7-C6	4.67	100.89	111.78	12	9
4	A	400	PX4	P1-O3-C1	4.66	99.07	121.26	5	13
4	A	404	PX4	C7-O7-C23	4.66	128.95	117.80	4	4
4	A	314	PX4	C5-N1-C3	4.66	121.21	108.98	12	3
4	A	358	PX4	C8-C7-C6	4.66	100.93	111.78	8	6
4	A	403	PX4	O5-C8-C7	4.65	121.81	108.40	5	5
4	A	382	PX4	O5-C8-C7	4.65	121.81	108.40	7	7
4	A	414	PX4	C5-N1-C3	4.65	96.76	108.98	12	2
4	A	384	PX4	C8-C7-C6	4.64	100.96	111.78	13	9
4	A	419	PX4	C5-N1-C4	4.64	96.79	108.98	9	3
4	A	425	PX4	C11-C10-C9	4.64	96.69	113.69	1	1
4	A	421	PX4	O7-C7-C8	4.64	124.98	108.34	13	9
4	A	408	PX4	O5-C8-C7	4.63	121.75	108.40	13	9
4	A	352	PX4	O5-C8-C7	4.63	121.74	108.40	1	10
4	A	367	PX4	C7-O7-C23	4.62	128.87	117.80	13	6
4	A	404	PX4	P1-O3-C1	4.62	99.25	121.26	9	12
4	A	408	PX4	C7-O7-C23	4.62	128.85	117.80	9	6
4	A	319	PX4	O5-C8-C7	4.62	121.70	108.40	2	10
4	A	393	PX4	O5-C8-C7	4.62	121.70	108.40	6	9
4	A	367	PX4	O5-C8-C7	4.61	121.68	108.40	8	12
4	A	353	PX4	P1-O3-C1	4.60	99.34	121.26	9	11
4	A	406	PX4	O5-C8-C7	4.60	121.67	108.40	9	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	306	PX4	O5-C8-C7	4.60	121.65	108.40	2	8
4	A	399	PX4	P1-O3-C1	4.60	99.38	121.26	10	11
4	A	415	PX4	C5-N1-C4	4.59	96.91	108.98	10	5
4	A	428	PX4	O7-C23-O8	4.59	112.97	123.70	4	4
4	A	418	PX4	C8-C7-C6	4.59	101.08	111.78	13	8
4	A	372	PX4	C8-C7-C6	4.59	101.09	111.78	14	8
4	A	399	PX4	C4-N1-C3	4.59	96.93	108.98	10	7
4	A	314	PX4	C7-O7-C23	4.58	128.77	117.80	14	2
4	A	313	PX4	C8-C7-C6	4.58	101.10	111.78	13	7
4	A	364	PX4	O7-C23-C24	4.58	121.39	111.48	14	9
4	A	416	PX4	C1-C2-N1	4.58	130.52	115.82	11	3
4	A	325	PX4	C8-C7-C6	4.58	101.11	111.78	11	12
4	A	354	PX4	O3-P1-O2	4.58	90.79	108.94	7	4
4	A	394	PX4	O3-P1-O2	4.58	90.79	108.94	5	2
4	A	323	PX4	P1-O3-C1	4.57	99.49	121.26	12	12
4	A	337	PX4	C26-C25-C24	4.57	96.33	113.13	12	3
4	A	397	PX4	O7-C23-O8	4.57	113.02	123.70	6	5
4	A	396	PX4	C4-N1-C3	4.57	120.98	108.98	3	3
4	A	349	PX4	O5-C8-C7	4.57	121.56	108.40	1	6
4	A	359	PX4	O7-C7-C8	4.56	124.71	108.34	9	6
4	A	364	PX4	O5-C8-C7	4.56	121.55	108.40	12	7
4	A	385	PX4	O5-C8-C7	4.56	121.54	108.40	13	9
4	A	336	PX4	C8-C7-C6	4.56	101.16	111.78	10	9
4	A	387	PX4	C5-N1-C3	4.55	97.01	108.98	14	5
4	A	350	PX4	O7-C23-O8	4.55	113.06	123.70	2	5
4	A	399	PX4	O5-C8-C7	4.55	121.52	108.40	2	8
4	A	395	PX4	O5-C8-C7	4.55	121.52	108.40	6	10
4	A	396	PX4	P1-O3-C1	4.55	99.60	121.26	8	10
4	A	310	PX4	P1-O3-C1	4.55	99.60	121.26	6	8
4	A	319	PX4	P1-O3-C1	4.55	99.60	121.26	13	11
4	A	347	PX4	C5-N1-C4	4.55	120.92	108.98	10	3
4	A	355	PX4	O7-C23-C24	4.55	121.32	111.48	4	5
4	A	423	PX4	P1-O4-C6	4.55	95.29	121.35	9	8
4	A	356	PX4	O5-C9-O6	4.55	112.26	123.63	14	2
4	A	373	PX4	O7-C23-C24	4.54	121.30	111.48	8	7
4	A	418	PX4	O7-C23-O8	4.54	113.09	123.70	5	7
4	A	421	PX4	C4-N1-C3	4.53	120.88	108.98	12	4
4	A	401	PX4	P1-O3-C1	4.53	99.69	121.26	6	11
4	A	348	PX4	O7-C23-C24	4.53	121.28	111.48	5	10
4	A	344	PX4	C7-O7-C23	4.53	128.63	117.80	14	4
4	A	346	PX4	O5-C8-C7	4.53	121.44	108.40	10	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	348	PX4	O5-C8-C7	4.52	121.44	108.40	3	9
4	A	364	PX4	O1-P1-O2	4.52	133.49	112.44	8	6
4	A	415	PX4	O7-C23-O8	4.52	113.13	123.70	13	3
4	A	411	PX4	C5-N1-C3	4.52	97.10	108.98	11	3
4	A	420	PX4	O5-C8-C7	4.51	121.41	108.40	13	7
4	A	372	PX4	C7-O7-C23	4.51	128.60	117.80	6	7
4	A	378	PX4	C8-C7-C6	4.51	101.27	111.78	8	5
4	A	397	PX4	C7-O7-C23	4.51	128.59	117.80	10	4
4	A	387	PX4	O5-C8-C7	4.51	121.39	108.40	6	10
4	A	378	PX4	O7-C23-O8	4.50	113.18	123.70	12	3
4	A	312	PX4	O7-C7-C8	4.50	124.49	108.34	7	11
4	A	411	PX4	O7-C23-O8	4.49	113.20	123.70	2	3
4	A	306	PX4	O7-C7-C8	4.49	124.45	108.34	1	9
4	A	373	PX4	C8-C7-C6	4.49	101.31	111.78	11	9
4	A	333	PX4	O7-C23-C24	4.49	121.19	111.48	9	6
4	A	374	PX4	O7-C7-C8	4.49	124.44	108.34	8	4
4	A	324	PX4	P1-O3-C1	4.48	99.95	121.26	10	11
4	A	332	PX4	C8-C7-C6	4.47	101.36	111.78	6	11
4	A	366	PX4	O5-C8-C7	4.47	121.28	108.40	7	10
4	A	311	PX4	C12-C11-C10	4.47	96.71	113.13	2	3
4	A	324	PX4	O5-C8-C7	4.47	121.28	108.40	5	7
4	A	394	PX4	O7-C23-O8	4.47	113.25	123.70	13	4
4	A	357	PX4	O7-C23-C24	4.47	121.14	111.48	2	6
4	A	409	PX4	O7-C23-C24	4.47	121.14	111.48	12	8
4	A	313	PX4	O7-C23-O8	4.46	113.28	123.70	7	6
4	A	333	PX4	O7-C7-C6	4.46	124.34	108.34	4	8
4	A	410	PX4	O7-C7-C8	4.45	124.32	108.34	13	11
4	A	307	PX4	O3-P1-O2	4.45	91.30	108.94	2	6
4	A	331	PX4	O5-C8-C7	4.45	121.22	108.40	12	9
4	A	310	PX4	P1-O4-C6	4.45	95.86	121.35	13	10
4	A	393	PX4	O7-C23-C24	4.45	121.10	111.48	8	7
4	A	310	PX4	C5-N1-C4	4.44	97.30	108.98	5	3
4	A	372	PX4	O7-C23-C24	4.44	121.09	111.48	10	5
4	A	403	PX4	C8-C7-C6	4.44	101.42	111.78	2	9
4	A	355	PX4	P1-O3-C1	4.44	100.12	121.26	12	12
4	A	423	PX4	C5-N1-C3	4.44	97.31	108.98	9	5
4	A	384	PX4	O5-C9-O6	4.44	112.52	123.63	10	4
4	A	330	PX4	O5-C8-C7	4.44	121.19	108.40	5	10
4	A	367	PX4	P1-O3-C1	4.44	100.14	121.26	9	12
4	A	412	PX4	O5-C8-C7	4.44	121.19	108.40	3	6
4	A	344	PX4	C4-N1-C3	4.43	97.34	108.98	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	C4-N1-C3	4.43	97.34	108.98	6	5
4	A	358	PX4	O5-C8-C7	4.43	121.16	108.40	10	8
4	A	371	PX4	P1-O3-C1	4.43	100.19	121.26	6	13
4	A	379	PX4	C5-N1-C3	4.43	97.35	108.98	10	4
4	A	371	PX4	C5-N1-C4	4.43	120.60	108.98	8	3
4	A	365	PX4	P1-O3-C1	4.42	100.21	121.26	13	10
4	A	309	PX4	P1-O3-C1	4.42	100.22	121.26	14	11
4	A	401	PX4	O7-C23-C24	4.42	121.05	111.48	3	6
4	A	345	PX4	O5-C9-C10	4.41	125.29	111.83	2	4
4	A	350	PX4	P1-O4-C6	4.41	96.06	121.35	12	4
4	A	381	PX4	O5-C8-C7	4.41	121.10	108.40	2	12
4	A	429	PX4	P1-O3-C1	4.41	100.28	121.26	5	11
4	A	386	PX4	O1-P1-O2	4.40	132.92	112.44	5	7
4	A	334	PX4	O5-C9-O6	4.40	112.63	123.63	5	2
4	A	356	PX4	C4-N1-C3	4.39	97.45	108.98	11	2
4	A	369	PX4	C8-C7-C6	4.39	101.55	111.78	8	7
4	A	430	PX4	O7-C23-C24	4.39	120.98	111.48	1	6
4	A	318	PX4	P1-O3-C1	4.39	100.38	121.26	4	9
4	A	338	PX4	O5-C8-C7	4.39	121.04	108.40	12	5
4	A	393	PX4	O3-P1-O2	4.39	91.55	108.94	9	3
4	A	309	PX4	O5-C8-C7	4.38	121.03	108.40	5	8
4	A	333	PX4	C7-O7-C23	4.38	128.28	117.80	6	4
4	A	355	PX4	C7-O7-C23	4.38	107.31	117.80	13	2
4	A	361	PX4	O5-C9-C10	4.38	125.19	111.83	2	2
4	A	383	PX4	O7-C23-C24	4.38	120.95	111.48	5	7
4	A	342	PX4	O5-C8-C7	4.38	121.02	108.40	2	6
4	A	428	PX4	P1-O4-C6	4.37	96.29	121.35	8	8
4	A	336	PX4	O4-P1-O2	4.37	126.26	108.94	14	4
4	A	370	PX4	O7-C23-C24	4.37	120.94	111.48	8	8
4	A	308	PX4	O7-C23-O8	4.37	113.50	123.70	3	5
4	A	327	PX4	O5-C8-C7	4.36	120.98	108.40	11	7
4	A	321	PX4	O5-C8-C7	4.36	120.98	108.40	13	7
4	A	371	PX4	C4-N1-C3	4.36	97.51	108.98	3	4
4	A	391	PX4	O7-C23-C24	4.36	120.92	111.48	2	7
4	A	414	PX4	O7-C23-O8	4.36	113.51	123.70	1	5
4	A	411	PX4	O7-C23-C24	4.36	120.91	111.48	7	6
4	A	426	PX4	P1-O3-C1	4.35	100.54	121.26	13	10
4	A	372	PX4	P1-O3-C1	4.35	100.55	121.26	4	9
4	A	376	PX4	P1-O3-C1	4.35	100.56	121.26	9	13
4	A	325	PX4	O7-C23-C24	4.35	120.89	111.48	12	7
4	A	328	PX4	O5-C8-C7	4.35	120.92	108.40	6	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	398	PX4	O3-P1-O2	4.34	91.72	108.94	3	6
4	A	417	PX4	O4-P1-O2	4.34	126.14	108.94	13	3
4	A	376	PX4	O7-C7-C8	4.34	123.91	108.34	1	7
4	A	419	PX4	P1-O3-C1	4.34	100.61	121.26	6	9
4	A	336	PX4	O5-C8-C7	4.34	120.90	108.40	10	9
4	A	373	PX4	O3-P1-O2	4.34	91.75	108.94	9	6
4	A	400	PX4	O7-C7-C8	4.34	123.90	108.34	7	7
4	A	355	PX4	C8-C7-C6	4.33	101.69	111.78	6	8
4	A	345	PX4	O7-C23-C24	4.33	120.84	111.48	10	7
4	A	366	PX4	P1-O3-C1	4.33	100.66	121.26	2	12
4	A	393	PX4	O7-C7-C8	4.33	123.87	108.34	13	7
4	A	416	PX4	O3-P1-O2	4.33	91.78	108.94	4	3
4	A	327	PX4	C5-N1-C3	4.32	97.62	108.98	8	3
4	A	416	PX4	C5-N1-C3	4.32	97.62	108.98	9	3
4	A	358	PX4	O7-C23-O8	4.32	113.60	123.70	1	5
4	A	326	PX4	O5-C9-C10	4.32	125.01	111.83	6	3
4	A	338	PX4	P1-O3-C1	4.32	100.69	121.26	3	13
4	A	347	PX4	O7-C7-C8	4.32	123.84	108.34	2	7
4	A	406	PX4	O3-P1-O2	4.32	91.81	108.94	1	4
4	A	321	PX4	C7-O7-C23	4.32	128.13	117.80	8	6
4	A	422	PX4	P1-O3-C1	4.32	100.72	121.26	10	7
4	A	397	PX4	P1-O3-C1	4.31	100.72	121.26	14	10
4	A	355	PX4	P1-O4-C6	4.31	96.66	121.35	1	10
4	A	420	PX4	P1-O3-C1	4.31	100.75	121.26	7	8
4	A	342	PX4	P1-O3-C1	4.31	100.76	121.26	10	14
4	A	344	PX4	O5-C8-C7	4.31	120.81	108.40	5	8
4	A	364	PX4	C8-C7-C6	4.31	101.75	111.78	13	9
4	A	416	PX4	C8-C7-C6	4.30	101.75	111.78	3	7
4	A	421	PX4	C7-O7-C23	4.31	128.10	117.80	12	5
4	A	384	PX4	O7-C23-O8	4.30	113.64	123.70	9	4
4	A	424	PX4	O5-C8-C7	4.30	120.80	108.40	5	8
4	A	371	PX4	O5-C8-C7	4.30	120.80	108.40	5	5
4	A	326	PX4	P1-O3-C1	4.30	100.79	121.26	7	13
4	A	419	PX4	O7-C23-C24	4.30	120.78	111.48	11	6
4	A	363	PX4	C4-N1-C3	4.30	97.69	108.98	9	2
4	A	360	PX4	O7-C23-C24	4.29	120.77	111.48	2	10
4	A	388	PX4	P1-O3-C1	4.29	100.82	121.26	6	8
4	A	427	PX4	O7-C7-C8	4.29	123.74	108.34	12	9
4	A	382	PX4	O7-C23-C24	4.29	120.76	111.48	8	6
4	A	388	PX4	O7-C23-C24	4.29	120.75	111.48	2	6
4	A	343	PX4	O5-C8-C7	4.28	120.74	108.40	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	398	PX4	O1-P1-O2	4.28	132.34	112.44	3	8
4	A	363	PX4	P1-O3-C1	4.28	100.91	121.26	8	8
4	A	392	PX4	O7-C23-C24	4.28	120.73	111.48	7	7
4	A	409	PX4	O3-P1-O2	4.27	92.01	108.94	8	6
4	A	390	PX4	O3-P1-O2	4.27	92.01	108.94	2	5
4	A	393	PX4	O1-P1-O2	4.27	132.30	112.44	9	9
4	A	403	PX4	C7-O7-C23	4.27	107.58	117.80	10	3
4	A	308	PX4	P1-O3-C1	4.26	100.96	121.26	7	9
4	A	339	PX4	P1-O3-C1	4.26	100.97	121.26	8	11
4	A	354	PX4	C5-N1-C4	4.26	97.78	108.98	14	5
4	A	421	PX4	P1-O3-C1	4.26	100.97	121.26	7	8
4	A	381	PX4	O7-C7-C8	4.26	123.63	108.34	10	8
4	A	354	PX4	O1-P1-O2	4.26	132.25	112.44	7	12
4	A	380	PX4	C7-O7-C23	4.26	107.61	117.80	5	6
4	A	316	PX4	O7-C23-C24	4.26	120.69	111.48	1	8
4	A	407	PX4	P1-O4-C6	4.26	96.96	121.35	7	7
4	A	329	PX4	O7-C23-O8	4.26	113.76	123.70	2	7
4	A	341	PX4	P1-O3-C1	4.25	101.02	121.26	4	12
4	A	416	PX4	P1-O4-C6	4.25	96.98	121.35	9	9
4	A	307	PX4	P1-O3-C1	4.25	101.03	121.26	2	9
4	A	389	PX4	O5-C8-C7	4.25	120.65	108.40	13	10
4	A	344	PX4	P1-O3-C1	4.25	101.04	121.26	7	11
4	A	390	PX4	C8-C7-C6	4.25	101.88	111.78	5	9
4	A	392	PX4	C1-C2-N1	4.25	129.45	115.82	9	4
4	A	317	PX4	C1-C2-N1	4.24	129.44	115.82	7	5
4	A	403	PX4	O1-P1-O4	4.24	126.80	107.57	9	5
4	A	350	PX4	O1-P1-O2	4.24	132.17	112.44	9	6
4	A	336	PX4	O1-P1-O2	4.24	132.16	112.44	7	8
4	A	341	PX4	O5-C8-C7	4.24	120.61	108.40	6	6
4	A	326	PX4	O7-C23-C24	4.23	120.64	111.48	5	5
4	A	351	PX4	O7-C7-C6	4.23	123.53	108.34	3	7
4	A	340	PX4	O5-C8-C7	4.23	120.59	108.40	3	12
4	A	389	PX4	O5-C9-C10	4.23	124.73	111.83	9	4
4	A	361	PX4	O7-C7-C6	4.23	123.51	108.34	8	3
4	A	364	PX4	C4-N1-C3	4.23	97.87	108.98	13	5
4	A	383	PX4	O5-C8-C7	4.23	120.59	108.40	3	10
4	A	416	PX4	O1-P1-O4	4.23	126.72	107.57	3	4
4	A	354	PX4	C8-C7-C6	4.22	101.94	111.78	1	7
4	A	392	PX4	P1-O3-C1	4.22	101.16	121.26	8	12
4	A	338	PX4	C7-O7-C23	4.22	127.90	117.80	12	3
4	A	340	PX4	C7-O7-C23	4.22	107.69	117.80	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	373	PX4	O1-P1-O2	4.22	132.09	112.44	5	10
4	A	342	PX4	C4-N1-C3	4.22	120.06	108.98	5	3
4	A	331	PX4	P1-O4-C6	4.22	97.17	121.35	14	8
4	A	362	PX4	O5-C8-C7	4.22	120.56	108.40	7	11
4	A	400	PX4	C5-N1-C4	4.22	120.05	108.98	10	1
4	A	343	PX4	O3-P1-O2	4.21	125.64	108.94	6	3
4	A	344	PX4	O5-C9-C10	4.22	124.69	111.83	7	6
4	A	421	PX4	O5-C9-O6	4.21	113.09	123.63	9	6
4	A	385	PX4	O7-C7-C6	4.21	123.46	108.34	2	4
4	A	399	PX4	C8-C7-C6	4.21	101.96	111.78	11	11
4	A	353	PX4	P1-O4-C6	4.21	97.22	121.35	12	9
4	A	426	PX4	C8-C7-C6	4.21	101.98	111.78	6	4
4	A	315	PX4	O5-C8-C7	4.20	120.51	108.40	2	6
4	A	366	PX4	O3-P1-O2	4.20	92.28	108.94	12	7
4	A	384	PX4	O7-C7-C8	4.20	123.42	108.34	3	5
4	A	421	PX4	O7-C23-O8	4.20	113.88	123.70	9	3
4	A	407	PX4	O7-C23-C24	4.20	120.57	111.48	8	8
4	A	424	PX4	O7-C23-O8	4.20	113.89	123.70	7	5
4	A	318	PX4	O1-P1-O2	4.20	131.97	112.44	10	5
4	A	325	PX4	C7-O7-C23	4.20	127.84	117.80	1	3
4	A	355	PX4	C5-N1-C4	4.20	97.95	108.98	7	6
4	A	313	PX4	C7-O7-C23	4.19	127.83	117.80	7	4
4	A	376	PX4	O7-C23-C24	4.19	120.55	111.48	14	7
4	A	402	PX4	O5-C8-C7	4.19	120.48	108.40	6	6
4	A	407	PX4	O7-C7-C8	4.19	123.38	108.34	9	7
4	A	309	PX4	O4-P1-O2	4.19	125.54	108.94	9	3
4	A	326	PX4	C4-N1-C3	4.19	97.98	108.98	1	1
4	A	356	PX4	C8-C7-C6	4.19	102.02	111.78	3	10
4	A	415	PX4	O1-P1-O2	4.19	131.93	112.44	8	8
4	A	403	PX4	O4-P1-O2	4.18	125.52	108.94	4	2
4	A	416	PX4	P1-O3-C1	4.19	101.34	121.26	12	10
4	A	338	PX4	C5-N1-C3	4.18	97.99	108.98	9	5
4	A	315	PX4	C4-N1-C3	4.18	98.00	108.98	14	7
4	A	383	PX4	O7-C7-C6	4.18	123.34	108.34	13	4
4	A	396	PX4	O5-C8-C7	4.18	120.44	108.40	2	10
4	A	376	PX4	O5-C9-O6	4.18	113.18	123.63	4	5
4	A	396	PX4	P1-O4-C6	4.18	97.42	121.35	4	8
4	A	338	PX4	C12-C11-C10	4.17	97.80	113.13	8	2
4	A	311	PX4	O7-C23-O8	4.17	113.96	123.70	2	4
4	A	409	PX4	O5-C9-O6	4.17	113.20	123.63	3	3
4	A	307	PX4	O5-C8-C7	4.17	120.41	108.40	8	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	309	PX4	O7-C23-O8	4.16	113.97	123.70	14	10
4	A	394	PX4	O7-C23-C24	4.16	120.49	111.48	6	8
4	A	343	PX4	P1-O3-C1	4.16	101.44	121.26	2	11
4	A	402	PX4	C1-C2-N1	4.16	129.19	115.82	8	4
4	A	409	PX4	C8-C7-C6	4.16	102.08	111.78	5	7
4	A	374	PX4	C8-C7-C6	4.16	102.08	111.78	8	6
4	A	388	PX4	P1-O4-C6	4.16	97.50	121.35	13	8
4	A	335	PX4	P1-O3-C1	4.16	101.45	121.26	4	8
4	A	396	PX4	O7-C7-C8	4.15	123.25	108.34	13	6
4	A	367	PX4	O5-C9-O6	4.15	113.24	123.63	8	5
4	A	359	PX4	P1-O3-C1	4.15	101.50	121.26	10	10
4	A	374	PX4	O5-C9-O6	4.15	113.25	123.63	2	3
4	A	382	PX4	O7-C7-C8	4.15	123.23	108.34	4	5
4	A	315	PX4	C8-C7-C6	4.15	102.11	111.78	10	9
4	A	327	PX4	C4-N1-C3	4.15	98.08	108.98	5	6
4	A	357	PX4	O5-C8-C7	4.15	120.35	108.40	3	8
4	A	414	PX4	P1-O3-C1	4.15	101.53	121.26	3	11
4	A	313	PX4	O5-C9-O6	4.14	113.27	123.63	2	7
4	A	335	PX4	C7-O7-C23	4.14	107.88	117.80	9	4
4	A	371	PX4	O1-P1-O4	4.14	126.34	107.57	12	3
4	A	405	PX4	P1-O4-C6	4.14	97.61	121.35	13	13
4	A	410	PX4	O1-P1-O2	4.14	131.72	112.44	5	5
4	A	413	PX4	O7-C23-C24	4.14	120.44	111.48	6	5
4	A	356	PX4	O7-C7-C8	4.14	123.20	108.34	14	7
4	A	330	PX4	O5-C9-O6	4.14	113.27	123.63	12	4
4	A	410	PX4	O7-C23-C24	4.14	120.44	111.48	7	4
4	A	349	PX4	C8-C7-C6	4.13	102.14	111.78	4	6
4	A	410	PX4	C4-N1-C3	4.14	119.84	108.98	13	2
4	A	400	PX4	O7-C23-O8	4.13	114.05	123.70	7	8
4	A	418	PX4	C4-N1-C3	4.13	98.13	108.98	9	4
4	A	426	PX4	C5-N1-C4	4.13	98.13	108.98	5	2
4	A	392	PX4	O7-C7-C8	4.13	123.15	108.34	8	5
4	A	337	PX4	O7-C7-C6	4.12	123.14	108.34	13	3
4	A	427	PX4	C4-N1-C3	4.12	98.15	108.98	12	2
4	A	331	PX4	P1-O3-C1	4.12	101.67	121.26	14	12
4	A	335	PX4	O7-C23-C24	4.11	120.38	111.48	3	7
4	A	375	PX4	C5-N1-C3	4.11	98.17	108.98	3	2
4	A	332	PX4	O5-C9-O6	4.11	113.35	123.63	13	4
4	A	398	PX4	P1-O3-C1	4.11	101.70	121.26	1	11
4	A	354	PX4	P1-O3-C1	4.11	101.71	121.26	12	13
4	A	319	PX4	O1-P1-O3	4.10	88.96	107.57	6	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	329	PX4	O7-C23-C24	4.10	120.36	111.48	12	10
4	A	352	PX4	O5-C9-O6	4.10	113.36	123.63	1	5
4	A	346	PX4	O1-P1-O3	4.10	88.97	107.57	14	2
4	A	373	PX4	O7-C7-C8	4.10	123.06	108.34	3	8
4	A	377	PX4	O7-C23-C24	4.10	120.36	111.48	7	9
4	A	406	PX4	O7-C7-C8	4.10	123.06	108.34	13	3
4	A	318	PX4	O5-C8-C7	4.10	120.22	108.40	13	10
4	A	325	PX4	O5-C8-C7	4.10	120.22	108.40	7	10
4	A	327	PX4	O7-C23-O8	4.10	114.12	123.70	4	6
4	A	341	PX4	C8-C7-C6	4.10	102.23	111.78	5	9
4	A	351	PX4	C4-N1-C3	4.10	98.21	108.98	2	2
4	A	386	PX4	P1-O4-C6	4.09	97.90	121.35	10	11
4	A	406	PX4	C8-C7-C6	4.09	102.24	111.78	6	9
4	A	325	PX4	O7-C23-O8	4.09	114.14	123.70	3	6
4	A	346	PX4	P1-O3-C1	4.09	101.79	121.26	10	13
4	A	363	PX4	O1-P1-O4	4.09	126.11	107.57	10	3
4	A	314	PX4	C8-C7-C6	4.09	102.26	111.78	2	12
4	A	316	PX4	O1-P1-O3	4.09	89.04	107.57	5	3
4	A	340	PX4	C26-C25-C24	4.09	98.11	113.13	11	2
4	A	319	PX4	O7-C23-C24	4.09	120.32	111.48	12	6
4	A	392	PX4	O1-P1-O2	4.09	131.46	112.44	7	5
4	A	357	PX4	O7-C23-O8	4.08	114.17	123.70	1	5
4	A	400	PX4	O7-C7-C6	4.08	122.98	108.34	1	5
4	A	404	PX4	O7-C7-C8	4.08	122.98	108.34	13	7
4	A	340	PX4	C5-N1-C4	4.08	98.27	108.98	5	2
4	A	425	PX4	P1-O3-C1	4.08	101.86	121.26	5	12
4	A	343	PX4	O7-C7-C6	4.07	122.95	108.34	9	6
4	A	377	PX4	P1-O4-C6	4.07	98.02	121.35	13	4
4	A	310	PX4	O5-C8-C7	4.07	120.13	108.40	8	4
4	A	318	PX4	P1-O4-C6	4.07	98.03	121.35	14	9
4	A	385	PX4	C5-N1-C4	4.07	98.29	108.98	6	1
4	A	347	PX4	C8-C7-C6	4.07	102.30	111.78	1	7
4	A	414	PX4	C5-N1-C4	4.07	98.29	108.98	12	4
4	A	365	PX4	O5-C9-C10	4.07	124.24	111.83	1	5
4	A	338	PX4	P1-O4-C6	4.06	98.06	121.35	10	13
4	A	401	PX4	O7-C7-C8	4.07	122.93	108.34	5	6
4	A	344	PX4	C5-N1-C3	4.06	98.30	108.98	2	5
4	A	399	PX4	C7-O7-C23	4.06	127.52	117.80	9	5
4	A	328	PX4	C8-C7-C6	4.06	102.32	111.78	2	11
4	A	310	PX4	O3-P1-O2	4.06	92.85	108.94	14	2
4	A	315	PX4	O7-C23-C24	4.06	120.26	111.48	12	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	350	PX4	O5-C8-C7	4.05	120.08	108.40	9	6
4	A	386	PX4	P1-O3-C1	4.05	101.98	121.26	6	11
4	A	349	PX4	O7-C7-C8	4.05	122.87	108.34	9	9
4	A	371	PX4	C1-C2-N1	4.05	128.81	115.82	4	4
4	A	384	PX4	O5-C9-C10	4.05	124.17	111.83	10	5
4	A	422	PX4	C8-C7-C6	4.05	102.35	111.78	11	8
4	A	414	PX4	O5-C9-C10	4.04	124.16	111.83	14	7
4	A	403	PX4	O7-C7-C6	4.04	122.84	108.34	6	5
4	A	420	PX4	C8-C7-C6	4.04	102.37	111.78	7	10
4	A	330	PX4	O1-P1-O2	4.04	131.22	112.44	3	9
4	A	417	PX4	C26-C25-C24	4.04	98.29	113.13	6	2
4	A	404	PX4	O7-C23-O8	4.04	114.27	123.70	4	8
4	A	374	PX4	P1-O3-C1	4.03	102.06	121.26	9	11
4	A	380	PX4	O7-C23-O8	4.03	114.28	123.70	6	5
4	A	414	PX4	O7-C23-C24	4.03	120.19	111.48	14	10
4	A	339	PX4	C7-O7-C23	4.03	127.43	117.80	12	3
4	A	412	PX4	C1-C2-N1	4.03	128.74	115.82	4	6
4	A	375	PX4	P1-O3-C1	4.02	102.12	121.26	1	11
4	A	417	PX4	C12-C11-C10	4.02	98.35	113.13	1	2
4	A	346	PX4	P1-O4-C6	4.02	98.33	121.35	14	11
4	A	352	PX4	C7-O7-C23	4.02	127.41	117.80	11	5
4	A	398	PX4	O7-C23-C24	4.02	120.17	111.48	9	9
4	A	422	PX4	O5-C9-C10	4.02	124.08	111.83	8	4
4	A	401	PX4	O7-C7-C6	4.01	122.75	108.34	9	9
4	A	402	PX4	C5-N1-C3	4.01	98.43	108.98	11	2
4	A	348	PX4	C5-N1-C4	4.01	98.44	108.98	7	3
4	A	405	PX4	C8-C7-C6	4.01	102.43	111.78	14	10
4	A	343	PX4	C5-N1-C3	4.01	98.45	108.98	6	2
4	A	420	PX4	C1-C2-N1	4.01	128.69	115.82	6	4
4	A	420	PX4	C4-N1-C3	4.01	98.46	108.98	5	4
4	A	361	PX4	O7-C23-C24	4.00	120.14	111.48	4	6
4	A	332	PX4	O7-C23-C24	4.00	120.13	111.48	9	4
4	A	397	PX4	O7-C7-C8	3.99	122.66	108.34	3	8
4	A	419	PX4	C8-C7-C6	3.99	102.48	111.78	6	12
4	A	332	PX4	O7-C7-C8	3.99	122.66	108.34	4	6
4	A	313	PX4	C12-C11-C10	3.99	98.47	113.13	2	4
4	A	356	PX4	O5-C8-C7	3.99	119.89	108.40	1	11
4	A	384	PX4	P1-O4-C6	3.99	98.49	121.35	5	9
4	A	398	PX4	O7-C7-C8	3.99	122.65	108.34	13	5
4	A	384	PX4	P1-O3-C1	3.99	102.28	121.26	2	11
4	A	319	PX4	O7-C7-C6	3.99	122.64	108.34	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	396	PX4	O7-C23-C24	3.99	120.10	111.48	10	5
4	A	377	PX4	P1-O3-C1	3.98	102.30	121.26	13	9
4	A	418	PX4	C12-C11-C10	3.98	98.49	113.13	5	2
4	A	322	PX4	P1-O3-C1	3.98	102.30	121.26	14	12
4	A	411	PX4	O7-C7-C8	3.98	122.63	108.34	12	6
4	A	306	PX4	C8-C7-C6	3.98	102.51	111.78	14	7
4	A	336	PX4	O1-P1-O3	3.98	89.54	107.57	14	1
4	A	337	PX4	O5-C8-C7	3.98	119.86	108.40	5	9
4	A	405	PX4	P1-O3-C1	3.98	102.32	121.26	9	12
4	A	314	PX4	P1-O3-C1	3.98	102.33	121.26	10	10
4	A	361	PX4	O5-C8-C7	3.98	119.86	108.40	1	6
4	A	394	PX4	C4-N1-C3	3.97	98.53	108.98	1	2
4	A	402	PX4	C8-C7-C6	3.97	102.52	111.78	3	9
4	A	356	PX4	O5-C9-C10	3.97	123.94	111.83	14	7
4	A	375	PX4	O7-C23-O8	3.97	114.42	123.70	8	5
4	A	338	PX4	O5-C9-O6	3.97	113.70	123.63	11	5
4	A	406	PX4	P1-O3-C1	3.96	102.39	121.26	3	9
4	A	419	PX4	O5-C9-O6	3.96	113.71	123.63	5	1
4	A	370	PX4	O7-C23-O8	3.96	114.44	123.70	9	7
4	A	380	PX4	P1-O3-C1	3.96	102.40	121.26	4	12
4	A	398	PX4	O4-P1-O2	3.96	124.64	108.94	5	2
4	A	408	PX4	C12-C11-C10	3.96	98.57	113.13	10	1
4	A	417	PX4	O7-C23-O8	3.96	114.44	123.70	6	4
4	A	376	PX4	O5-C9-C10	3.96	123.91	111.83	8	3
4	A	409	PX4	P1-O3-C1	3.96	102.40	121.26	1	11
4	A	375	PX4	P1-O4-C6	3.96	98.66	121.35	10	9
4	A	419	PX4	P1-O4-C6	3.96	98.66	121.35	3	9
4	A	399	PX4	O5-C9-O6	3.96	113.73	123.63	3	4
4	A	364	PX4	P1-O3-C1	3.96	102.43	121.26	9	12
4	A	423	PX4	P1-O3-C1	3.95	102.44	121.26	14	10
4	A	347	PX4	O1-P1-O2	3.95	130.82	112.44	2	10
4	A	357	PX4	C7-O7-C23	3.95	127.25	117.80	6	5
4	A	377	PX4	O7-C7-C8	3.95	122.51	108.34	8	4
4	A	402	PX4	C7-O7-C23	3.95	127.25	117.80	5	4
4	A	309	PX4	O1-P1-O2	3.95	130.81	112.44	11	9
4	A	409	PX4	C7-O7-C23	3.95	108.35	117.80	14	6
4	A	369	PX4	C25-C24-C23	3.94	99.24	113.69	1	3
4	A	373	PX4	C5-N1-C4	3.94	98.62	108.98	12	3
4	A	411	PX4	C5-N1-C4	3.94	98.62	108.98	1	5
4	A	403	PX4	C1-C2-N1	3.94	128.47	115.82	12	5
4	A	404	PX4	P1-O4-C6	3.94	98.77	121.35	5	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	380	PX4	O5-C9-C10	3.94	123.84	111.83	1	6
4	A	419	PX4	O1-P1-O3	3.94	89.71	107.57	2	3
4	A	427	PX4	O5-C9-C10	3.94	123.85	111.83	3	3
4	A	317	PX4	O5-C8-C7	3.94	119.74	108.40	14	8
4	A	363	PX4	C5-N1-C3	3.94	119.31	108.98	9	3
4	A	376	PX4	O3-P1-O2	3.94	93.34	108.94	10	3
4	A	425	PX4	O7-C7-C8	3.93	122.45	108.34	1	7
4	A	322	PX4	O5-C9-O6	3.93	113.79	123.63	10	3
4	A	344	PX4	O7-C23-C24	3.93	119.99	111.48	14	6
4	A	408	PX4	O7-C7-C8	3.93	122.45	108.34	5	5
4	A	311	PX4	O5-C9-O6	3.93	113.80	123.63	10	5
4	A	324	PX4	O7-C7-C6	3.93	122.44	108.34	6	8
4	A	357	PX4	O5-C9-O6	3.93	113.80	123.63	12	9
4	A	378	PX4	O7-C23-C24	3.93	119.98	111.48	11	5
4	A	414	PX4	C1-C2-N1	3.93	128.44	115.82	11	3
4	A	315	PX4	P1-O4-C6	3.93	98.86	121.35	5	8
4	A	423	PX4	O5-C9-C10	3.93	123.81	111.83	4	1
4	A	341	PX4	O5-C9-O6	3.93	113.81	123.63	14	4
4	A	326	PX4	C11-C10-C9	3.92	99.32	113.69	4	2
4	A	379	PX4	O5-C9-C10	3.92	123.79	111.83	4	4
4	A	387	PX4	C5-N1-C4	3.92	98.68	108.98	13	4
4	A	412	PX4	C4-N1-C3	3.92	119.27	108.98	9	2
4	A	327	PX4	P1-O3-C1	3.92	102.62	121.26	13	12
4	A	351	PX4	O1-P1-O2	3.91	130.65	112.44	10	9
4	A	407	PX4	C4-N1-C3	3.91	98.70	108.98	8	3
4	A	418	PX4	P1-O4-C6	3.91	98.93	121.35	4	10
4	A	317	PX4	P1-O3-C1	3.91	102.64	121.26	5	9
4	A	349	PX4	P1-O3-C1	3.91	102.64	121.26	9	12
4	A	372	PX4	O5-C8-C7	3.91	119.67	108.40	8	8
4	A	369	PX4	C5-N1-C4	3.91	98.71	108.98	4	6
4	A	309	PX4	O5-C9-O6	3.91	113.86	123.63	14	5
4	A	353	PX4	O7-C23-O8	3.91	114.58	123.70	4	3
4	A	313	PX4	P1-O3-C1	3.90	102.68	121.26	8	11
4	A	358	PX4	O7-C23-C24	3.90	119.92	111.48	13	8
4	A	408	PX4	P1-O3-C1	3.90	102.69	121.26	8	12
4	A	343	PX4	P1-O4-C6	3.90	99.01	121.35	8	8
4	A	394	PX4	O1-P1-O2	3.90	130.58	112.44	5	12
4	A	320	PX4	P1-O3-C1	3.90	102.71	121.26	6	8
4	A	324	PX4	P1-O4-C6	3.90	99.02	121.35	1	10
4	A	323	PX4	P1-O4-C6	3.90	99.03	121.35	14	12
4	A	424	PX4	P1-O4-C6	3.90	99.03	121.35	14	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	314	PX4	C5-N1-C4	3.89	98.75	108.98	11	5
4	A	383	PX4	O1-P1-O2	3.89	130.55	112.44	3	8
4	A	415	PX4	C7-O7-C23	3.89	127.11	117.80	14	2
4	A	416	PX4	C7-O7-C23	3.89	127.11	117.80	3	3
4	A	306	PX4	C7-O7-C23	3.89	127.10	117.80	13	5
4	A	391	PX4	P1-O4-C6	3.89	99.07	121.35	9	9
4	A	368	PX4	O1-P1-O4	3.89	125.18	107.57	11	1
4	A	408	PX4	C5-N1-C4	3.89	98.77	108.98	5	3
4	A	309	PX4	C4-N1-C3	3.88	98.77	108.98	9	3
4	A	402	PX4	C5-N1-C4	3.88	98.77	108.98	14	4
4	A	356	PX4	P1-O3-C1	3.88	102.77	121.26	9	8
4	A	378	PX4	O5-C9-C10	3.88	123.68	111.83	6	2
4	A	368	PX4	O7-C7-C8	3.88	122.27	108.34	3	8
4	A	353	PX4	O7-C7-C8	3.88	122.26	108.34	6	8
4	A	400	PX4	P1-O4-C6	3.88	99.12	121.35	8	9
4	A	401	PX4	C1-C2-N1	3.88	128.27	115.82	4	4
4	A	309	PX4	O7-C7-C6	3.88	122.25	108.34	7	4
4	A	347	PX4	O1-P1-O3	3.88	90.00	107.57	2	1
4	A	369	PX4	O7-C23-C24	3.88	119.87	111.48	7	4
4	A	369	PX4	O7-C7-C8	3.88	122.25	108.34	10	6
4	A	369	PX4	O5-C8-C7	3.87	119.56	108.40	8	5
4	A	410	PX4	C26-C25-C24	3.87	98.89	113.13	5	2
4	A	425	PX4	O1-P1-O2	3.87	130.47	112.44	1	11
4	A	428	PX4	O5-C9-O6	3.87	113.94	123.63	2	4
4	A	315	PX4	O7-C7-C8	3.87	122.23	108.34	1	6
4	A	369	PX4	C7-O7-C23	3.87	108.53	117.80	1	3
4	A	407	PX4	O5-C9-O6	3.87	113.94	123.63	12	4
4	A	429	PX4	O4-P1-O2	3.87	124.27	108.94	2	2
4	A	347	PX4	O5-C9-O6	3.87	113.96	123.63	8	3
4	A	385	PX4	P1-O3-C1	3.87	102.85	121.26	9	9
4	A	334	PX4	P1-O3-C1	3.86	102.87	121.26	8	7
4	A	349	PX4	O1-P1-O2	3.86	130.41	112.44	11	10
4	A	370	PX4	O5-C9-C10	3.86	123.62	111.83	3	3
4	A	354	PX4	P1-O4-C6	3.86	99.22	121.35	13	8
4	A	385	PX4	O1-P1-O2	3.86	130.41	112.44	10	8
4	A	310	PX4	C7-O7-C23	3.86	127.04	117.80	4	4
4	A	358	PX4	O1-P1-O2	3.86	130.41	112.44	8	9
4	A	424	PX4	P1-O3-C1	3.86	102.88	121.26	1	10
4	A	393	PX4	O7-C23-O8	3.86	114.69	123.70	2	4
4	A	372	PX4	C5-N1-C3	3.85	98.85	108.98	3	3
4	A	410	PX4	P1-O4-C6	3.85	99.26	121.35	7	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	394	PX4	O5-C9-C10	3.85	123.58	111.83	3	6
4	A	321	PX4	O7-C7-C8	3.85	122.15	108.34	3	7
4	A	346	PX4	C7-O7-C23	3.85	127.00	117.80	9	4
4	A	416	PX4	O7-C7-C6	3.85	122.14	108.34	3	7
4	A	342	PX4	C5-N1-C3	3.85	98.88	108.98	12	3
4	A	417	PX4	O1-P1-O2	3.85	130.34	112.44	9	6
4	A	332	PX4	O7-C23-O8	3.84	114.72	123.70	1	5
4	A	423	PX4	O7-C23-O8	3.84	114.72	123.70	9	4
4	A	351	PX4	P1-O3-C1	3.84	102.97	121.26	5	8
4	A	357	PX4	P1-O3-C1	3.84	102.97	121.26	8	8
4	A	416	PX4	C5-N1-C4	3.84	119.07	108.98	8	5
4	A	308	PX4	C8-C7-C6	3.84	102.83	111.78	4	10
4	A	379	PX4	C1-C2-N1	3.84	128.14	115.82	4	2
4	A	389	PX4	O7-C7-C8	3.84	122.12	108.34	10	8
4	A	391	PX4	O7-C7-C8	3.84	122.11	108.34	12	5
4	A	418	PX4	O7-C7-C8	3.84	122.11	108.34	10	6
4	A	315	PX4	C12-C11-C10	3.84	99.03	113.13	11	2
4	A	383	PX4	O7-C7-C8	3.84	122.10	108.34	8	5
4	A	337	PX4	O5-C9-O6	3.83	114.04	123.63	14	4
4	A	344	PX4	P1-O4-C6	3.83	99.38	121.35	9	7
4	A	399	PX4	C5-N1-C4	3.83	119.05	108.98	10	4
4	A	359	PX4	O7-C23-O8	3.83	114.75	123.70	7	8
4	A	373	PX4	C11-C10-C9	3.83	99.67	113.69	10	3
4	A	429	PX4	O1-P1-O4	3.83	124.91	107.57	13	4
4	A	325	PX4	O5-C9-C10	3.83	123.50	111.83	9	4
4	A	330	PX4	P1-O4-C6	3.83	99.43	121.35	14	12
4	A	363	PX4	O7-C23-C24	3.82	119.75	111.48	3	3
4	A	390	PX4	O5-C9-O6	3.82	114.07	123.63	12	2
4	A	336	PX4	P1-O3-C1	3.82	103.07	121.26	6	9
4	A	396	PX4	O5-C9-C10	3.82	123.48	111.83	7	1
4	A	426	PX4	C7-O7-C23	3.81	126.92	117.80	5	11
4	A	373	PX4	O1-P1-O3	3.81	90.30	107.57	3	3
4	A	389	PX4	O7-C23-O8	3.81	114.80	123.70	11	7
4	A	418	PX4	C5-N1-C3	3.81	98.98	108.98	2	2
4	A	308	PX4	C25-C24-C23	3.81	99.75	113.69	13	1
4	A	367	PX4	C5-N1-C2	3.81	94.78	109.91	10	2
4	A	346	PX4	O1-P1-O2	3.80	130.14	112.44	12	6
4	A	430	PX4	C5-N1-C3	3.81	98.98	108.98	3	3
4	A	320	PX4	O7-C23-C24	3.80	119.70	111.48	1	6
4	A	337	PX4	P1-O3-C1	3.80	103.18	121.26	10	11
4	A	382	PX4	O7-C23-O8	3.80	114.82	123.70	13	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	354	PX4	O7-C23-O8	3.80	114.83	123.70	6	7
4	A	382	PX4	O3-P1-O2	3.80	93.89	108.94	13	3
4	A	385	PX4	C8-O5-C9	3.80	103.24	117.12	7	2
4	A	327	PX4	O7-C7-C6	3.80	121.96	108.34	14	4
4	A	349	PX4	O7-C23-O8	3.80	114.83	123.70	8	4
4	A	317	PX4	O7-C23-C24	3.79	119.69	111.48	1	7
4	A	322	PX4	O7-C23-O8	3.79	114.84	123.70	1	4
4	A	326	PX4	P1-O4-C6	3.79	99.61	121.35	9	10
4	A	397	PX4	C4-N1-C3	3.79	99.01	108.98	8	4
4	A	343	PX4	C8-C7-C6	3.79	102.95	111.78	9	9
4	A	364	PX4	P1-O4-C6	3.79	99.63	121.35	12	7
4	A	314	PX4	C12-C11-C10	3.79	99.21	113.13	10	3
4	A	338	PX4	O7-C7-C8	3.79	121.93	108.34	4	7
4	A	354	PX4	C4-N1-C3	3.79	99.03	108.98	2	1
4	A	359	PX4	P1-O4-C6	3.79	99.66	121.35	9	8
4	A	368	PX4	P1-O3-C1	3.79	103.24	121.26	4	9
4	A	429	PX4	C5-N1-C4	3.79	118.92	108.98	1	2
4	A	336	PX4	O7-C23-C24	3.78	119.67	111.48	11	5
4	A	418	PX4	P1-O3-C1	3.78	103.25	121.26	3	9
4	A	306	PX4	O5-C9-O6	3.78	114.17	123.63	7	5
4	A	329	PX4	P1-O4-C6	3.78	99.69	121.35	6	8
4	A	356	PX4	C26-C25-C24	3.78	99.24	113.13	8	3
4	A	396	PX4	O1-P1-O2	3.78	130.03	112.44	3	6
4	A	331	PX4	O7-C7-C8	3.78	121.89	108.34	13	7
4	A	352	PX4	O7-C23-C24	3.78	119.65	111.48	13	8
4	A	391	PX4	C5-N1-C4	3.78	99.05	108.98	3	3
4	A	398	PX4	C5-N1-C3	3.78	99.05	108.98	10	3
4	A	359	PX4	O7-C7-C6	3.78	121.89	108.34	4	8
4	A	404	PX4	O1-P1-O3	3.77	90.46	107.57	13	1
4	A	408	PX4	O1-P1-O2	3.78	130.01	112.44	3	8
4	A	380	PX4	O3-P1-O2	3.77	93.98	108.94	9	4
4	A	307	PX4	O1-P1-O2	3.77	130.00	112.44	10	8
4	A	320	PX4	C1-C2-N1	3.77	127.93	115.82	2	2
4	A	407	PX4	O5-C8-C7	3.77	119.27	108.40	1	10
4	A	419	PX4	O5-C9-C10	3.77	123.34	111.83	5	4
4	A	331	PX4	O3-P1-O2	3.77	93.99	108.94	4	3
4	A	331	PX4	O1-P1-O2	3.77	129.98	112.44	1	6
4	A	334	PX4	O7-C23-C24	3.77	119.64	111.48	11	7
4	A	391	PX4	O5-C8-C7	3.77	119.26	108.40	1	10
4	A	330	PX4	O7-C7-C8	3.77	121.85	108.34	9	8
4	A	315	PX4	P1-O3-C1	3.76	103.35	121.26	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	323	PX4	C7-O7-C23	3.76	126.80	117.80	10	5
4	A	326	PX4	O1-P1-O2	3.76	129.95	112.44	2	11
4	A	369	PX4	O1-P1-O2	3.76	129.96	112.44	7	9
4	A	342	PX4	O7-C23-O8	3.76	114.91	123.70	7	7
4	A	346	PX4	C4-N1-C3	3.76	99.10	108.98	7	4
4	A	415	PX4	O7-C7-C8	3.76	121.83	108.34	4	5
4	A	354	PX4	C1-C2-N1	3.76	127.88	115.82	9	1
4	A	369	PX4	O7-C23-O8	3.76	114.92	123.70	7	3
4	A	418	PX4	O1-P1-O2	3.76	129.93	112.44	14	6
4	A	397	PX4	O3-P1-O2	3.76	94.05	108.94	4	3
4	A	321	PX4	P1-O3-C1	3.76	103.38	121.26	14	12
4	A	325	PX4	C4-N1-C3	3.76	99.11	108.98	11	4
4	A	395	PX4	O5-C9-O6	3.76	114.23	123.63	1	3
4	A	323	PX4	C4-N1-C2	3.75	95.00	109.91	8	3
4	A	338	PX4	O3-P1-O2	3.75	94.09	108.94	4	2
4	A	376	PX4	O1-P1-O2	3.74	129.87	112.44	11	10
4	A	393	PX4	O7-C7-C6	3.75	121.78	108.34	9	7
4	A	329	PX4	O5-C9-C10	3.74	123.25	111.83	8	3
4	A	407	PX4	P1-O3-C1	3.74	103.44	121.26	10	10
4	A	371	PX4	O7-C7-C8	3.74	121.77	108.34	9	9
4	A	314	PX4	O7-C23-C24	3.74	103.39	111.48	10	7
4	A	330	PX4	O7-C7-C6	3.74	121.76	108.34	13	3
4	A	359	PX4	O3-P1-O2	3.74	94.12	108.94	11	4
4	A	374	PX4	C1-C2-N1	3.74	127.82	115.82	13	6
4	A	321	PX4	C11-C10-C9	3.74	100.00	113.69	12	1
4	A	386	PX4	C8-C7-C6	3.74	103.08	111.78	9	8
4	A	405	PX4	O1-P1-O3	3.74	90.63	107.57	9	2
4	A	391	PX4	O5-C9-O6	3.73	114.29	123.63	10	3
4	A	314	PX4	C4-N1-C3	3.73	99.17	108.98	7	6
4	A	349	PX4	P1-O4-C6	3.73	99.97	121.35	11	10
4	A	332	PX4	P1-O3-C1	3.73	103.52	121.26	7	11
4	A	336	PX4	O7-C23-O8	3.73	114.99	123.70	3	4
4	A	345	PX4	O3-P1-O2	3.73	94.16	108.94	1	3
4	A	409	PX4	O7-C23-O8	3.73	114.98	123.70	8	5
4	A	379	PX4	O7-C7-C8	3.73	121.72	108.34	7	6
4	A	367	PX4	O7-C7-C6	3.73	121.71	108.34	9	5
4	A	389	PX4	O5-C9-O6	3.72	114.31	123.63	7	5
4	A	422	PX4	O7-C7-C8	3.72	121.70	108.34	14	4
4	A	423	PX4	O7-C7-C8	3.72	121.70	108.34	3	5
4	A	314	PX4	O7-C7-C6	3.72	121.69	108.34	12	7
4	A	314	PX4	O5-C9-O6	3.72	114.32	123.63	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	344	PX4	C13-C12-C11	3.72	95.56	114.37	7	3
4	A	425	PX4	O3-P1-O2	3.72	94.19	108.94	6	3
4	A	312	PX4	C12-C11-C10	3.72	99.46	113.13	2	1
4	A	340	PX4	P1-O3-C1	3.72	103.56	121.26	9	12
4	A	395	PX4	O7-C7-C8	3.72	121.68	108.34	7	8
4	A	325	PX4	O1-P1-O4	3.71	124.41	107.57	5	4
4	A	318	PX4	C5-N1-C3	3.71	99.22	108.98	9	4
4	A	352	PX4	P1-O3-C1	3.71	103.59	121.26	10	7
4	A	348	PX4	O5-C9-O6	3.71	114.34	123.63	14	8
4	A	382	PX4	P1-O3-C1	3.71	103.60	121.26	6	10
4	A	398	PX4	C8-C7-C6	3.71	103.13	111.78	13	6
4	A	409	PX4	P1-O4-C6	3.71	100.09	121.35	14	11
4	A	390	PX4	P1-O3-C1	3.71	103.60	121.26	11	10
4	A	343	PX4	O5-C9-C10	3.71	123.14	111.83	5	4
4	A	345	PX4	P1-O3-C1	3.71	103.62	121.26	8	11
4	A	423	PX4	C8-C7-C6	3.71	103.14	111.78	8	8
4	A	366	PX4	O5-C9-C10	3.71	123.13	111.83	1	3
4	A	392	PX4	O7-C7-C6	3.70	121.64	108.34	1	7
4	A	402	PX4	O7-C23-O8	3.71	115.04	123.70	9	4
4	A	345	PX4	O5-C9-O6	3.70	114.36	123.63	7	2
4	A	321	PX4	O7-C23-C24	3.70	119.49	111.48	4	10
4	A	321	PX4	C8-O5-C9	3.70	103.58	117.12	12	1
4	A	339	PX4	C27-C26-C25	3.70	95.66	114.37	5	2
4	A	352	PX4	O1-P1-O2	3.70	129.65	112.44	3	10
4	A	327	PX4	O5-C9-O6	3.70	114.38	123.63	10	5
4	A	317	PX4	C5-N1-C3	3.69	118.68	108.98	14	5
4	A	348	PX4	P1-O3-C1	3.69	103.68	121.26	11	11
4	A	386	PX4	O5-C9-C10	3.69	123.09	111.83	5	6
4	A	410	PX4	O5-C9-C10	3.69	123.09	111.83	7	3
4	A	415	PX4	C5-N1-C2	3.69	95.24	109.91	3	2
4	A	419	PX4	O5-C8-C7	3.69	119.04	108.40	13	7
4	A	321	PX4	C1-C2-N1	3.69	127.66	115.82	4	3
4	A	330	PX4	C15-C14-C13	3.69	95.72	114.37	13	1
4	A	395	PX4	C5-N1-C4	3.69	99.29	108.98	6	2
4	A	349	PX4	O5-C9-C10	3.69	123.08	111.83	8	3
4	A	323	PX4	O7-C23-O8	3.69	115.09	123.70	8	4
4	A	331	PX4	C4-N1-C3	3.69	99.30	108.98	11	3
4	A	372	PX4	C19-C18-C17	3.68	95.74	114.37	5	1
4	A	321	PX4	O1-P1-O2	3.68	129.58	112.44	10	8
4	A	342	PX4	O1-P1-O2	3.68	129.57	112.44	4	10
4	A	386	PX4	O3-P1-O2	3.68	94.35	108.94	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	387	PX4	C7-O7-C23	3.68	126.60	117.80	5	5
4	A	430	PX4	O7-C7-C8	3.68	121.53	108.34	8	6
4	A	345	PX4	P1-O4-C6	3.67	100.31	121.35	14	8
4	A	358	PX4	P1-O4-C6	3.67	100.33	121.35	7	11
4	A	391	PX4	O1-P1-O2	3.67	129.51	112.44	4	8
4	A	393	PX4	C7-O7-C23	3.67	126.57	117.80	5	2
4	A	367	PX4	P1-O4-C6	3.67	100.34	121.35	7	6
4	A	422	PX4	O5-C9-O6	3.67	114.46	123.63	5	6
4	A	360	PX4	O7-C7-C6	3.66	121.49	108.34	10	4
4	A	347	PX4	O3-P1-O2	3.66	94.42	108.94	2	5
4	A	371	PX4	O1-P1-O2	3.66	129.48	112.44	4	10
4	A	317	PX4	C4-N1-C3	3.66	99.37	108.98	4	5
4	A	357	PX4	C25-C24-C23	3.66	127.10	113.69	8	3
4	A	361	PX4	O7-C7-C8	3.66	121.47	108.34	4	6
4	A	374	PX4	P1-O4-C6	3.66	100.39	121.35	13	11
4	A	393	PX4	C5-N1-C3	3.66	118.58	108.98	2	8
4	A	396	PX4	C7-O7-C23	3.66	126.55	117.80	10	4
4	A	403	PX4	P1-O3-C1	3.66	103.86	121.26	14	9
4	A	310	PX4	C5-N1-C3	3.65	99.39	108.98	13	5
4	A	335	PX4	P1-O4-C6	3.65	100.45	121.35	6	5
4	A	346	PX4	C8-O5-C9	3.65	130.45	117.12	2	2
4	A	406	PX4	O1-P1-O2	3.65	129.41	112.44	3	8
4	A	314	PX4	C32-C31-C30	3.64	95.95	114.37	10	2
4	A	403	PX4	O5-C9-C10	3.64	122.94	111.83	10	5
4	A	429	PX4	O5-C9-C10	3.64	122.95	111.83	13	3
4	A	400	PX4	C8-O5-C9	3.64	103.80	117.12	9	3
4	A	341	PX4	C5-N1-C4	3.64	99.42	108.98	1	3
4	A	343	PX4	O1-P1-O2	3.64	129.38	112.44	6	8
4	A	401	PX4	P1-O4-C6	3.64	100.50	121.35	13	11
4	A	324	PX4	O5-C9-C10	3.64	122.92	111.83	13	3
4	A	365	PX4	C5-N1-C4	3.64	99.42	108.98	3	3
4	A	368	PX4	C1-C2-N1	3.64	127.50	115.82	5	6
4	A	380	PX4	C17-C16-C15	3.64	95.99	114.37	2	2
4	A	357	PX4	P1-O4-C6	3.63	100.53	121.35	14	9
4	A	370	PX4	C5-N1-C4	3.63	118.52	108.98	11	2
4	A	427	PX4	C4-N1-C2	3.63	95.47	109.91	5	4
4	A	340	PX4	C25-C24-C23	3.63	100.39	113.69	7	4
4	A	357	PX4	O1-P1-O3	3.63	91.12	107.57	2	2
4	A	414	PX4	C7-O7-C23	3.63	126.48	117.80	6	4
4	A	429	PX4	O1-P1-O3	3.63	91.12	107.57	2	5
4	A	395	PX4	O7-C7-C6	3.63	121.36	108.34	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	363	PX4	P1-O4-C6	3.63	100.56	121.35	11	9
4	A	307	PX4	O7-C7-C8	3.63	121.35	108.34	9	4
4	A	405	PX4	O5-C9-O6	3.63	114.56	123.63	12	6
4	A	369	PX4	C26-C25-C24	3.62	99.81	113.13	5	3
4	A	396	PX4	O1-P1-O3	3.62	124.00	107.57	12	4
4	A	324	PX4	O7-C7-C8	3.62	121.34	108.34	9	5
4	A	388	PX4	O3-P1-O2	3.62	94.58	108.94	5	2
4	A	325	PX4	O5-C9-O6	3.62	114.57	123.63	4	3
4	A	392	PX4	C4-N1-C3	3.62	99.47	108.98	10	5
4	A	325	PX4	P1-O4-C6	3.62	100.62	121.35	12	10
4	A	332	PX4	O1-P1-O2	3.62	129.27	112.44	14	6
4	A	374	PX4	O7-C23-C24	3.62	119.30	111.48	6	6
4	A	393	PX4	P1-O4-C6	3.62	100.63	121.35	3	9
4	A	428	PX4	O7-C23-C24	3.61	119.30	111.48	12	8
4	A	318	PX4	O7-C7-C6	3.61	121.30	108.34	4	8
4	A	343	PX4	C1-C2-N1	3.61	127.41	115.82	4	6
4	A	362	PX4	C5-N1-C4	3.61	99.49	108.98	14	2
4	A	376	PX4	C13-C12-C11	3.61	96.12	114.37	11	3
4	A	349	PX4	O5-C9-O6	3.61	114.60	123.63	12	5
4	A	335	PX4	O4-P1-O2	3.61	123.23	108.94	9	3
4	A	361	PX4	P1-O3-C1	3.61	104.09	121.26	4	12
4	A	362	PX4	O7-C23-C24	3.61	119.28	111.48	13	7
4	A	409	PX4	C5-N1-C3	3.60	99.51	108.98	6	4
4	A	423	PX4	O7-C23-C24	3.60	119.28	111.48	2	5
4	A	339	PX4	O1-P1-O2	3.60	129.21	112.44	12	7
4	A	380	PX4	O7-C7-C8	3.60	121.27	108.34	13	9
4	A	343	PX4	C7-O7-C23	3.60	109.18	117.80	8	6
4	A	429	PX4	C25-C24-C23	3.60	100.50	113.69	11	1
4	A	360	PX4	C1-C2-N1	3.60	127.37	115.82	7	4
4	A	382	PX4	P1-O4-C6	3.60	100.74	121.35	13	9
4	A	336	PX4	C26-C25-C24	3.60	99.91	113.13	10	4
4	A	392	PX4	C5-N1-C3	3.60	118.42	108.98	9	4
4	A	372	PX4	P1-O4-C6	3.59	100.75	121.35	7	10
4	A	385	PX4	O3-C1-C2	3.59	126.94	109.65	9	1
4	A	309	PX4	C8-C7-C6	3.59	103.41	111.78	2	7
4	A	311	PX4	P1-O3-C1	3.59	104.16	121.26	11	9
4	A	374	PX4	O7-C7-C6	3.59	121.23	108.34	6	5
4	A	328	PX4	P1-O4-C6	3.59	100.78	121.35	14	11
4	A	360	PX4	O7-C23-O8	3.59	115.31	123.70	14	4
4	A	332	PX4	C1-C2-N1	3.59	127.34	115.82	8	5
4	A	361	PX4	C5-N1-C3	3.59	99.55	108.98	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	323	PX4	O5-C9-O6	3.58	114.66	123.63	9	3
4	A	343	PX4	O1-P1-O3	3.59	91.32	107.57	14	1
4	A	419	PX4	O7-C7-C8	3.59	95.48	108.34	3	6
4	A	398	PX4	O5-C9-C10	3.58	122.75	111.83	7	3
4	A	427	PX4	P1-O4-C6	3.58	100.83	121.35	1	9
4	A	357	PX4	C5-N1-C3	3.58	99.57	108.98	4	4
4	A	381	PX4	C25-C24-C23	3.58	100.58	113.69	1	2
4	A	308	PX4	O7-C7-C6	3.58	121.18	108.34	3	6
4	A	336	PX4	C5-N1-C3	3.58	99.58	108.98	11	5
4	A	327	PX4	O3-P1-O2	3.58	94.76	108.94	12	6
4	A	381	PX4	O7-C23-O8	3.58	115.34	123.70	13	5
4	A	371	PX4	C5-N1-C3	3.57	99.59	108.98	12	3
4	A	390	PX4	O4-P1-O2	3.58	123.11	108.94	5	4
4	A	407	PX4	O7-C7-C6	3.58	121.17	108.34	11	3
4	A	324	PX4	O7-C23-C24	3.57	119.21	111.48	9	5
4	A	336	PX4	P1-O4-C6	3.57	100.87	121.35	8	9
4	A	380	PX4	O7-C7-C6	3.57	121.16	108.34	7	3
4	A	334	PX4	O7-C7-C6	3.57	121.16	108.34	10	8
4	A	306	PX4	C5-N1-C4	3.57	118.35	108.98	3	3
4	A	409	PX4	O1-P1-O2	3.57	129.05	112.44	13	9
4	A	309	PX4	C1-C2-N1	3.57	127.27	115.82	11	1
4	A	312	PX4	O7-C23-O8	3.57	115.36	123.70	13	2
4	A	373	PX4	O5-C9-C10	3.57	122.71	111.83	13	4
4	A	379	PX4	O5-C9-O6	3.57	114.70	123.63	1	5
4	A	415	PX4	O1-P1-O3	3.56	91.41	107.57	1	2
4	A	340	PX4	O7-C7-C6	3.56	121.13	108.34	5	10
4	A	415	PX4	P1-O4-C6	3.56	100.93	121.35	9	10
4	A	322	PX4	O7-C7-C8	3.56	121.12	108.34	8	6
4	A	330	PX4	C33-C32-C31	3.56	96.37	114.37	3	3
4	A	390	PX4	C5-N1-C3	3.56	99.63	108.98	2	5
4	A	340	PX4	O7-C23-O8	3.56	115.39	123.70	12	4
4	A	374	PX4	C7-O7-C23	3.56	126.31	117.80	3	7
4	A	371	PX4	O5-C9-C10	3.55	122.67	111.83	12	5
4	A	395	PX4	P1-O3-C1	3.55	104.34	121.26	12	13
4	A	325	PX4	C13-C12-C11	3.55	96.41	114.37	12	2
4	A	325	PX4	P1-O3-C1	3.55	104.35	121.26	11	6
4	A	311	PX4	O1-P1-O2	3.55	128.96	112.44	13	11
4	A	379	PX4	C8-C7-C6	3.55	103.51	111.78	1	8
4	A	319	PX4	O7-C7-C8	3.55	121.08	108.34	6	6
4	A	373	PX4	C7-O7-C23	3.55	126.29	117.80	6	2
4	A	396	PX4	C1-C2-N1	3.55	127.21	115.82	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	C7-O7-C23	3.55	109.31	117.80	8	1
4	A	424	PX4	O7-C7-C8	3.55	121.06	108.34	1	3
4	A	405	PX4	C7-O7-C23	3.54	126.28	117.80	14	4
4	A	409	PX4	O1-P1-O4	3.54	123.63	107.57	3	3
4	A	412	PX4	O5-C9-O6	3.54	114.76	123.63	3	5
4	A	318	PX4	O7-C23-C24	3.54	119.14	111.48	2	6
4	A	427	PX4	C1-C2-N1	3.54	127.19	115.82	8	7
4	A	378	PX4	O1-P1-O2	3.54	128.92	112.44	4	8
4	A	348	PX4	O3-P1-O2	3.54	94.91	108.94	12	2
4	A	352	PX4	O5-C9-C10	3.54	122.63	111.83	12	5
4	A	382	PX4	O1-P1-O2	3.54	128.91	112.44	11	10
4	A	388	PX4	O1-P1-O2	3.54	128.91	112.44	11	7
4	A	427	PX4	C5-N1-C3	3.54	99.68	108.98	2	3
4	A	312	PX4	O4-P1-O2	3.54	122.95	108.94	14	2
4	A	319	PX4	O7-C23-O8	3.54	115.44	123.70	1	4
4	A	356	PX4	C5-N1-C3	3.53	99.69	108.98	13	4
4	A	377	PX4	O5-C9-C10	3.53	122.61	111.83	14	3
4	A	425	PX4	O5-C9-C10	3.53	122.61	111.83	9	2
4	A	330	PX4	C7-O7-C23	3.53	126.25	117.80	11	5
4	A	334	PX4	O3-P1-O2	3.53	94.94	108.94	8	4
4	A	362	PX4	C4-N1-C3	3.53	118.25	108.98	11	3
4	A	363	PX4	O1-P1-O2	3.53	128.88	112.44	12	5
4	A	385	PX4	O5-C9-C10	3.53	122.61	111.83	10	3
4	A	410	PX4	C5-N1-C3	3.53	99.70	108.98	10	4
4	A	424	PX4	O1-P1-O2	3.53	128.86	112.44	11	12
4	A	426	PX4	O7-C7-C8	3.53	121.00	108.34	6	8
4	A	349	PX4	O1-P1-O3	3.53	91.58	107.57	14	2
4	A	378	PX4	C31-C30-C29	3.53	96.54	114.37	9	1
4	A	381	PX4	O1-P1-O2	3.53	128.85	112.44	8	10
4	A	422	PX4	P1-O4-C6	3.53	101.14	121.35	10	7
4	A	401	PX4	O5-C9-C10	3.53	122.59	111.83	14	5
4	A	429	PX4	P1-O4-C6	3.53	101.14	121.35	8	9
4	A	319	PX4	O5-C9-C10	3.52	122.58	111.83	12	4
4	A	325	PX4	O7-C7-C6	3.52	120.98	108.34	13	5
4	A	352	PX4	O7-C23-O8	3.52	115.47	123.70	5	5
4	A	369	PX4	C3-N1-C2	3.52	123.90	109.91	11	4
4	A	416	PX4	C4-N1-C3	3.52	99.73	108.98	10	5
4	A	344	PX4	O5-C9-O6	3.52	114.83	123.63	5	3
4	A	356	PX4	C5-N1-C4	3.51	99.74	108.98	10	4
4	A	427	PX4	O3-P1-O2	3.52	95.00	108.94	9	5
4	A	340	PX4	C1-C2-N1	3.51	127.10	115.82	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	O7-C7-C6	3.51	120.95	108.34	7	6
4	A	332	PX4	C13-C12-C11	3.51	96.61	114.37	6	1
4	A	357	PX4	C5-N1-C4	3.51	99.75	108.98	5	5
4	A	411	PX4	O1-P1-O2	3.51	128.79	112.44	14	10
4	A	381	PX4	O5-C9-O6	3.51	114.84	123.63	3	7
4	A	326	PX4	C5-N1-C4	3.51	118.19	108.98	11	2
4	A	328	PX4	O1-P1-O2	3.51	128.77	112.44	3	7
4	A	351	PX4	C26-C25-C24	3.51	100.23	113.13	11	2
4	A	374	PX4	O1-P1-O2	3.51	128.77	112.44	4	8
4	A	391	PX4	C4-N1-C3	3.51	99.76	108.98	9	3
4	A	406	PX4	O7-C7-C6	3.51	120.93	108.34	8	5
4	A	418	PX4	O1-P1-O4	3.51	123.47	107.57	11	1
4	A	344	PX4	O7-C7-C6	3.51	120.93	108.34	5	4
4	A	382	PX4	O5-C9-C10	3.51	122.53	111.83	9	3
4	A	401	PX4	O7-C23-O8	3.51	115.50	123.70	7	3
4	A	357	PX4	C8-C7-C6	3.50	103.61	111.78	13	7
4	A	366	PX4	P1-O4-C6	3.50	101.27	121.35	3	12
4	A	402	PX4	P1-O4-C6	3.50	101.29	121.35	4	7
4	A	375	PX4	O1-P1-O2	3.50	128.72	112.44	2	7
4	A	397	PX4	P1-O4-C6	3.50	101.30	121.35	13	8
4	A	367	PX4	C1-C2-N1	3.50	127.05	115.82	8	1
4	A	372	PX4	O1-P1-O2	3.50	128.71	112.44	8	7
4	A	313	PX4	O1-P1-O2	3.49	128.70	112.44	1	11
4	A	343	PX4	O7-C7-C8	3.49	120.88	108.34	2	2
4	A	405	PX4	O7-C7-C6	3.49	120.88	108.34	7	5
4	A	329	PX4	C5-N1-C4	3.49	118.15	108.98	2	2
4	A	340	PX4	C11-C10-C9	3.49	100.91	113.69	6	2
4	A	342	PX4	P1-O4-C6	3.49	101.35	121.35	11	9
4	A	355	PX4	O7-C7-C8	3.49	120.86	108.34	3	7
4	A	386	PX4	O5-C9-O6	3.49	114.90	123.63	5	3
4	A	393	PX4	O5-C9-O6	3.49	114.90	123.63	1	5
4	A	415	PX4	C19-C18-C17	3.49	96.73	114.37	6	1
4	A	409	PX4	C25-C24-C23	3.49	100.92	113.69	8	3
4	A	315	PX4	C5-N1-C4	3.49	99.82	108.98	6	4
4	A	323	PX4	O7-C7-C8	3.49	120.85	108.34	10	3
4	A	370	PX4	P1-O4-C6	3.48	101.38	121.35	12	8
4	A	331	PX4	C26-C25-C24	3.48	100.33	113.13	2	3
4	A	331	PX4	O5-C9-C10	3.48	122.45	111.83	12	1
4	A	383	PX4	C11-C10-C9	3.48	100.93	113.69	5	3
4	A	334	PX4	O1-P1-O2	3.48	128.63	112.44	4	10
4	A	319	PX4	O1-P1-O2	3.48	128.63	112.44	11	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	O7-C7-C6	3.48	120.82	108.34	7	5
4	A	326	PX4	C1-C2-N1	3.48	126.98	115.82	2	6
4	A	332	PX4	O5-C9-C10	3.48	122.44	111.83	13	2
4	A	360	PX4	C5-N1-C4	3.48	99.84	108.98	11	3
4	A	372	PX4	C4-N1-C2	3.48	96.09	109.91	10	1
4	A	339	PX4	O7-C7-C6	3.48	120.81	108.34	9	7
4	A	404	PX4	O7-C23-C24	3.48	119.00	111.48	13	9
4	A	329	PX4	O1-P1-O2	3.47	128.60	112.44	2	9
4	A	337	PX4	P1-O4-C6	3.47	101.44	121.35	2	6
4	A	322	PX4	O1-P1-O3	3.47	91.84	107.57	2	3
4	A	332	PX4	O5-C8-C7	3.47	118.40	108.40	4	6
4	A	372	PX4	C4-N1-C3	3.47	99.86	108.98	2	3
4	A	383	PX4	O7-C23-O8	3.47	115.59	123.70	2	4
4	A	404	PX4	C1-C2-N1	3.47	126.96	115.82	2	4
4	A	404	PX4	C5-N1-C3	3.47	99.86	108.98	14	5
4	A	389	PX4	P1-O4-C6	3.47	101.47	121.35	7	9
4	A	411	PX4	P1-O4-C6	3.47	101.47	121.35	9	12
4	A	340	PX4	O5-C9-O6	3.47	114.95	123.63	3	3
4	A	395	PX4	C4-N1-C3	3.47	99.87	108.98	7	1
4	A	314	PX4	P1-O4-C6	3.46	101.50	121.35	3	10
4	A	340	PX4	C5-N1-C3	3.46	99.88	108.98	4	2
4	A	363	PX4	O7-C7-C6	3.46	120.77	108.34	9	5
4	A	382	PX4	C1-C2-N1	3.46	126.93	115.82	9	3
4	A	419	PX4	O3-P1-O2	3.46	95.21	108.94	1	7
4	A	309	PX4	C7-O7-C23	3.46	109.52	117.80	13	4
4	A	399	PX4	C5-N1-C3	3.46	118.06	108.98	3	2
4	A	414	PX4	P1-O4-C6	3.46	101.53	121.35	3	11
4	A	338	PX4	C26-C25-C24	3.46	100.42	113.13	4	6
4	A	426	PX4	O4-P1-O2	3.46	122.64	108.94	11	1
4	A	333	PX4	C5-N1-C3	3.46	99.90	108.98	13	5
4	A	354	PX4	O7-C7-C6	3.45	120.74	108.34	12	7
4	A	355	PX4	O5-C9-O6	3.46	114.98	123.63	5	4
4	A	360	PX4	C26-C25-C24	3.46	100.43	113.13	12	2
4	A	370	PX4	P1-O3-C1	3.46	104.80	121.26	11	10
4	A	336	PX4	C5-N1-C4	3.46	99.90	108.98	7	6
4	A	362	PX4	O7-C7-C8	3.46	120.74	108.34	11	9
4	A	368	PX4	O5-C9-O6	3.45	114.99	123.63	13	3
4	A	391	PX4	C1-C2-N1	3.45	126.91	115.82	13	3
4	A	348	PX4	P1-O4-C6	3.45	101.57	121.35	10	8
4	A	379	PX4	P1-O4-C6	3.45	101.57	121.35	12	11
4	A	348	PX4	C30-C29-C28	3.45	96.93	114.37	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	395	PX4	O4-P1-O2	3.45	122.61	108.94	7	2
4	A	426	PX4	C1-C2-N1	3.45	126.90	115.82	10	3
4	A	360	PX4	P1-O4-C6	3.45	101.58	121.35	6	8
4	A	313	PX4	P1-O4-C6	3.45	101.59	121.35	12	6
4	A	429	PX4	C27-C26-C25	3.45	96.94	114.37	1	3
4	A	415	PX4	O3-P1-O2	3.45	95.27	108.94	9	4
4	A	311	PX4	C4-N1-C2	3.45	123.60	109.91	14	2
4	A	349	PX4	O7-C7-C6	3.45	120.70	108.34	7	4
4	A	392	PX4	O7-C23-O8	3.45	115.65	123.70	7	4
4	A	375	PX4	O7-C7-C8	3.44	120.70	108.34	10	9
4	A	310	PX4	O7-C7-C6	3.44	120.69	108.34	12	6
4	A	340	PX4	C15-C14-C13	3.44	96.98	114.37	13	1
4	A	350	PX4	O5-C9-C10	3.44	122.32	111.83	4	7
4	A	403	PX4	O7-C7-C8	3.44	120.69	108.34	12	5
4	A	405	PX4	O7-C23-C24	3.44	118.92	111.48	5	11
4	A	427	PX4	O1-P1-O2	3.44	128.44	112.44	7	6
4	A	361	PX4	P1-O4-C6	3.44	101.65	121.35	9	6
4	A	377	PX4	C5-N1-C3	3.44	99.95	108.98	11	5
4	A	365	PX4	O3-P1-O2	3.44	95.32	108.94	9	2
4	A	379	PX4	O7-C7-C6	3.43	120.67	108.34	13	6
4	A	391	PX4	C7-O7-C23	3.43	126.01	117.80	9	3
4	A	375	PX4	O5-C9-C10	3.43	122.30	111.83	7	5
4	A	307	PX4	C12-C11-C10	3.43	100.53	113.13	9	3
4	A	312	PX4	C4-N1-C3	3.43	117.98	108.98	4	2
4	A	350	PX4	C20-C19-C18	3.43	97.03	114.37	14	2
4	A	361	PX4	O7-C23-O8	3.43	115.69	123.70	6	3
4	A	417	PX4	C7-O7-C23	3.43	109.59	117.80	11	3
4	A	369	PX4	C4-N1-C3	3.43	117.97	108.98	5	2
4	A	428	PX4	O7-C7-C6	3.42	120.63	108.34	8	2
4	A	352	PX4	O7-C7-C6	3.42	120.62	108.34	5	8
4	A	343	PX4	C4-N1-C3	3.42	117.96	108.98	7	4
4	A	413	PX4	C5-N1-C4	3.42	99.99	108.98	4	4
4	A	341	PX4	P1-O4-C6	3.42	101.76	121.35	6	10
4	A	354	PX4	O7-C7-C8	3.42	120.61	108.34	4	7
4	A	318	PX4	O7-C7-C8	3.42	120.60	108.34	9	4
4	A	430	PX4	O3-P1-O2	3.42	95.39	108.94	7	5
4	A	344	PX4	O3-P1-O2	3.41	95.40	108.94	12	5
4	A	354	PX4	O1-P1-O3	3.42	92.09	107.57	4	4
4	A	350	PX4	O7-C7-C6	3.41	120.59	108.34	12	4
4	A	382	PX4	C7-O7-C23	3.41	125.97	117.80	10	5
4	A	394	PX4	P1-O4-C6	3.41	101.79	121.35	10	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	356	PX4	P1-O4-C6	3.41	101.80	121.35	1	2
4	A	380	PX4	O1-P1-O2	3.41	128.32	112.44	10	9
4	A	382	PX4	O1-P1-O4	3.41	123.03	107.57	13	1
4	A	366	PX4	C4-N1-C3	3.41	100.02	108.98	11	2
4	A	357	PX4	O1-P1-O2	3.41	128.30	112.44	2	10
4	A	339	PX4	O7-C23-O8	3.41	115.74	123.70	12	3
4	A	374	PX4	O7-C23-O8	3.41	115.74	123.70	11	4
4	A	415	PX4	C12-C11-C10	3.41	100.61	113.13	6	5
4	A	330	PX4	P1-O3-C1	3.41	105.05	121.26	6	9
4	A	335	PX4	O5-C9-O6	3.40	115.11	123.63	11	5
4	A	336	PX4	C12-C11-C10	3.40	100.62	113.13	10	1
4	A	376	PX4	C5-N1-C3	3.41	100.03	108.98	1	3
4	A	306	PX4	O7-C7-C6	3.40	120.55	108.34	4	6
4	A	312	PX4	P1-O3-C1	3.40	105.07	121.26	11	5
4	A	319	PX4	P1-O4-C6	3.40	101.86	121.35	10	8
4	A	347	PX4	O7-C23-O8	3.40	115.75	123.70	4	5
4	A	324	PX4	O1-P1-O2	3.40	128.27	112.44	12	10
4	A	341	PX4	C25-C24-C23	3.40	126.16	113.69	12	3
4	A	351	PX4	O7-C23-C24	3.40	118.84	111.48	12	9
4	A	387	PX4	O7-C23-O8	3.40	115.75	123.70	12	5
4	A	346	PX4	C5-N1-C4	3.40	100.05	108.98	5	4
4	A	381	PX4	C19-C18-C17	3.40	97.18	114.37	5	1
4	A	321	PX4	O7-C23-O8	3.40	115.76	123.70	4	4
4	A	369	PX4	O1-P1-O4	3.40	122.97	107.57	14	2
4	A	306	PX4	O1-P1-O2	3.40	128.24	112.44	3	10
4	A	321	PX4	O5-C9-C10	3.39	122.18	111.83	14	3
4	A	363	PX4	O7-C7-C8	3.39	120.52	108.34	7	9
4	A	367	PX4	C14-C13-C12	3.40	97.21	114.37	11	2
4	A	425	PX4	P1-O4-C6	3.40	101.89	121.35	10	10
4	A	322	PX4	O3-P1-O2	3.39	95.49	108.94	2	4
4	A	331	PX4	C7-O7-C23	3.39	125.92	117.80	8	2
4	A	337	PX4	C25-C24-C23	3.39	101.27	113.69	14	2
4	A	360	PX4	O1-P1-O2	3.39	128.23	112.44	13	7
4	A	425	PX4	C5-N1-C3	3.39	100.06	108.98	4	3
4	A	389	PX4	C28-C27-C26	3.39	97.22	114.37	9	1
4	A	383	PX4	C13-C12-C11	3.39	97.24	114.37	12	2
4	A	400	PX4	O5-C9-C10	3.39	122.17	111.83	12	3
4	A	413	PX4	O1-P1-O2	3.39	128.22	112.44	4	7
4	A	329	PX4	O3-P1-O2	3.39	95.51	108.94	9	3
4	A	365	PX4	O1-P1-O2	3.39	128.20	112.44	8	6
4	A	430	PX4	O7-C7-C6	3.39	120.50	108.34	7	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	308	PX4	O1-P1-O2	3.39	128.19	112.44	8	9
4	A	345	PX4	O4-P1-O2	3.38	122.35	108.94	8	1
4	A	368	PX4	O1-P1-O2	3.38	128.19	112.44	1	10
4	A	326	PX4	O7-C7-C6	3.38	120.48	108.34	12	3
4	A	331	PX4	O5-C9-O6	3.38	115.17	123.63	7	5
4	A	420	PX4	O5-C9-C10	3.38	122.15	111.83	8	2
4	A	387	PX4	P1-O4-C6	3.38	101.97	121.35	12	11
4	A	401	PX4	O1-P1-O2	3.38	128.17	112.44	3	9
4	A	339	PX4	O4-P1-O2	3.38	122.33	108.94	1	3
4	A	411	PX4	C12-C11-C10	3.38	100.71	113.13	10	1
4	A	350	PX4	C7-O7-C23	3.38	125.88	117.80	1	4
4	A	318	PX4	C7-O7-C23	3.38	125.88	117.80	13	5
4	A	334	PX4	C4-N1-C3	3.38	100.11	108.98	2	4
4	A	357	PX4	O5-C9-C10	3.38	122.13	111.83	3	4
4	A	379	PX4	O1-P1-O2	3.38	128.15	112.44	4	9
4	A	418	PX4	O3-P1-O2	3.38	95.56	108.94	10	4
4	A	308	PX4	C5-N1-C3	3.37	100.11	108.98	3	6
4	A	342	PX4	C26-C25-C24	3.37	100.73	113.13	8	1
4	A	381	PX4	P1-O4-C6	3.37	102.02	121.35	6	10
4	A	385	PX4	C4-N1-C3	3.37	100.11	108.98	4	4
4	A	309	PX4	P1-O4-C6	3.37	102.03	121.35	12	10
4	A	413	PX4	C5-N1-C3	3.37	100.12	108.98	6	2
4	A	361	PX4	C4-N1-C3	3.37	100.13	108.98	4	3
4	A	369	PX4	P1-O4-C6	3.37	102.05	121.35	12	10
4	A	392	PX4	C5-N1-C4	3.37	117.82	108.98	5	6
4	A	408	PX4	O5-C9-C10	3.37	122.11	111.83	3	4
4	A	415	PX4	O7-C23-C24	3.37	118.77	111.48	7	8
4	A	319	PX4	C13-C12-C11	3.37	97.35	114.37	8	1
4	A	420	PX4	C7-O7-C23	3.37	125.86	117.80	6	4
4	A	332	PX4	C8-O5-C9	3.37	104.81	117.12	7	4
4	A	399	PX4	P1-O4-C6	3.37	102.06	121.35	12	7
4	A	355	PX4	C5-N1-C3	3.36	100.14	108.98	14	3
4	A	317	PX4	C18-C17-C16	3.36	97.38	114.37	10	3
4	A	372	PX4	O1-P1-O3	3.36	92.33	107.57	8	2
4	A	429	PX4	O3-P1-O2	3.36	95.61	108.94	8	6
4	A	425	PX4	O5-C8-C7	3.36	118.08	108.40	11	10
4	A	321	PX4	O3-P1-O2	3.35	95.64	108.94	6	4
4	A	419	PX4	O1-P1-O2	3.35	128.05	112.44	4	11
4	A	420	PX4	O7-C7-C8	3.35	120.38	108.34	2	5
4	A	422	PX4	C5-N1-C2	3.35	96.57	109.91	3	1
4	A	362	PX4	O7-C23-O8	3.35	115.86	123.70	4	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	381	PX4	O7-C7-C6	3.35	120.37	108.34	13	4
4	A	401	PX4	O1-P1-O3	3.35	92.37	107.57	5	3
4	A	342	PX4	O7-C7-C8	3.35	120.36	108.34	8	5
4	A	352	PX4	O7-C7-C8	3.35	120.36	108.34	12	7
4	A	422	PX4	O7-C7-C6	3.35	120.36	108.34	11	3
4	A	328	PX4	O7-C23-O8	3.35	115.88	123.70	8	6
4	A	329	PX4	C5-N1-C3	3.35	100.19	108.98	6	4
4	A	348	PX4	C5-N1-C3	3.35	100.19	108.98	5	3
4	A	369	PX4	C18-C17-C16	3.35	97.45	114.37	5	2
4	A	383	PX4	O1-P1-O4	3.35	122.73	107.57	11	3
4	A	313	PX4	C4-N1-C3	3.34	100.19	108.98	3	2
4	A	350	PX4	O7-C23-C24	3.34	118.71	111.48	8	6
4	A	356	PX4	C1-C2-N1	3.34	126.55	115.82	1	5
4	A	406	PX4	O1-P1-O4	3.34	122.72	107.57	1	3
4	A	408	PX4	P1-O4-C6	3.34	102.19	121.35	4	10
4	A	311	PX4	O7-C7-C6	3.34	120.33	108.34	2	5
4	A	308	PX4	C1-C2-N1	3.34	126.54	115.82	5	4
4	A	335	PX4	C12-C11-C10	3.34	100.86	113.13	6	4
4	A	366	PX4	O7-C23-C24	3.34	118.71	111.48	6	9
4	A	312	PX4	C5-N1-C3	3.34	100.21	108.98	11	2
4	A	338	PX4	O1-P1-O2	3.34	127.97	112.44	7	9
4	A	352	PX4	C4-N1-C3	3.34	100.21	108.98	3	2
4	A	414	PX4	O5-C8-C7	3.34	118.02	108.40	3	8
4	A	333	PX4	O5-C9-C10	3.33	122.00	111.83	6	6
4	A	342	PX4	O3-P1-O2	3.33	95.72	108.94	4	3
4	A	367	PX4	C26-C25-C24	3.33	100.88	113.13	10	1
4	A	420	PX4	C5-N1-C2	3.33	123.16	109.91	12	2
4	A	326	PX4	O3-P1-O2	3.33	95.73	108.94	12	2
4	A	376	PX4	C1-C2-N1	3.33	126.52	115.82	13	4
4	A	422	PX4	O3-P1-O2	3.33	95.73	108.94	10	3
4	A	430	PX4	C27-C26-C25	3.33	97.53	114.37	14	3
4	A	322	PX4	O7-C7-C6	3.33	120.28	108.34	2	6
4	A	326	PX4	C7-O7-C23	3.33	125.76	117.80	3	3
4	A	333	PX4	O3-P1-O2	3.33	95.74	108.94	8	4
4	A	394	PX4	C5-N1-C3	3.33	117.72	108.98	1	1
4	A	349	PX4	C5-N1-C4	3.33	117.72	108.98	6	4
4	A	411	PX4	O5-C9-O6	3.33	115.30	123.63	2	3
4	A	376	PX4	C5-N1-C4	3.33	100.23	108.98	3	4
4	A	406	PX4	P1-O4-C6	3.33	102.28	121.35	7	11
4	A	379	PX4	C29-C28-C27	3.33	97.55	114.37	13	1
4	A	390	PX4	C7-O7-C23	3.33	125.76	117.80	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	C5-N1-C4	3.32	117.71	108.98	9	3
4	A	307	PX4	C3-N1-C2	3.32	123.13	109.91	6	2
4	A	403	PX4	P1-O4-C6	3.33	102.30	121.35	12	6
4	A	371	PX4	P1-O4-C6	3.32	102.31	121.35	8	10
4	A	410	PX4	O7-C7-C6	3.32	120.26	108.34	7	4
4	A	338	PX4	O4-P1-O2	3.32	122.10	108.94	4	4
4	A	363	PX4	C12-C11-C10	3.32	100.92	113.13	3	4
4	A	364	PX4	C5-N1-C3	3.32	100.25	108.98	2	5
4	A	416	PX4	O7-C7-C8	3.32	120.26	108.34	9	5
4	A	326	PX4	C12-C11-C10	3.32	100.93	113.13	8	1
4	A	335	PX4	C5-N1-C3	3.32	117.69	108.98	13	1
4	A	385	PX4	O5-C9-O6	3.32	115.33	123.63	14	5
4	A	372	PX4	O5-C9-C10	3.32	121.95	111.83	5	7
4	A	421	PX4	C1-C2-N1	3.31	126.46	115.82	12	3
4	A	422	PX4	O7-C23-O8	3.31	115.95	123.70	1	5
4	A	427	PX4	O7-C7-C6	3.31	120.22	108.34	12	6
4	A	345	PX4	O1-P1-O2	3.31	127.84	112.44	13	7
4	A	381	PX4	C5-N1-C3	3.31	100.28	108.98	7	5
4	A	340	PX4	P1-O4-C6	3.31	102.39	121.35	2	8
4	A	375	PX4	C26-C25-C24	3.31	100.97	113.13	9	3
4	A	398	PX4	O5-C9-O6	3.31	115.35	123.63	10	3
4	A	394	PX4	C11-C10-C9	3.31	101.57	113.69	1	1
4	A	342	PX4	O5-C9-C10	3.31	121.92	111.83	8	2
4	A	361	PX4	C25-C24-C23	3.31	101.58	113.69	4	3
4	A	373	PX4	C15-C14-C13	3.31	97.66	114.37	13	1
4	A	428	PX4	C5-N1-C3	3.31	100.29	108.98	1	1
4	A	429	PX4	O1-P1-O2	3.31	127.82	112.44	7	9
4	A	389	PX4	O1-P1-O2	3.30	127.82	112.44	8	8
4	A	371	PX4	C19-C18-C17	3.30	97.67	114.37	4	3
4	A	418	PX4	O5-C9-O6	3.30	115.36	123.63	13	5
4	A	401	PX4	C26-C25-C24	3.30	100.99	113.13	12	2
4	A	341	PX4	C26-C25-C24	3.30	101.01	113.13	6	3
4	A	411	PX4	P1-O3-C1	3.30	105.56	121.26	5	12
4	A	312	PX4	O3-P1-O2	3.30	122.00	108.94	5	9
4	A	398	PX4	O7-C23-O8	3.30	116.00	123.70	3	2
4	A	430	PX4	O5-C9-O6	3.30	115.39	123.63	13	3
4	A	322	PX4	O1-P1-O2	3.29	127.76	112.44	4	9
4	A	375	PX4	O3-P1-O2	3.29	95.89	108.94	8	3
4	A	388	PX4	O7-C23-O8	3.29	116.01	123.70	12	7
4	A	414	PX4	O1-P1-O2	3.29	127.76	112.44	13	7
4	A	324	PX4	C5-N1-C4	3.29	100.33	108.98	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	361	PX4	O3-P1-O2	3.29	95.89	108.94	9	6
4	A	377	PX4	O1-P1-O2	3.29	127.75	112.44	2	5
4	A	410	PX4	O4-P1-O2	3.29	121.97	108.94	13	3
4	A	353	PX4	C5-N1-C4	3.29	117.61	108.98	8	1
4	A	355	PX4	O3-P1-O2	3.29	95.90	108.94	1	4
4	A	368	PX4	C28-C27-C26	3.29	97.75	114.37	13	1
4	A	376	PX4	O5-C8-C7	3.29	117.88	108.40	3	7
4	A	373	PX4	C5-N1-C3	3.29	100.34	108.98	1	2
4	A	386	PX4	O3-C1-C2	3.29	125.47	109.65	8	1
4	A	401	PX4	C5-N1-C4	3.29	100.34	108.98	5	4
4	A	389	PX4	C4-N1-C3	3.29	100.34	108.98	7	4
4	A	423	PX4	O4-P1-O2	3.29	121.96	108.94	9	1
4	A	367	PX4	O7-C23-O8	3.29	116.02	123.70	5	4
4	A	375	PX4	C4-N1-C3	3.28	100.35	108.98	3	3
4	A	426	PX4	P1-O4-C6	3.28	102.53	121.35	5	7
4	A	324	PX4	O7-C23-O8	3.28	116.04	123.70	7	3
4	A	396	PX4	C5-N1-C2	3.28	96.87	109.91	3	4
4	A	415	PX4	C32-C31-C30	3.28	97.79	114.37	7	3
4	A	360	PX4	C8-O5-C9	3.28	105.14	117.12	8	2
4	A	307	PX4	O5-C9-O6	3.28	115.43	123.63	13	3
4	A	362	PX4	C5-N1-C3	3.28	100.37	108.98	1	2
4	A	421	PX4	O1-P1-O2	3.28	127.69	112.44	14	8
4	A	363	PX4	C5-N1-C4	3.28	100.37	108.98	12	3
4	A	378	PX4	O7-C7-C8	3.27	120.09	108.34	11	5
4	A	398	PX4	O7-C7-C6	3.27	120.09	108.34	7	4
4	A	325	PX4	C3-N1-C2	3.27	122.92	109.91	11	3
4	A	336	PX4	O7-C7-C6	3.27	120.08	108.34	11	6
4	A	354	PX4	C18-C17-C16	3.27	97.82	114.37	2	1
4	A	404	PX4	C8-O5-C9	3.27	105.16	117.12	9	2
4	A	412	PX4	O7-C7-C6	3.27	120.08	108.34	1	4
4	A	377	PX4	O7-C23-O8	3.27	116.06	123.70	11	4
4	A	398	PX4	P1-O4-C6	3.27	102.62	121.35	3	12
4	A	413	PX4	O7-C23-O8	3.27	116.06	123.70	12	3
4	A	332	PX4	C12-C11-C10	3.27	101.12	113.13	14	1
4	A	384	PX4	C5-N1-C4	3.27	117.56	108.98	10	1
4	A	401	PX4	O3-P1-O2	3.27	95.98	108.94	13	4
4	A	402	PX4	O5-C9-C10	3.27	121.80	111.83	2	3
4	A	311	PX4	O3-P1-O2	3.26	96.00	108.94	1	8
4	A	320	PX4	C7-O7-C23	3.26	125.61	117.80	11	3
4	A	345	PX4	O7-C7-C8	3.26	120.05	108.34	7	3
4	A	393	PX4	C12-C11-C10	3.26	101.14	113.13	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	399	PX4	O7-C7-C6	3.26	120.05	108.34	4	3
4	A	419	PX4	C4-N1-C3	3.26	100.41	108.98	13	4
4	A	314	PX4	C3-N1-C2	3.26	96.95	109.91	8	2
4	A	331	PX4	O7-C7-C6	3.26	120.04	108.34	11	6
4	A	363	PX4	O5-C9-O6	3.26	115.47	123.63	3	3
4	A	399	PX4	O7-C23-O8	3.26	116.09	123.70	10	4
4	A	403	PX4	C8-O5-C9	3.26	105.21	117.12	3	3
4	A	312	PX4	C1-C2-N1	3.26	126.27	115.82	11	3
4	A	351	PX4	O7-C7-C8	3.26	120.03	108.34	2	8
4	A	427	PX4	O4-P1-O2	3.26	121.85	108.94	14	2
4	A	364	PX4	C1-C2-N1	3.25	126.27	115.82	12	5
4	A	366	PX4	O4-P1-O2	3.25	121.83	108.94	12	4
4	A	341	PX4	C7-O7-C23	3.25	125.58	117.80	11	5
4	A	393	PX4	C1-C2-N1	3.25	126.26	115.82	11	4
4	A	306	PX4	P1-O3-C1	3.25	105.79	121.26	14	11
4	A	317	PX4	P1-O4-C6	3.25	102.73	121.35	1	9
4	A	351	PX4	P1-O4-C6	3.25	102.73	121.35	1	8
4	A	412	PX4	C30-C29-C28	3.25	97.94	114.37	14	3
4	A	379	PX4	O7-C23-O8	3.25	116.11	123.70	4	4
4	A	315	PX4	C7-O7-C23	3.25	125.56	117.80	5	6
4	A	329	PX4	C1-C2-N1	3.25	126.24	115.82	2	4
4	A	323	PX4	C4-N1-C3	3.25	117.50	108.98	10	3
4	A	351	PX4	O7-C23-O8	3.25	116.12	123.70	8	2
4	A	420	PX4	O1-P1-O4	3.24	92.87	107.57	14	1
4	A	331	PX4	C5-N1-C3	3.24	100.46	108.98	13	6
4	A	335	PX4	O7-C7-C8	3.24	119.98	108.34	11	5
4	A	360	PX4	C4-N1-C3	3.24	100.46	108.98	14	4
4	A	371	PX4	O1-P1-O3	3.24	92.88	107.57	10	4
4	A	420	PX4	C5-N1-C3	3.24	117.49	108.98	5	1
4	A	320	PX4	C5-N1-C3	3.24	117.48	108.98	14	6
4	A	321	PX4	C26-C25-C24	3.24	101.23	113.13	10	4
4	A	344	PX4	O7-C7-C8	3.24	119.96	108.34	8	6
4	A	360	PX4	O5-C9-C10	3.24	121.71	111.83	9	4
4	A	370	PX4	O7-C7-C8	3.24	119.97	108.34	2	7
4	A	378	PX4	O7-C7-C6	3.24	119.96	108.34	8	9
4	A	417	PX4	P1-O3-C1	3.24	105.84	121.26	3	9
4	A	329	PX4	C25-C24-C23	3.24	101.83	113.69	6	1
4	A	339	PX4	C26-C25-C24	3.24	101.24	113.13	5	4
4	A	344	PX4	O7-C23-O8	3.24	116.14	123.70	10	4
4	A	381	PX4	O1-P1-O3	3.23	92.91	107.57	6	4
4	A	388	PX4	C28-C27-C26	3.24	98.02	114.37	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	C18-C17-C16	3.24	98.01	114.37	10	1
4	A	391	PX4	O7-C7-C6	3.23	119.95	108.34	14	4
4	A	420	PX4	O7-C23-O8	3.23	116.14	123.70	2	3
4	A	310	PX4	C1-C2-N1	3.23	126.20	115.82	1	4
4	A	320	PX4	C5-N1-C4	3.23	100.49	108.98	7	2
4	A	350	PX4	O7-C7-C8	3.23	119.94	108.34	8	4
4	A	368	PX4	O5-C9-C10	3.23	121.69	111.83	6	4
4	A	408	PX4	C1-C2-N1	3.23	126.20	115.82	6	4
4	A	426	PX4	O7-C7-C6	3.23	119.94	108.34	13	7
4	A	368	PX4	O7-C7-C6	3.23	119.92	108.34	5	4
4	A	376	PX4	P1-O4-C6	3.23	102.85	121.35	14	8
4	A	323	PX4	O1-P1-O2	3.23	127.45	112.44	10	5
4	A	418	PX4	O7-C7-C6	3.23	119.92	108.34	5	2
4	A	324	PX4	C5-N1-C2	3.22	97.09	109.91	5	1
4	A	319	PX4	O4-P1-O2	3.22	121.71	108.94	6	3
4	A	333	PX4	C1-C2-N1	3.22	126.17	115.82	1	3
4	A	341	PX4	O1-P1-O4	3.22	122.17	107.57	14	2
4	A	411	PX4	C3-N1-C2	3.22	122.72	109.91	3	1
4	A	405	PX4	O4-P1-O2	3.22	121.70	108.94	9	3
4	A	334	PX4	O7-C23-O8	3.22	116.18	123.70	9	4
4	A	355	PX4	C4-N1-C3	3.22	117.43	108.98	5	7
4	A	423	PX4	O3-P1-O2	3.22	96.17	108.94	1	3
4	A	430	PX4	P1-O4-C6	3.22	102.90	121.35	4	8
4	A	362	PX4	P1-O4-C6	3.22	102.91	121.35	9	6
4	A	332	PX4	O1-P1-O3	3.22	92.99	107.57	13	3
4	A	343	PX4	O4-P1-O2	3.22	96.18	108.94	6	1
4	A	344	PX4	O4-P1-O2	3.22	121.68	108.94	10	3
4	A	359	PX4	C5-N1-C4	3.22	117.43	108.98	2	4
4	A	352	PX4	P1-O4-C6	3.22	102.92	121.35	6	6
4	A	359	PX4	C14-C13-C12	3.22	98.11	114.37	9	1
4	A	397	PX4	C1-C2-N1	3.22	126.15	115.82	6	2
4	A	310	PX4	O1-P1-O2	3.21	127.40	112.44	2	8
4	A	319	PX4	O5-C9-O6	3.22	115.59	123.63	7	3
4	A	313	PX4	C5-N1-C4	3.21	100.54	108.98	7	2
4	A	365	PX4	P1-O4-C6	3.21	102.94	121.35	11	8
4	A	386	PX4	O7-C7-C6	3.21	119.87	108.34	5	3
4	A	324	PX4	C14-C13-C12	3.21	98.14	114.37	5	2
4	A	408	PX4	O5-C9-O6	3.21	115.59	123.63	4	3
4	A	333	PX4	P1-O3-C1	3.21	105.98	121.26	4	5
4	A	308	PX4	P1-O4-C6	3.21	102.97	121.35	9	9
4	A	347	PX4	P1-O4-C6	3.21	102.96	121.35	4	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	330	PX4	C27-C26-C25	3.21	98.16	114.37	9	2
4	A	329	PX4	O5-C9-O6	3.21	115.61	123.63	10	6
4	A	363	PX4	O7-C23-O8	3.21	116.21	123.70	7	5
4	A	375	PX4	C28-C27-C26	3.21	98.17	114.37	11	1
4	A	378	PX4	C25-C24-C23	3.21	101.95	113.69	1	2
4	A	328	PX4	O3-P1-O2	3.20	96.24	108.94	3	4
4	A	331	PX4	C8-O5-C9	3.20	105.41	117.12	6	3
4	A	349	PX4	C20-C19-C18	3.20	98.17	114.37	11	1
4	A	352	PX4	C26-C25-C24	3.20	101.36	113.13	8	2
4	A	406	PX4	C5-N1-C2	3.20	122.64	109.91	12	3
4	A	423	PX4	C1-C2-N1	3.20	126.10	115.82	12	4
4	A	306	PX4	O1-P1-O4	3.20	122.08	107.57	1	2
4	A	358	PX4	C5-N1-C3	3.20	100.57	108.98	14	3
4	A	381	PX4	C4-N1-C2	3.20	97.19	109.91	13	5
4	A	346	PX4	O7-C7-C6	3.20	119.82	108.34	14	3
4	A	352	PX4	C32-C31-C30	3.20	98.21	114.37	12	1
4	A	424	PX4	O5-C9-O6	3.20	115.63	123.63	1	5
4	A	306	PX4	O7-C23-O8	3.19	116.24	123.70	4	6
4	A	387	PX4	C27-C26-C25	3.19	98.22	114.37	7	2
4	A	383	PX4	O5-C9-O6	3.19	115.64	123.63	14	4
4	A	412	PX4	O5-C9-C10	3.19	121.57	111.83	3	6
4	A	415	PX4	O7-C7-C6	3.19	119.80	108.34	3	5
4	A	418	PX4	C34-C33-C32	3.19	98.23	114.37	6	2
4	A	335	PX4	C19-C18-C17	3.19	98.25	114.37	4	2
4	A	362	PX4	O5-C9-O6	3.19	115.65	123.63	5	3
4	A	412	PX4	C7-O7-C23	3.19	125.43	117.80	1	3
4	A	427	PX4	O5-C9-O6	3.19	115.65	123.63	3	8
4	A	368	PX4	O7-C23-C24	3.19	118.38	111.48	7	5
4	A	312	PX4	C16-C15-C14	3.19	98.26	114.37	9	2
4	A	373	PX4	C4-N1-C3	3.19	100.61	108.98	10	4
4	A	314	PX4	O1-P1-O2	3.18	127.26	112.44	3	6
4	A	320	PX4	O7-C7-C6	3.18	119.77	108.34	4	7
4	A	323	PX4	C8-O5-C9	3.18	105.48	117.12	3	3
4	A	346	PX4	O7-C7-C8	3.18	119.77	108.34	10	10
4	A	336	PX4	O5-C9-C10	3.18	121.54	111.83	4	2
4	A	324	PX4	O3-P1-O2	3.18	96.32	108.94	12	1
4	A	403	PX4	C5-N1-C4	3.18	100.62	108.98	12	3
4	A	336	PX4	O5-C9-O6	3.18	115.67	123.63	5	5
4	A	358	PX4	O3-P1-O2	3.18	96.33	108.94	8	3
4	A	415	PX4	C5-N1-C3	3.18	117.33	108.98	1	3
4	A	307	PX4	C4-N1-C3	3.18	100.62	108.98	9	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	329	PX4	O7-C7-C8	3.18	119.75	108.34	5	5
4	A	336	PX4	C7-O7-C23	3.18	125.40	117.80	14	4
4	A	357	PX4	O7-C7-C8	3.18	119.75	108.34	11	4
4	A	383	PX4	O5-C9-C10	3.18	121.52	111.83	11	3
4	A	390	PX4	O1-P1-O3	3.18	93.16	107.57	11	3
4	A	337	PX4	O1-P1-O2	3.18	127.22	112.44	12	9
4	A	365	PX4	C8-O5-C9	3.18	105.51	117.12	10	4
4	A	378	PX4	C27-C26-C25	3.18	98.31	114.37	8	1
4	A	309	PX4	O7-C7-C8	3.17	119.73	108.34	8	3
4	A	417	PX4	O5-C9-C10	3.17	121.51	111.83	1	5
4	A	345	PX4	O1-P1-O4	3.17	121.94	107.57	10	2
4	A	349	PX4	C4-N1-C3	3.17	100.64	108.98	5	4
4	A	323	PX4	O5-C8-C7	3.17	117.54	108.40	12	6
4	A	380	PX4	O5-C9-O6	3.17	115.70	123.63	7	2
4	A	417	PX4	C20-C19-C18	3.17	98.35	114.37	4	1
4	A	425	PX4	O7-C23-O8	3.17	116.29	123.70	2	3
4	A	312	PX4	P1-O4-C6	3.17	103.19	121.35	9	6
4	A	377	PX4	O3-P1-O2	3.17	96.38	108.94	11	2
4	A	388	PX4	C1-C2-N1	3.17	125.99	115.82	7	2
4	A	403	PX4	O7-C23-O8	3.17	116.30	123.70	2	5
4	A	430	PX4	C5-N1-C4	3.17	100.65	108.98	12	3
4	A	332	PX4	C5-N1-C3	3.17	117.29	108.98	3	2
4	A	358	PX4	C17-C16-C15	3.17	98.36	114.37	2	2
4	A	359	PX4	C29-C28-C27	3.17	98.36	114.37	8	1
4	A	377	PX4	C1-C2-N1	3.17	125.98	115.82	1	3
4	A	398	PX4	C1-C2-N1	3.17	125.98	115.82	11	5
4	A	426	PX4	O5-C9-C10	3.17	121.49	111.83	6	5
4	A	424	PX4	C4-N1-C2	3.17	122.49	109.91	12	3
4	A	336	PX4	C4-N1-C3	3.16	100.67	108.98	5	4
4	A	358	PX4	O4-P1-O2	3.16	121.47	108.94	1	3
4	A	367	PX4	O1-P1-O3	3.16	93.23	107.57	8	2
4	A	307	PX4	P1-O4-C6	3.16	103.23	121.35	7	7
4	A	313	PX4	O7-C7-C8	3.16	119.69	108.34	11	6
4	A	385	PX4	O6-C9-C10	3.16	111.41	123.78	4	1
4	A	339	PX4	C20-C19-C18	3.16	98.40	114.37	6	1
4	A	340	PX4	O1-P1-O2	3.16	127.15	112.44	6	9
4	A	428	PX4	O1-P1-O2	3.16	127.13	112.44	11	7
4	A	430	PX4	C4-N1-C3	3.16	117.27	108.98	6	4
4	A	335	PX4	C3-N1-C2	3.16	97.36	109.91	13	2
4	A	378	PX4	P1-O4-C6	3.16	103.27	121.35	3	8
4	A	395	PX4	O1-P1-O4	3.16	121.87	107.57	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	317	PX4	C26-C25-C24	3.15	101.54	113.13	13	3
4	A	370	PX4	C25-C24-C23	3.15	102.14	113.69	1	2
4	A	379	PX4	C8-O5-C9	3.15	105.59	117.12	5	3
4	A	316	PX4	C7-O7-C23	3.15	125.34	117.80	14	2
4	A	371	PX4	O3-C1-C2	3.15	124.81	109.65	3	4
4	A	373	PX4	O5-C9-O6	3.15	115.75	123.63	6	5
4	A	412	PX4	C8-C7-C6	3.15	104.44	111.78	8	6
4	A	424	PX4	C8-O5-C9	3.15	105.60	117.12	13	1
4	A	368	PX4	C12-C11-C10	3.15	101.56	113.13	6	3
4	A	410	PX4	O7-C23-O8	3.15	116.34	123.70	14	4
4	A	385	PX4	P1-O4-C6	3.15	103.32	121.35	2	9
4	A	413	PX4	O7-C7-C6	3.15	119.64	108.34	7	5
4	A	338	PX4	O7-C23-O8	3.15	116.35	123.70	13	5
4	A	352	PX4	C5-N1-C3	3.15	100.71	108.98	12	1
4	A	407	PX4	O5-C9-C10	3.15	121.43	111.83	10	4
4	A	391	PX4	C31-C30-C29	3.14	98.47	114.37	9	1
4	A	330	PX4	C5-N1-C2	3.14	122.40	109.91	1	1
4	A	342	PX4	C15-C14-C13	3.14	98.48	114.37	5	1
4	A	364	PX4	C5-N1-C4	3.14	100.72	108.98	8	3
4	A	375	PX4	O7-C7-C6	3.14	119.62	108.34	5	5
4	A	394	PX4	O7-C7-C6	3.14	119.62	108.34	14	5
4	A	361	PX4	C8-O5-C9	3.14	105.64	117.12	10	1
4	A	369	PX4	C1-C2-N1	3.14	125.90	115.82	14	4
4	A	424	PX4	C5-N1-C2	3.14	97.43	109.91	5	2
4	A	392	PX4	C12-C11-C10	3.14	101.59	113.13	14	3
4	A	412	PX4	C5-N1-C4	3.14	100.73	108.98	13	2
4	A	311	PX4	O4-P1-O2	3.14	121.37	108.94	5	1
4	A	335	PX4	O7-C23-O8	3.14	116.37	123.70	3	2
4	A	354	PX4	O1-P1-O4	3.14	121.79	107.57	4	2
4	A	430	PX4	O1-P1-O2	3.14	127.05	112.44	11	6
4	A	397	PX4	O5-C9-C10	3.14	121.39	111.83	12	2
4	A	379	PX4	C26-C25-C24	3.13	101.61	113.13	11	2
4	A	398	PX4	C32-C31-C30	3.13	98.53	114.37	12	2
4	A	420	PX4	P1-O4-C6	3.13	103.40	121.35	11	11
4	A	345	PX4	C5-N1-C3	3.13	100.75	108.98	10	3
4	A	426	PX4	O1-P1-O2	3.13	127.01	112.44	13	8
4	A	320	PX4	O5-C9-O6	3.13	115.80	123.63	10	5
4	A	333	PX4	O1-P1-O2	3.13	127.00	112.44	3	9
4	A	414	PX4	C12-C11-C10	3.13	124.63	113.13	4	3
4	A	412	PX4	C12-C11-C10	3.13	101.63	113.13	11	3
4	A	371	PX4	C16-C15-C14	3.13	98.57	114.37	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	339	PX4	P1-O4-C6	3.12	103.45	121.35	1	7
4	A	341	PX4	O1-P1-O2	3.12	126.97	112.44	7	8
4	A	345	PX4	C4-N1-C3	3.12	100.77	108.98	6	1
4	A	365	PX4	C1-C2-N1	3.12	125.84	115.82	4	5
4	A	420	PX4	C4-N1-C2	3.12	122.32	109.91	3	2
4	A	316	PX4	O7-C23-O8	3.12	116.41	123.70	10	6
4	A	326	PX4	O7-C7-C8	3.12	119.53	108.34	2	5
4	A	333	PX4	C5-N1-C4	3.12	117.17	108.98	9	2
4	A	376	PX4	O7-C23-O8	3.12	116.41	123.70	3	4
4	A	418	PX4	C26-C25-C24	3.12	101.66	113.13	4	3
4	A	353	PX4	O5-C9-C10	3.12	121.34	111.83	2	5
4	A	360	PX4	C7-O7-C23	3.12	125.26	117.80	2	4
4	A	374	PX4	C18-C17-C16	3.12	98.60	114.37	13	3
4	A	313	PX4	O8-C23-C24	3.12	111.59	123.78	6	2
4	A	362	PX4	C26-C25-C24	3.12	101.67	113.13	2	5
4	A	372	PX4	C27-C26-C25	3.12	98.61	114.37	7	4
4	A	364	PX4	O5-C9-C10	3.12	121.34	111.83	13	4
4	A	366	PX4	C29-C28-C27	3.12	98.62	114.37	1	5
4	A	386	PX4	C5-N1-C3	3.12	100.79	108.98	9	4
4	A	353	PX4	C4-N1-C3	3.11	100.80	108.98	4	5
4	A	330	PX4	C29-C28-C27	3.11	98.63	114.37	13	3
4	A	384	PX4	C4-N1-C3	3.11	100.80	108.98	10	3
4	A	420	PX4	C5-N1-C4	3.11	100.80	108.98	3	5
4	A	355	PX4	O5-C9-C10	3.11	121.32	111.83	2	3
4	A	361	PX4	O1-P1-O4	3.11	121.67	107.57	4	3
4	A	404	PX4	C4-N1-C3	3.11	100.81	108.98	1	5
4	A	319	PX4	C5-N1-C4	3.11	100.81	108.98	14	2
4	A	342	PX4	C20-C19-C18	3.11	98.65	114.37	4	2
4	A	327	PX4	O7-C7-C8	3.11	119.49	108.34	7	5
4	A	339	PX4	O3-C1-C2	3.11	124.60	109.65	8	1
4	A	365	PX4	C5-N1-C2	3.11	122.26	109.91	1	1
4	A	356	PX4	O1-P1-O2	3.11	126.89	112.44	14	10
4	A	366	PX4	O1-P1-O4	3.11	121.65	107.57	5	5
4	A	398	PX4	C7-O7-C23	3.11	110.36	117.80	1	1
4	A	423	PX4	C26-C25-C24	3.11	101.71	113.13	3	1
4	A	419	PX4	O4-P1-O2	3.11	121.24	108.94	3	3
4	A	357	PX4	O7-C7-C6	3.10	119.48	108.34	8	7
4	A	402	PX4	O7-C7-C8	3.10	119.48	108.34	2	7
4	A	322	PX4	C26-C25-C24	3.10	101.72	113.13	3	7
4	A	419	PX4	C1-C2-N1	3.10	125.78	115.82	3	5
4	A	320	PX4	O1-P1-O2	3.10	126.87	112.44	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	351	PX4	O1-P1-O3	3.10	93.51	107.57	8	1
4	A	401	PX4	O5-C9-O6	3.10	115.87	123.63	8	6
4	A	408	PX4	O7-C23-O8	3.10	116.45	123.70	1	5
4	A	307	PX4	C17-C16-C15	3.10	98.71	114.37	12	2
4	A	325	PX4	C5-N1-C3	3.10	100.83	108.98	3	2
4	A	357	PX4	C31-C30-C29	3.10	98.70	114.37	7	1
4	A	413	PX4	P1-O4-C6	3.10	103.58	121.35	7	10
4	A	382	PX4	C8-O5-C9	3.10	128.44	117.12	7	4
4	A	308	PX4	C7-O7-C23	3.10	110.39	117.80	9	2
4	A	364	PX4	C34-C33-C32	3.10	98.72	114.37	5	1
4	A	399	PX4	C34-C33-C32	3.09	98.72	114.37	3	2
4	A	416	PX4	C8-O5-C9	3.10	105.80	117.12	13	3
4	A	382	PX4	O5-C9-O6	3.09	115.89	123.63	6	6
4	A	405	PX4	C5-N1-C3	3.09	117.10	108.98	8	4
4	A	337	PX4	O7-C23-O8	3.09	116.48	123.70	7	3
4	A	345	PX4	O3-C1-C2	3.09	124.53	109.65	7	2
4	A	357	PX4	C1-C2-N1	3.09	125.74	115.82	14	2
4	A	405	PX4	C5-N1-C4	3.09	117.10	108.98	3	3
4	A	429	PX4	O7-C7-C8	3.09	119.43	108.34	2	5
4	A	351	PX4	O5-C9-O6	3.09	115.90	123.63	8	3
4	A	359	PX4	C7-O7-C23	3.09	110.40	117.80	11	5
4	A	382	PX4	O7-C7-C6	3.09	119.43	108.34	8	4
4	A	360	PX4	O7-C7-C8	3.09	119.42	108.34	7	3
4	A	318	PX4	C1-C2-N1	3.09	125.73	115.82	11	6
4	A	408	PX4	O7-C7-C6	3.09	119.42	108.34	5	5
4	A	316	PX4	O3-P1-O2	3.08	96.71	108.94	5	3
4	A	334	PX4	C8-O5-C9	3.08	105.85	117.12	4	3
4	A	344	PX4	O1-P1-O4	3.08	121.55	107.57	3	4
4	A	380	PX4	C33-C32-C31	3.08	98.78	114.37	5	1
4	A	406	PX4	O7-C23-O8	3.08	116.50	123.70	4	4
4	A	422	PX4	O1-P1-O2	3.08	126.79	112.44	1	9
4	A	373	PX4	C1-C2-N1	3.08	125.71	115.82	2	7
4	A	316	PX4	P1-O4-C6	3.08	103.70	121.35	10	7
4	A	325	PX4	O4-P1-O2	3.08	121.14	108.94	8	2
4	A	362	PX4	C12-C11-C10	3.08	101.81	113.13	6	1
4	A	388	PX4	O5-C9-C10	3.08	121.22	111.83	5	2
4	A	314	PX4	O1-P1-O3	3.08	93.62	107.57	13	1
4	A	313	PX4	C26-C25-C24	3.08	101.83	113.13	14	3
4	A	382	PX4	C19-C18-C17	3.08	98.82	114.37	3	2
4	A	421	PX4	O4-P1-O2	3.08	96.74	108.94	13	2
4	A	388	PX4	C8-O5-C9	3.07	105.88	117.12	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	394	PX4	C5-N1-C4	3.07	117.05	108.98	4	5
4	A	426	PX4	C5-N1-C3	3.07	100.90	108.98	14	4
4	A	411	PX4	C26-C25-C24	3.07	101.84	113.13	7	3
4	A	311	PX4	O1-P1-O4	3.07	121.49	107.57	12	4
4	A	391	PX4	O1-P1-O4	3.07	121.48	107.57	9	3
4	A	406	PX4	C33-C32-C31	3.07	98.85	114.37	3	2
4	A	418	PX4	O5-C9-C10	3.07	121.20	111.83	8	5
4	A	341	PX4	C5-N1-C3	3.07	100.91	108.98	3	3
4	A	368	PX4	C25-C24-C23	3.07	102.44	113.69	4	2
4	A	307	PX4	C4-N1-C2	3.07	97.72	109.91	6	4
4	A	328	PX4	C4-N1-C3	3.07	100.92	108.98	2	4
4	A	412	PX4	P1-O4-C6	3.07	103.76	121.35	10	5
4	A	384	PX4	C7-O7-C23	3.07	110.45	117.80	12	1
4	A	412	PX4	O7-C7-C8	3.07	119.35	108.34	14	5
4	A	308	PX4	O5-C9-C10	3.07	121.19	111.83	11	4
4	A	322	PX4	P1-O4-C6	3.07	103.78	121.35	6	8
4	A	323	PX4	C5-N1-C3	3.07	117.03	108.98	9	4
4	A	333	PX4	O5-C9-O6	3.07	115.96	123.63	7	6
4	A	342	PX4	C7-O7-C23	3.07	125.13	117.80	3	3
4	A	360	PX4	O3-P1-O2	3.07	96.78	108.94	2	4
4	A	404	PX4	O7-C7-C6	3.07	119.34	108.34	2	6
4	A	347	PX4	O7-C7-C6	3.06	119.33	108.34	12	4
4	A	352	PX4	O1-P1-O4	3.06	121.45	107.57	5	2
4	A	412	PX4	O1-P1-O2	3.06	126.69	112.44	14	4
4	A	309	PX4	C5-N1-C4	3.06	100.94	108.98	7	4
4	A	367	PX4	C5-N1-C4	3.06	100.93	108.98	12	2
4	A	375	PX4	C25-C24-C23	3.06	102.48	113.69	6	2
4	A	405	PX4	O7-C7-C8	3.06	119.32	108.34	14	3
4	A	321	PX4	O5-C9-O6	3.06	115.98	123.63	1	3
4	A	323	PX4	O4-P1-O2	3.06	121.05	108.94	8	1
4	A	417	PX4	C33-C32-C31	3.06	98.91	114.37	1	3
4	A	422	PX4	C5-N1-C4	3.06	117.01	108.98	9	1
4	A	316	PX4	O4-P1-O2	3.06	121.05	108.94	4	2
4	A	335	PX4	O7-C7-C6	3.06	119.31	108.34	3	4
4	A	366	PX4	C30-C29-C28	3.06	98.92	114.37	10	2
4	A	384	PX4	O4-P1-O2	3.06	96.82	108.94	4	3
4	A	423	PX4	O1-P1-O2	3.06	126.66	112.44	9	5
4	A	353	PX4	C28-C27-C26	3.05	98.93	114.37	1	1
4	A	381	PX4	C26-C25-C24	3.05	101.90	113.13	14	4
4	A	380	PX4	C5-N1-C2	3.05	122.04	109.91	6	1
4	A	387	PX4	O1-P1-O3	3.05	93.73	107.57	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	C3-N1-C2	3.05	122.04	109.91	3	2
4	A	425	PX4	C5-N1-C4	3.05	100.96	108.98	13	1
4	A	365	PX4	O7-C7-C8	3.05	119.28	108.34	7	4
4	A	375	PX4	C5-N1-C4	3.05	100.97	108.98	1	4
4	A	409	PX4	C26-C25-C24	3.05	101.92	113.13	11	2
4	A	333	PX4	P1-O4-C6	3.05	103.89	121.35	9	8
4	A	333	PX4	C29-C28-C27	3.05	98.97	114.37	1	2
4	A	407	PX4	O3-C1-C2	3.05	124.31	109.65	4	1
4	A	313	PX4	O4-P1-O2	3.04	121.00	108.94	13	2
4	A	322	PX4	O5-C8-C7	3.04	117.17	108.40	6	7
4	A	331	PX4	C11-C10-C9	3.04	102.54	113.69	6	1
4	A	388	PX4	C7-O7-C23	3.04	110.51	117.80	13	6
4	A	343	PX4	C11-C10-C9	3.04	102.55	113.69	3	2
4	A	384	PX4	C1-C2-N1	3.04	125.57	115.82	4	4
4	A	387	PX4	O5-C9-C10	3.04	121.10	111.83	14	4
4	A	399	PX4	O1-P1-O2	3.04	126.58	112.44	11	7
4	A	405	PX4	O1-P1-O2	3.04	126.58	112.44	6	8
4	A	339	PX4	C32-C31-C30	3.04	99.01	114.37	12	2
4	A	398	PX4	C4-N1-C3	3.04	101.00	108.98	7	3
4	A	410	PX4	O5-C8-C7	3.04	117.15	108.40	12	3
4	A	424	PX4	O1-P1-O3	3.04	93.80	107.57	1	4
4	A	311	PX4	P1-O4-C6	3.04	103.96	121.35	1	4
4	A	354	PX4	C26-C25-C24	3.03	101.98	113.13	10	1
4	A	397	PX4	C15-C14-C13	3.03	99.03	114.37	13	1
4	A	308	PX4	O1-P1-O3	3.03	93.83	107.57	8	1
4	A	337	PX4	C5-N1-C4	3.03	101.02	108.98	14	3
4	A	373	PX4	C16-C15-C14	3.03	99.05	114.37	3	4
4	A	383	PX4	C5-N1-C4	3.03	101.02	108.98	13	5
4	A	409	PX4	C5-N1-C4	3.03	101.01	108.98	14	5
4	A	387	PX4	O1-P1-O2	3.03	126.54	112.44	4	10
4	A	388	PX4	O7-C7-C8	3.03	119.21	108.34	12	3
4	A	340	PX4	C19-C18-C17	3.03	99.07	114.37	10	2
4	A	315	PX4	O7-C23-O8	3.02	116.63	123.70	3	3
4	A	320	PX4	O5-C9-C10	3.03	121.06	111.83	11	4
4	A	352	PX4	C1-C2-N1	3.03	125.53	115.82	11	5
4	A	354	PX4	C12-C11-C10	3.03	102.01	113.13	9	2
4	A	355	PX4	O7-C23-O8	3.03	116.63	123.70	2	4
4	A	413	PX4	C8-O5-C9	3.03	106.05	117.12	2	5
4	A	411	PX4	C5-N1-C2	3.03	121.94	109.91	6	2
4	A	329	PX4	C4-N1-C3	3.02	101.03	108.98	13	2
4	A	330	PX4	C8-O5-C9	3.02	106.06	117.12	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	338	PX4	C25-C24-C23	3.02	102.61	113.69	5	2
4	A	348	PX4	O7-C7-C6	3.02	119.19	108.34	8	5
4	A	385	PX4	C5-N1-C3	3.02	101.03	108.98	14	6
4	A	399	PX4	O7-C7-C8	3.02	119.19	108.34	7	4
4	A	430	PX4	C8-O5-C9	3.02	106.06	117.12	7	6
4	A	414	PX4	O7-C7-C8	3.02	119.19	108.34	12	6
4	A	414	PX4	O7-C7-C6	3.02	119.19	108.34	4	3
4	A	384	PX4	C12-C11-C10	3.02	102.03	113.13	3	1
4	A	316	PX4	C4-N1-C3	3.02	101.04	108.98	1	2
4	A	412	PX4	C5-N1-C3	3.02	116.91	108.98	10	2
4	A	327	PX4	P1-O4-C6	3.02	104.05	121.35	7	5
4	A	372	PX4	O7-C23-O8	3.02	116.65	123.70	7	3
4	A	428	PX4	C3-N1-C2	3.02	97.91	109.91	9	1
4	A	326	PX4	C5-N1-C3	3.02	101.05	108.98	12	3
4	A	354	PX4	C33-C32-C31	3.02	99.11	114.37	2	1
4	A	332	PX4	C5-N1-C4	3.02	101.05	108.98	14	3
4	A	359	PX4	O1-P1-O2	3.02	126.48	112.44	1	7
4	A	368	PX4	O7-C23-O8	3.02	116.65	123.70	14	4
4	A	390	PX4	C5-N1-C4	3.02	116.91	108.98	8	3
4	A	378	PX4	C26-C25-C24	3.02	124.21	113.13	6	2
4	A	415	PX4	O4-P1-O2	3.02	120.89	108.94	9	1
4	A	426	PX4	C8-O5-C9	3.02	128.14	117.12	6	3
4	A	341	PX4	C11-C10-C9	3.01	102.65	113.69	1	2
4	A	394	PX4	C7-O7-C23	3.01	125.01	117.80	1	3
4	A	366	PX4	O7-C7-C8	3.01	119.15	108.34	13	6
4	A	335	PX4	C26-C25-C24	3.01	102.06	113.13	11	2
4	A	391	PX4	C14-C13-C12	3.01	99.15	114.37	14	1
4	A	424	PX4	C5-N1-C3	3.01	101.06	108.98	6	4
4	A	430	PX4	C7-O7-C23	3.01	110.59	117.80	7	3
4	A	355	PX4	O1-P1-O2	3.01	126.45	112.44	7	8
4	A	376	PX4	O1-P1-O3	3.01	121.21	107.57	7	1
4	A	422	PX4	C19-C18-C17	3.01	99.16	114.37	3	1
4	A	324	PX4	C4-N1-C3	3.01	116.87	108.98	5	3
4	A	339	PX4	C15-C14-C13	3.01	99.17	114.37	4	2
4	A	350	PX4	C1-C2-N1	3.01	125.47	115.82	4	3
4	A	395	PX4	O1-P1-O2	3.01	126.42	112.44	13	7
4	A	402	PX4	O3-P1-O2	3.01	97.02	108.94	6	2
4	A	316	PX4	O7-C7-C6	3.00	119.12	108.34	1	5
4	A	316	PX4	O1-P1-O2	3.00	126.41	112.44	9	8
4	A	328	PX4	C7-O7-C23	3.00	124.98	117.80	13	2
4	A	386	PX4	C4-N1-C3	3.00	101.09	108.98	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	C7-O7-C23	3.00	124.98	117.80	6	2
4	A	397	PX4	O1-P1-O3	3.00	93.95	107.57	11	1
4	A	395	PX4	C1-C2-N1	3.00	125.46	115.82	11	4
4	A	346	PX4	C12-C11-C10	3.00	124.15	113.13	7	3
4	A	348	PX4	O5-C9-C10	3.00	120.98	111.83	7	5
4	A	316	PX4	P1-O3-C1	3.00	106.99	121.26	14	9
4	A	336	PX4	O7-C7-C8	3.00	119.10	108.34	10	7
4	A	366	PX4	C28-C27-C26	3.00	99.21	114.37	2	1
4	A	421	PX4	O5-C9-C10	3.00	120.98	111.83	5	5
4	A	315	PX4	O7-C7-C6	3.00	119.09	108.34	8	3
4	A	318	PX4	C26-C25-C24	3.00	102.11	113.13	1	2
4	A	338	PX4	C18-C17-C16	3.00	99.22	114.37	5	3
4	A	358	PX4	C15-C14-C13	3.00	99.22	114.37	3	2
4	A	361	PX4	C20-C19-C18	3.00	99.22	114.37	14	1
4	A	371	PX4	C17-C16-C15	3.00	99.22	114.37	2	1
4	A	386	PX4	C8-O5-C9	3.00	106.17	117.12	5	4
4	A	388	PX4	O1-P1-O3	3.00	93.99	107.57	10	2
4	A	397	PX4	C25-C24-C23	3.00	102.72	113.69	1	2
4	A	310	PX4	O5-C9-O6	2.99	116.14	123.63	12	4
4	A	340	PX4	C12-C11-C10	2.99	102.12	113.13	8	2
4	A	400	PX4	O1-P1-O4	2.99	121.14	107.57	4	2
4	A	323	PX4	O7-C7-C6	2.99	119.08	108.34	14	2
4	A	378	PX4	C4-N1-C3	2.99	116.84	108.98	13	4
4	A	323	PX4	C3-N1-C2	2.99	121.80	109.91	12	2
4	A	324	PX4	C17-C16-C15	2.99	99.26	114.37	2	2
4	A	332	PX4	O4-P1-O2	2.99	120.78	108.94	13	2
4	A	340	PX4	C5-N1-C2	2.99	121.80	109.91	4	3
4	A	394	PX4	C30-C29-C28	2.99	99.25	114.37	11	1
4	A	345	PX4	C8-O5-C9	2.99	106.19	117.12	10	2
4	A	364	PX4	C16-C15-C14	2.99	99.27	114.37	12	2
4	A	422	PX4	O1-P1-O3	2.99	94.02	107.57	6	1
4	A	328	PX4	C1-C2-N1	2.99	125.40	115.82	3	3
4	A	333	PX4	O7-C7-C8	2.99	119.06	108.34	6	2
4	A	359	PX4	C32-C31-C30	2.98	99.29	114.37	6	1
4	A	421	PX4	C30-C29-C28	2.98	99.28	114.37	9	3
4	A	376	PX4	C29-C28-C27	2.98	99.30	114.37	10	2
4	A	401	PX4	C32-C31-C30	2.98	99.30	114.37	4	1
4	A	312	PX4	C26-C25-C24	2.98	124.07	113.13	6	3
4	A	350	PX4	C4-N1-C3	2.98	101.16	108.98	3	2
4	A	356	PX4	O7-C23-O8	2.98	116.74	123.70	12	5
4	A	362	PX4	O5-C9-C10	2.98	120.92	111.83	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	C19-C18-C17	2.98	99.31	114.37	9	1
4	A	386	PX4	C26-C25-C24	2.98	102.18	113.13	12	1
4	A	402	PX4	O1-P1-O2	2.98	126.30	112.44	4	5
4	A	388	PX4	C11-C10-C9	2.98	102.78	113.69	12	2
4	A	410	PX4	C15-C14-C13	2.98	99.31	114.37	14	2
4	A	307	PX4	O1-P1-O4	2.97	121.05	107.57	3	7
4	A	350	PX4	O4-P1-O2	2.98	120.73	108.94	1	3
4	A	379	PX4	C14-C13-C12	2.97	99.33	114.37	6	2
4	A	381	PX4	C1-C2-N1	2.98	125.37	115.82	14	3
4	A	348	PX4	C12-C11-C10	2.97	124.05	113.13	8	1
4	A	334	PX4	O5-C9-C10	2.97	120.90	111.83	5	6
4	A	389	PX4	C5-N1-C3	2.97	101.17	108.98	1	4
4	A	397	PX4	O7-C7-C6	2.97	119.01	108.34	2	1
4	A	419	PX4	O7-C7-C6	2.97	119.01	108.34	6	5
4	A	362	PX4	C29-C28-C27	2.97	99.35	114.37	5	2
4	A	307	PX4	C27-C26-C25	2.97	99.36	114.37	4	3
4	A	308	PX4	C4-N1-C3	2.97	101.18	108.98	13	4
4	A	361	PX4	O5-C9-O6	2.97	116.20	123.63	12	3
4	A	403	PX4	C26-C25-C24	2.97	102.22	113.13	11	2
4	A	423	PX4	O1-P1-O3	2.97	94.11	107.57	12	2
4	A	342	PX4	C5-N1-C4	2.97	101.18	108.98	12	5
4	A	307	PX4	C1-C2-N1	2.97	125.34	115.82	1	3
4	A	380	PX4	P1-O4-C6	2.97	104.35	121.35	12	9
4	A	394	PX4	C25-C24-C23	2.97	102.82	113.69	6	2
4	A	322	PX4	O4-P1-O2	2.97	120.69	108.94	6	3
4	A	325	PX4	O7-C7-C8	2.97	118.98	108.34	4	4
4	A	337	PX4	O4-P1-O2	2.97	120.69	108.94	1	1
4	A	338	PX4	C4-N1-C3	2.96	116.76	108.98	5	1
4	A	409	PX4	C34-C33-C32	2.97	99.38	114.37	14	2
4	A	310	PX4	O5-C9-C10	2.96	120.87	111.83	10	5
4	A	342	PX4	O5-C9-O6	2.96	116.22	123.63	8	4
4	A	329	PX4	O7-C7-C6	2.96	118.96	108.34	2	6
4	A	343	PX4	O7-C23-O8	2.96	116.78	123.70	13	6
4	A	405	PX4	C29-C28-C27	2.96	99.40	114.37	13	1
4	A	417	PX4	P1-O4-C6	2.96	104.38	121.35	12	9
4	A	406	PX4	O5-C9-O6	2.96	116.22	123.63	5	2
4	A	310	PX4	O1-P1-O4	2.96	120.97	107.57	14	1
4	A	408	PX4	O1-P1-O4	2.96	120.98	107.57	13	2
4	A	417	PX4	C4-N1-C3	2.96	101.20	108.98	5	3
4	A	344	PX4	C26-C25-C24	2.96	102.26	113.13	12	1
4	A	384	PX4	C5-N1-C3	2.96	101.21	108.98	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C12-C11-C10	2.96	102.26	113.13	4	6
4	A	339	PX4	C4-N1-C2	2.95	121.65	109.91	5	2
4	A	412	PX4	O7-C23-O8	2.95	116.80	123.70	8	4
4	A	417	PX4	O3-P1-O2	2.95	97.23	108.94	7	5
4	A	312	PX4	C7-O7-C23	2.95	124.86	117.80	2	2
4	A	327	PX4	O1-P1-O2	2.95	126.18	112.44	9	7
4	A	340	PX4	O1-P1-O3	2.95	94.18	107.57	14	3
4	A	313	PX4	C1-C2-N1	2.95	125.29	115.82	1	1
4	A	341	PX4	C1-C2-N1	2.95	125.29	115.82	1	2
4	A	350	PX4	C5-N1-C3	2.95	101.23	108.98	10	4
4	A	354	PX4	C5-N1-C3	2.95	101.23	108.98	10	1
4	A	346	PX4	C25-C24-C23	2.95	102.89	113.69	2	1
4	A	354	PX4	C20-C19-C18	2.95	99.47	114.37	3	3
4	A	376	PX4	C7-O7-C23	2.95	110.74	117.80	7	4
4	A	398	PX4	O1-P1-O4	2.95	120.92	107.57	2	4
4	A	324	PX4	C7-O7-C23	2.94	110.75	117.80	6	2
4	A	337	PX4	C31-C30-C29	2.95	99.48	114.37	12	1
4	A	374	PX4	C11-C10-C9	2.95	102.90	113.69	10	3
4	A	407	PX4	O7-C23-O8	2.95	116.82	123.70	1	4
4	A	350	PX4	P1-O3-C1	2.94	107.25	121.26	7	8
4	A	318	PX4	C8-O5-C9	2.94	106.36	117.12	4	1
4	A	413	PX4	C11-C10-C9	2.94	102.91	113.69	1	2
4	A	319	PX4	C5-N1-C3	2.94	101.25	108.98	1	4
4	A	325	PX4	O1-P1-O2	2.94	126.13	112.44	6	7
4	A	417	PX4	C4-N1-C2	2.94	121.60	109.91	5	4
4	A	395	PX4	O1-P1-O3	2.94	94.24	107.57	12	2
4	A	399	PX4	O5-C9-C10	2.94	120.80	111.83	3	5
4	A	410	PX4	C11-C10-C9	2.94	102.92	113.69	9	3
4	A	318	PX4	C13-C12-C11	2.94	99.51	114.37	9	1
4	A	308	PX4	C26-C25-C24	2.94	102.33	113.13	6	2
4	A	317	PX4	O1-P1-O2	2.94	126.11	112.44	1	4
4	A	347	PX4	O4-P1-O2	2.94	120.57	108.94	4	3
4	A	346	PX4	O4-P1-O2	2.94	120.57	108.94	8	3
4	A	359	PX4	O5-C9-O6	2.93	130.97	123.63	10	1
4	A	388	PX4	C12-C11-C10	2.93	102.34	113.13	4	4
4	A	390	PX4	P1-O4-C6	2.93	104.54	121.35	3	8
4	A	396	PX4	C5-N1-C3	2.93	101.27	108.98	1	4
4	A	429	PX4	O7-C23-O8	2.93	116.84	123.70	12	3
4	A	417	PX4	C8-O5-C9	2.93	106.40	117.12	9	3
4	A	328	PX4	O5-C9-C10	2.93	120.77	111.83	5	3
4	A	328	PX4	O4-P1-O2	2.93	120.55	108.94	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	336	PX4	C11-C10-C9	2.93	102.96	113.69	10	3
4	A	342	PX4	C12-C11-C10	2.93	102.36	113.13	5	3
4	A	363	PX4	C7-O7-C23	2.93	124.81	117.80	3	3
4	A	395	PX4	P1-O4-C6	2.93	104.56	121.35	14	10
4	A	405	PX4	C4-N1-C2	2.93	98.26	109.91	10	2
4	A	428	PX4	C26-C25-C24	2.93	102.36	113.13	1	4
4	A	308	PX4	O7-C7-C8	2.93	118.85	108.34	1	5
4	A	312	PX4	O5-C9-O6	2.93	116.30	123.63	1	5
4	A	331	PX4	C14-C13-C12	2.93	99.56	114.37	5	3
4	A	368	PX4	C7-O7-C23	2.93	124.81	117.80	3	3
4	A	406	PX4	O5-C9-C10	2.93	120.76	111.83	7	1
4	A	428	PX4	C5-N1-C4	2.93	101.29	108.98	5	5
4	A	430	PX4	O5-C9-C10	2.93	120.76	111.83	13	4
4	A	352	PX4	C13-C12-C11	2.93	99.57	114.37	5	1
4	A	306	PX4	C1-C2-N1	2.92	125.21	115.82	6	3
4	A	322	PX4	O1-P1-O4	2.92	120.82	107.57	2	4
4	A	362	PX4	O1-P1-O2	2.92	126.05	112.44	14	5
4	A	373	PX4	O7-C23-O8	2.92	116.87	123.70	5	4
4	A	400	PX4	C33-C32-C31	2.92	99.59	114.37	9	1
4	A	430	PX4	O4-P1-O2	2.92	120.53	108.94	4	5
4	A	372	PX4	C29-C28-C27	2.92	99.60	114.37	1	2
4	A	381	PX4	O1-P1-O4	2.92	120.81	107.57	9	3
4	A	413	PX4	C1-C2-N1	2.92	125.20	115.82	8	4
4	A	408	PX4	C8-O5-C9	2.92	106.44	117.12	7	2
4	A	340	PX4	O4-P1-O2	2.92	120.51	108.94	4	4
4	A	367	PX4	C11-C10-C9	2.92	102.99	113.69	2	1
4	A	315	PX4	C5-N1-C3	2.92	101.31	108.98	12	2
4	A	407	PX4	O1-P1-O2	2.92	126.03	112.44	1	9
4	A	345	PX4	C5-N1-C4	2.92	101.31	108.98	14	4
4	A	347	PX4	C11-C10-C9	2.92	103.00	113.69	10	1
4	A	370	PX4	O3-P1-O2	2.92	97.37	108.94	3	3
4	A	373	PX4	C8-O5-C9	2.92	106.45	117.12	6	2
4	A	400	PX4	C32-C31-C30	2.92	99.62	114.37	9	1
4	A	401	PX4	C12-C11-C10	2.92	102.41	113.13	10	3
4	A	319	PX4	C26-C25-C24	2.92	102.42	113.13	5	2
4	A	327	PX4	C1-C2-N1	2.91	125.18	115.82	13	5
4	A	371	PX4	C3-N1-C2	2.91	121.50	109.91	13	4
4	A	328	PX4	C12-C11-C10	2.91	102.42	113.13	9	2
4	A	337	PX4	O5-C9-C10	2.91	120.72	111.83	10	2
4	A	363	PX4	C5-N1-C2	2.91	98.33	109.91	4	1
4	A	318	PX4	C4-N1-C3	2.91	116.62	108.98	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	318	PX4	C33-C32-C31	2.91	99.65	114.37	2	1
4	A	354	PX4	C25-C24-C23	2.91	103.02	113.69	5	5
4	A	380	PX4	O1-P1-O3	2.91	94.36	107.57	1	3
4	A	389	PX4	O3-C1-C2	2.91	123.66	109.65	5	2
4	A	397	PX4	C20-C19-C18	2.91	99.64	114.37	2	1
4	A	408	PX4	O8-C23-C24	2.91	112.39	123.78	3	1
4	A	417	PX4	O1-P1-O3	2.91	94.36	107.57	5	1
4	A	349	PX4	C5-N1-C3	2.91	116.62	108.98	13	2
4	A	328	PX4	O7-C7-C6	2.91	118.78	108.34	14	2
4	A	429	PX4	O5-C9-O6	2.91	116.35	123.63	8	4
4	A	380	PX4	O6-C9-C10	2.91	112.42	123.78	5	1
4	A	392	PX4	O5-C9-O6	2.91	116.36	123.63	6	4
4	A	327	PX4	C33-C32-C31	2.90	99.69	114.37	3	1
4	A	335	PX4	O1-P1-O2	2.90	125.96	112.44	10	8
4	A	338	PX4	C32-C31-C30	2.90	99.69	114.37	6	3
4	A	374	PX4	C4-N1-C3	2.90	101.35	108.98	10	4
4	A	387	PX4	C26-C25-C24	2.90	102.46	113.13	11	2
4	A	404	PX4	O3-P1-O2	2.90	120.44	108.94	3	2
4	A	420	PX4	O1-P1-O2	2.90	125.96	112.44	12	9
4	A	337	PX4	O7-C23-C24	2.90	117.76	111.48	1	4
4	A	394	PX4	O5-C9-O6	2.90	116.36	123.63	3	4
4	A	429	PX4	C12-C11-C10	2.90	123.80	113.13	8	2
4	A	344	PX4	O1-P1-O2	2.90	125.95	112.44	6	7
4	A	352	PX4	O1-P1-O3	2.90	94.41	107.57	5	1
4	A	399	PX4	O1-P1-O3	2.90	94.41	107.57	4	2
4	A	425	PX4	C34-C33-C32	2.90	99.70	114.37	10	2
4	A	413	PX4	O1-P1-O3	2.90	94.42	107.57	14	2
4	A	311	PX4	C1-C2-N1	2.90	125.13	115.82	12	3
4	A	331	PX4	C18-C17-C16	2.90	99.72	114.37	4	2
4	A	337	PX4	C17-C16-C15	2.90	99.72	114.37	1	3
4	A	350	PX4	C8-O5-C9	2.90	106.53	117.12	2	4
4	A	358	PX4	C1-C2-N1	2.90	125.12	115.82	8	1
4	A	367	PX4	O3-P1-O2	2.90	97.45	108.94	7	3
4	A	332	PX4	C19-C18-C17	2.90	99.73	114.37	2	1
4	A	340	PX4	C30-C29-C28	2.90	99.73	114.37	12	1
4	A	354	PX4	C7-O7-C23	2.90	124.73	117.80	1	5
4	A	359	PX4	O1-P1-O4	2.90	120.70	107.57	13	3
4	A	360	PX4	O5-C9-O6	2.90	116.38	123.63	14	6
4	A	366	PX4	O1-P1-O2	2.90	125.92	112.44	1	6
4	A	377	PX4	C4-N1-C3	2.90	101.36	108.98	4	3
4	A	392	PX4	C7-O7-C23	2.90	124.73	117.80	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	396	PX4	C5-N1-C4	2.89	116.58	108.98	6	3
4	A	311	PX4	C5-N1-C2	2.89	98.41	109.91	3	4
4	A	321	PX4	C12-C11-C10	2.89	102.50	113.13	2	1
4	A	404	PX4	C19-C18-C17	2.89	99.74	114.37	11	1
4	A	417	PX4	O7-C7-C8	2.89	118.72	108.34	2	8
4	A	423	PX4	C16-C15-C14	2.89	99.75	114.37	4	2
4	A	361	PX4	C5-N1-C2	2.89	121.40	109.91	11	2
4	A	364	PX4	O7-C7-C6	2.89	118.71	108.34	13	4
4	A	366	PX4	O7-C7-C6	2.89	118.71	108.34	3	4
4	A	402	PX4	C4-N1-C2	2.89	121.40	109.91	11	1
4	A	413	PX4	C4-N1-C3	2.89	101.38	108.98	2	4
4	A	395	PX4	O7-C23-O8	2.89	130.46	123.70	6	4
4	A	361	PX4	C32-C31-C30	2.89	99.77	114.37	13	2
4	A	307	PX4	C5-N1-C3	2.89	116.56	108.98	12	3
4	A	324	PX4	C19-C18-C17	2.89	99.78	114.37	12	2
4	A	311	PX4	C32-C31-C30	2.88	99.79	114.37	2	1
4	A	323	PX4	C27-C26-C25	2.88	99.79	114.37	1	1
4	A	345	PX4	O7-C7-C6	2.88	118.69	108.34	10	2
4	A	306	PX4	C4-N1-C2	2.88	121.37	109.91	14	3
4	A	315	PX4	O1-P1-O2	2.88	125.86	112.44	9	7
4	A	361	PX4	O6-C9-C10	2.88	112.50	123.78	2	2
4	A	382	PX4	C5-N1-C4	2.88	101.40	108.98	8	3
4	A	387	PX4	O5-C9-O6	2.88	116.41	123.63	13	6
4	A	325	PX4	C5-N1-C2	2.88	121.36	109.91	4	4
4	A	327	PX4	C8-O5-C9	2.88	106.58	117.12	12	3
4	A	340	PX4	C4-N1-C3	2.88	101.41	108.98	14	3
4	A	352	PX4	C11-C10-C9	2.88	103.13	113.69	6	1
4	A	351	PX4	C4-N1-C2	2.88	98.46	109.91	6	2
4	A	375	PX4	C19-C18-C17	2.88	99.80	114.37	11	1
4	A	408	PX4	C32-C31-C30	2.88	99.80	114.37	5	1
4	A	316	PX4	O5-C9-O6	2.88	116.42	123.63	14	3
4	A	319	PX4	C18-C17-C16	2.88	99.82	114.37	1	1
4	A	325	PX4	O3-P1-O2	2.88	97.52	108.94	4	4
4	A	350	PX4	C30-C29-C28	2.88	99.81	114.37	2	2
4	A	389	PX4	O1-P1-O3	2.88	94.51	107.57	14	3
4	A	427	PX4	O1-P1-O3	2.88	94.51	107.57	3	3
4	A	342	PX4	C13-C12-C11	2.88	99.82	114.37	11	1
4	A	346	PX4	O5-C9-O6	2.88	116.43	123.63	3	4
4	A	350	PX4	C27-C26-C25	2.88	99.82	114.37	5	3
4	A	365	PX4	C5-N1-C3	2.88	101.42	108.98	10	2
4	A	385	PX4	O7-C7-C8	2.88	118.67	108.34	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	O7-C7-C8	2.88	118.67	108.34	2	5
4	A	370	PX4	O1-P1-O4	2.88	120.61	107.57	3	2
4	A	374	PX4	C5-N1-C3	2.88	101.42	108.98	11	3
4	A	369	PX4	C30-C29-C28	2.87	99.84	114.37	2	3
4	A	383	PX4	C7-O7-C23	2.88	110.91	117.80	13	4
4	A	314	PX4	C18-C17-C16	2.87	99.85	114.37	14	1
4	A	332	PX4	O1-P1-O4	2.87	120.58	107.57	2	3
4	A	344	PX4	C31-C30-C29	2.87	99.85	114.37	2	1
4	A	416	PX4	O5-C9-C10	2.87	120.59	111.83	7	6
4	A	310	PX4	O7-C7-C8	2.87	118.64	108.34	1	5
4	A	328	PX4	O1-P1-O4	2.87	120.58	107.57	7	3
4	A	351	PX4	C16-C15-C14	2.87	99.86	114.37	11	2
4	A	371	PX4	O5-C9-O6	2.87	116.44	123.63	7	1
4	A	376	PX4	C4-N1-C2	2.87	121.32	109.91	7	3
4	A	317	PX4	C29-C28-C27	2.87	99.87	114.37	5	3
4	A	329	PX4	C20-C19-C18	2.87	99.87	114.37	8	1
4	A	332	PX4	P1-O4-C6	2.87	104.92	121.35	12	10
4	A	334	PX4	C5-N1-C4	2.87	101.44	108.98	1	3
4	A	340	PX4	O3-C1-C2	2.87	123.45	109.65	9	3
4	A	347	PX4	C18-C17-C16	2.87	99.88	114.37	10	1
4	A	362	PX4	C19-C18-C17	2.87	99.87	114.37	12	1
4	A	367	PX4	O1-P1-O2	2.87	125.78	112.44	14	2
4	A	372	PX4	O4-P1-O2	2.87	120.30	108.94	8	2
4	A	409	PX4	O1-P1-O3	2.87	94.56	107.57	12	4
4	A	368	PX4	C5-N1-C3	2.87	101.44	108.98	4	3
4	A	373	PX4	C31-C30-C29	2.87	99.88	114.37	4	3
4	A	413	PX4	O5-C9-C10	2.87	120.58	111.83	6	2
4	A	428	PX4	C11-C10-C9	2.87	103.19	113.69	8	1
4	A	323	PX4	C5-N1-C2	2.87	98.52	109.91	12	3
4	A	395	PX4	O3-P1-O2	2.87	97.58	108.94	13	4
4	A	306	PX4	O5-C9-C10	2.86	120.56	111.83	4	4
4	A	337	PX4	C30-C29-C28	2.86	99.89	114.37	9	3
4	A	338	PX4	O1-P1-O3	2.86	94.59	107.57	4	3
4	A	379	PX4	O1-P1-O4	2.86	120.54	107.57	14	2
4	A	383	PX4	C26-C25-C24	2.86	102.61	113.13	14	2
4	A	410	PX4	C1-C2-N1	2.86	125.02	115.82	9	6
4	A	390	PX4	C14-C13-C12	2.86	99.90	114.37	6	1
4	A	358	PX4	C34-C33-C32	2.86	99.90	114.37	13	2
4	A	420	PX4	C13-C12-C11	2.86	99.91	114.37	12	2
4	A	310	PX4	C12-C11-C10	2.86	102.63	113.13	4	2
4	A	379	PX4	C3-N1-C2	2.86	98.55	109.91	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	412	PX4	C25-C24-C23	2.86	103.22	113.69	6	4
4	A	335	PX4	O3-P1-O2	2.86	97.62	108.94	12	2
4	A	340	PX4	C8-O5-C9	2.86	127.56	117.12	7	3
4	A	374	PX4	O1-P1-O3	2.86	94.62	107.57	13	2
4	A	377	PX4	O1-P1-O3	2.86	120.51	107.57	1	1
4	A	404	PX4	O1-P1-O2	2.86	125.73	112.44	12	2
4	A	347	PX4	O5-C9-C10	2.85	120.54	111.83	10	6
4	A	382	PX4	C13-C12-C11	2.85	99.94	114.37	7	1
4	A	421	PX4	C26-C25-C24	2.85	102.64	113.13	8	3
4	A	320	PX4	C16-C15-C14	2.85	99.95	114.37	4	2
4	A	324	PX4	C1-C2-N1	2.85	124.97	115.82	13	2
4	A	342	PX4	C31-C30-C29	2.85	99.96	114.37	5	3
4	A	361	PX4	C5-N1-C4	2.85	116.47	108.98	2	3
4	A	373	PX4	C26-C25-C24	2.85	102.65	113.13	14	3
4	A	392	PX4	O3-P1-O2	2.85	97.64	108.94	7	2
4	A	407	PX4	C5-N1-C4	2.85	101.49	108.98	12	3
4	A	425	PX4	O7-C7-C6	2.85	118.57	108.34	9	2
4	A	378	PX4	C1-C2-N1	2.85	124.97	115.82	7	2
4	A	328	PX4	O7-C7-C8	2.85	118.56	108.34	10	4
4	A	397	PX4	C5-N1-C4	2.85	101.50	108.98	5	3
4	A	405	PX4	C4-N1-C3	2.85	101.49	108.98	14	3
4	A	406	PX4	C7-O7-C23	2.85	110.98	117.80	7	2
4	A	333	PX4	C4-N1-C3	2.85	101.50	108.98	4	2
4	A	346	PX4	C1-C2-N1	2.85	124.96	115.82	11	4
4	A	356	PX4	C8-O5-C9	2.85	106.71	117.12	3	3
4	A	350	PX4	C33-C32-C31	2.85	99.98	114.37	4	2
4	A	409	PX4	O7-C7-C6	2.85	118.55	108.34	12	3
4	A	328	PX4	C5-N1-C3	2.84	116.45	108.98	10	1
4	A	335	PX4	C4-N1-C3	2.84	101.51	108.98	7	4
4	A	339	PX4	C4-N1-C3	2.84	101.51	108.98	4	3
4	A	347	PX4	C7-O7-C23	2.84	110.99	117.80	2	4
4	A	320	PX4	C4-N1-C3	2.84	116.44	108.98	3	2
4	A	341	PX4	C20-C19-C18	2.84	100.00	114.37	3	1
4	A	379	PX4	C4-N1-C3	2.84	101.51	108.98	11	1
4	A	386	PX4	C18-C17-C16	2.84	100.01	114.37	14	1
4	A	390	PX4	C5-N1-C2	2.84	121.20	109.91	1	3
4	A	409	PX4	O7-C7-C8	2.84	118.54	108.34	9	8
4	A	400	PX4	C4-N1-C3	2.84	101.52	108.98	4	5
4	A	407	PX4	C32-C31-C30	2.84	100.02	114.37	1	1
4	A	427	PX4	C5-N1-C4	2.84	101.52	108.98	7	1
4	A	346	PX4	C15-C14-C13	2.84	100.02	114.37	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	355	PX4	O7-C7-C6	2.84	118.53	108.34	13	5
4	A	370	PX4	O1-P1-O2	2.84	125.65	112.44	2	6
4	A	374	PX4	O5-C9-C10	2.84	120.49	111.83	1	5
4	A	358	PX4	O1-P1-O4	2.84	120.42	107.57	9	2
4	A	368	PX4	C4-N1-C2	2.84	121.19	109.91	4	3
4	A	373	PX4	P1-O4-C6	2.84	105.09	121.35	8	10
4	A	379	PX4	O3-P1-O2	2.84	97.70	108.94	1	5
4	A	383	PX4	C5-N1-C3	2.84	101.53	108.98	2	2
4	A	318	PX4	C16-C15-C14	2.83	100.04	114.37	8	2
4	A	366	PX4	O5-C9-O6	2.84	116.54	123.63	14	2
4	A	422	PX4	C8-O5-C9	2.84	106.75	117.12	6	2
4	A	372	PX4	C12-C11-C10	2.83	102.71	113.13	12	2
4	A	391	PX4	C4-N1-C2	2.83	121.18	109.91	14	2
4	A	422	PX4	O1-P1-O4	2.84	120.42	107.57	6	2
4	A	326	PX4	C31-C30-C29	2.83	100.04	114.37	11	1
4	A	355	PX4	O4-P1-O2	2.83	97.70	108.94	11	3
4	A	362	PX4	O7-C7-C6	2.83	118.51	108.34	4	4
4	A	367	PX4	O5-C9-C10	2.83	120.48	111.83	5	3
4	A	311	PX4	C3-N1-C2	2.83	121.17	109.91	3	3
4	A	388	PX4	O7-C7-C6	2.83	118.51	108.34	13	4
4	A	359	PX4	O6-C9-C10	2.83	112.70	123.78	10	2
4	A	427	PX4	C7-O7-C23	2.83	124.58	117.80	4	4
4	A	385	PX4	C26-C25-C24	2.83	102.72	113.13	3	1
4	A	322	PX4	C27-C26-C25	2.83	100.06	114.37	3	2
4	A	337	PX4	O3-C1-C2	2.83	123.27	109.65	2	4
4	A	389	PX4	C30-C29-C28	2.83	100.06	114.37	7	2
4	A	389	PX4	C12-C11-C10	2.83	102.73	113.13	12	2
4	A	403	PX4	O5-C9-O6	2.83	116.55	123.63	14	3
4	A	342	PX4	C17-C16-C15	2.83	100.07	114.37	14	1
4	A	323	PX4	C25-C24-C23	2.83	103.33	113.69	10	3
4	A	377	PX4	C4-N1-C2	2.83	98.67	109.91	6	2
4	A	393	PX4	C14-C13-C12	2.83	100.07	114.37	12	3
4	A	398	PX4	C5-N1-C4	2.83	101.55	108.98	14	2
4	A	429	PX4	C7-O7-C23	2.83	111.03	117.80	10	1
4	A	307	PX4	C26-C25-C24	2.83	102.74	113.13	12	2
4	A	361	PX4	C11-C10-C9	2.83	103.34	113.69	5	2
4	A	374	PX4	O4-P1-O2	2.83	97.74	108.94	6	2
4	A	377	PX4	C28-C27-C26	2.83	100.08	114.37	5	2
4	A	383	PX4	P1-O4-C6	2.83	105.16	121.35	6	3
4	A	368	PX4	P1-O4-C6	2.83	105.16	121.35	4	8
4	A	403	PX4	C16-C15-C14	2.83	100.08	114.37	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	344	PX4	C12-C11-C10	2.82	102.75	113.13	9	2
4	A	346	PX4	O6-C9-C10	2.82	112.74	123.78	6	1
4	A	374	PX4	O3-C1-C2	2.82	123.24	109.65	7	2
4	A	403	PX4	O1-P1-O2	2.83	125.59	112.44	11	5
4	A	367	PX4	C4-N1-C3	2.82	101.56	108.98	6	2
4	A	400	PX4	C34-C33-C32	2.82	100.09	114.37	2	2
4	A	316	PX4	O1-P1-O4	2.82	120.36	107.57	5	3
4	A	320	PX4	O4-P1-O2	2.82	97.75	108.94	11	1
4	A	379	PX4	C15-C14-C13	2.82	100.11	114.37	8	3
4	A	378	PX4	C5-N1-C4	2.82	116.38	108.98	5	4
4	A	389	PX4	C34-C33-C32	2.82	100.11	114.37	13	1
4	A	360	PX4	C25-C24-C23	2.82	103.36	113.69	9	2
4	A	324	PX4	C12-C11-C10	2.82	102.78	113.13	2	2
4	A	329	PX4	C8-O5-C9	2.82	106.82	117.12	6	2
4	A	343	PX4	C4-N1-C2	2.82	121.11	109.91	8	2
4	A	367	PX4	C4-N1-C2	2.82	121.11	109.91	7	1
4	A	422	PX4	O4-P1-O2	2.82	120.10	108.94	8	2
4	A	423	PX4	C12-C11-C10	2.82	123.48	113.13	3	2
4	A	344	PX4	C18-C17-C16	2.81	100.14	114.37	12	3
4	A	351	PX4	C12-C11-C10	2.81	102.79	113.13	3	2
4	A	309	PX4	C5-N1-C3	2.81	101.59	108.98	2	4
4	A	315	PX4	C1-C2-N1	2.81	124.85	115.82	4	2
4	A	329	PX4	C27-C26-C25	2.81	128.58	114.37	13	1
4	A	346	PX4	C26-C25-C24	2.81	102.79	113.13	14	3
4	A	355	PX4	C11-C10-C9	2.81	124.00	113.69	1	4
4	A	356	PX4	C15-C14-C13	2.81	100.15	114.37	14	1
4	A	388	PX4	C20-C19-C18	2.81	100.16	114.37	12	3
4	A	395	PX4	C26-C25-C24	2.81	123.46	113.13	4	2
4	A	407	PX4	C5-N1-C2	2.81	121.09	109.91	11	1
4	A	306	PX4	C28-C27-C26	2.81	100.16	114.37	12	2
4	A	317	PX4	C4-N1-C2	2.81	121.08	109.91	2	2
4	A	389	PX4	C5-N1-C2	2.81	98.74	109.91	12	3
4	A	402	PX4	C20-C19-C18	2.81	100.16	114.37	2	2
4	A	414	PX4	O6-C9-C10	2.81	112.79	123.78	12	2
4	A	342	PX4	C1-C2-N1	2.81	124.84	115.82	11	3
4	A	426	PX4	O5-C9-O6	2.81	116.60	123.63	8	4
4	A	362	PX4	C3-N1-C2	2.81	98.75	109.91	11	2
4	A	393	PX4	O3-C1-C2	2.81	123.16	109.65	14	1
4	A	364	PX4	C4-N1-C2	2.81	121.06	109.91	14	1
4	A	367	PX4	C5-N1-C3	2.81	101.60	108.98	6	2
4	A	376	PX4	C4-N1-C3	2.81	101.60	108.98	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	330	PX4	C26-C25-C24	2.81	102.82	113.13	12	3
4	A	416	PX4	O5-C8-C7	2.81	116.48	108.40	10	5
4	A	314	PX4	C1-C2-N1	2.80	124.82	115.82	10	1
4	A	320	PX4	P1-O4-C6	2.80	105.28	121.35	1	10
4	A	370	PX4	O3-C1-C2	2.80	123.14	109.65	12	3
4	A	398	PX4	O6-C9-C10	2.80	112.81	123.78	7	1
4	A	416	PX4	O5-C9-O6	2.80	116.61	123.63	10	4
4	A	429	PX4	O7-C7-C6	2.80	118.40	108.34	10	3
4	A	306	PX4	C5-N1-C3	2.80	116.34	108.98	10	2
4	A	313	PX4	C17-C16-C15	2.80	100.20	114.37	11	1
4	A	368	PX4	C5-N1-C4	2.80	101.61	108.98	5	4
4	A	395	PX4	C27-C26-C25	2.80	100.20	114.37	10	2
4	A	357	PX4	O1-P1-O4	2.80	120.26	107.57	8	3
4	A	397	PX4	C8-O5-C9	2.80	106.88	117.12	3	1
4	A	346	PX4	O7-C23-O8	2.80	117.16	123.70	11	2
4	A	388	PX4	O4-P1-O2	2.80	120.03	108.94	8	2
4	A	315	PX4	C26-C25-C24	2.80	102.85	113.13	2	1
4	A	330	PX4	O1-P1-O4	2.80	94.89	107.57	3	1
4	A	422	PX4	C1-C2-N1	2.80	124.80	115.82	12	1
4	A	325	PX4	C12-C11-C10	2.79	102.86	113.13	1	2
4	A	381	PX4	C8-O5-C9	2.79	106.91	117.12	5	2
4	A	377	PX4	C8-O5-C9	2.79	106.91	117.12	9	3
4	A	389	PX4	C11-C10-C9	2.79	103.46	113.69	3	2
4	A	414	PX4	C4-N1-C3	2.79	116.31	108.98	12	2
4	A	414	PX4	C20-C19-C18	2.79	100.26	114.37	7	2
4	A	422	PX4	C30-C29-C28	2.79	100.25	114.37	8	2
4	A	384	PX4	C3-N1-C2	2.79	121.00	109.91	6	2
4	A	385	PX4	C18-C17-C16	2.79	100.26	114.37	12	3
4	A	395	PX4	O5-C9-C10	2.79	120.34	111.83	13	3
4	A	400	PX4	O5-C9-O6	2.79	116.65	123.63	3	3
4	A	419	PX4	C5-N1-C2	2.79	121.00	109.91	13	1
4	A	312	PX4	O7-C7-C6	2.79	118.34	108.34	12	3
4	A	425	PX4	C7-O7-C23	2.79	124.47	117.80	4	2
4	A	316	PX4	C18-C17-C16	2.79	100.28	114.37	14	1
4	A	326	PX4	O3-C1-C2	2.79	123.06	109.65	11	1
4	A	397	PX4	O1-P1-O2	2.79	125.41	112.44	7	6
4	A	401	PX4	C4-N1-C3	2.79	101.66	108.98	8	1
4	A	420	PX4	C15-C14-C13	2.79	100.28	114.37	8	1
4	A	333	PX4	C13-C12-C11	2.79	100.29	114.37	3	1
4	A	344	PX4	C4-N1-C2	2.78	120.98	109.91	11	2
4	A	349	PX4	C1-C2-N1	2.78	124.76	115.82	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	381	PX4	C16-C15-C14	2.78	100.30	114.37	4	3
4	A	414	PX4	O1-P1-O3	2.78	120.19	107.57	14	2
4	A	416	PX4	C26-C25-C24	2.78	102.90	113.13	10	1
4	A	326	PX4	C16-C15-C14	2.78	100.30	114.37	8	1
4	A	308	PX4	O1-P1-O4	2.78	120.18	107.57	11	2
4	A	351	PX4	C36-C35-C34	2.78	94.59	113.36	14	1
4	A	381	PX4	C5-N1-C4	2.78	101.67	108.98	1	3
4	A	410	PX4	C18-C17-C16	2.78	100.31	114.37	14	3
4	A	308	PX4	C4-N1-C2	2.78	98.87	109.91	1	1
4	A	335	PX4	C14-C13-C12	2.78	100.33	114.37	2	1
4	A	362	PX4	C1-C2-N1	2.78	124.74	115.82	8	3
4	A	394	PX4	O7-C7-C8	2.78	118.31	108.34	12	5
4	A	430	PX4	C12-C11-C10	2.78	123.34	113.13	8	4
4	A	364	PX4	O5-C9-O6	2.78	116.68	123.63	1	2
4	A	317	PX4	O7-C7-C6	2.78	118.30	108.34	4	6
4	A	344	PX4	C32-C31-C30	2.78	100.33	114.37	6	2
4	A	387	PX4	C31-C30-C29	2.78	100.33	114.37	13	1
4	A	363	PX4	C26-C25-C24	2.78	102.93	113.13	3	1
4	A	389	PX4	C20-C19-C18	2.78	100.33	114.37	10	1
4	A	386	PX4	O7-C23-O8	2.78	117.22	123.70	2	5
4	A	316	PX4	C11-C10-C9	2.77	123.86	113.69	14	2
4	A	325	PX4	C30-C29-C28	2.77	100.35	114.37	11	2
4	A	327	PX4	C30-C29-C28	2.77	100.35	114.37	2	1
4	A	388	PX4	C15-C14-C13	2.77	100.35	114.37	7	1
4	A	415	PX4	C11-C10-C9	2.77	103.53	113.69	5	2
4	A	370	PX4	C4-N1-C3	2.77	101.70	108.98	2	3
4	A	372	PX4	C30-C29-C28	2.77	100.36	114.37	9	3
4	A	393	PX4	C33-C32-C31	2.77	100.36	114.37	7	1
4	A	422	PX4	C5-N1-C3	2.77	116.25	108.98	10	3
4	A	429	PX4	C11-C10-C9	2.77	103.54	113.69	8	2
4	A	399	PX4	C4-N1-C2	2.77	98.90	109.91	3	1
4	A	328	PX4	C8-O5-C9	2.77	107.00	117.12	3	2
4	A	337	PX4	C5-N1-C3	2.77	101.70	108.98	12	4
4	A	400	PX4	C7-O7-C23	2.77	124.42	117.80	2	3
4	A	344	PX4	C33-C32-C31	2.77	100.38	114.37	13	3
4	A	353	PX4	C1-C2-N1	2.77	124.70	115.82	1	2
4	A	370	PX4	C1-C2-N1	2.77	124.70	115.82	11	3
4	A	426	PX4	C34-C33-C32	2.77	100.38	114.37	12	3
4	A	320	PX4	O1-P1-O4	2.77	120.10	107.57	7	3
4	A	375	PX4	C32-C31-C30	2.76	100.39	114.37	13	2
4	A	379	PX4	C25-C24-C23	2.77	103.56	113.69	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	400	PX4	O1-P1-O2	2.77	125.31	112.44	8	8
4	A	312	PX4	O5-C9-C10	2.76	120.26	111.83	4	3
4	A	423	PX4	C7-O7-C23	2.76	124.41	117.80	2	4
4	A	424	PX4	C29-C28-C27	2.76	100.39	114.37	6	1
4	A	425	PX4	O1-P1-O3	2.76	95.04	107.57	4	3
4	A	430	PX4	O1-P1-O4	2.76	120.09	107.57	3	3
4	A	325	PX4	C27-C26-C25	2.76	100.40	114.37	12	4
4	A	334	PX4	P1-O4-C6	2.76	105.52	121.35	13	6
4	A	396	PX4	O7-C23-O8	2.76	130.16	123.70	9	2
4	A	411	PX4	O5-C9-C10	2.76	120.25	111.83	13	5
4	A	385	PX4	O4-P1-O2	2.76	119.87	108.94	13	1
4	A	387	PX4	O3-P1-O2	2.76	98.00	108.94	11	2
4	A	410	PX4	O5-C9-O6	2.76	116.73	123.63	2	2
4	A	414	PX4	O3-C1-C2	2.76	122.93	109.65	4	2
4	A	366	PX4	C5-N1-C3	2.76	116.22	108.98	10	3
4	A	319	PX4	O3-P1-O2	2.76	98.01	108.94	1	2
4	A	327	PX4	C29-C28-C27	2.76	100.44	114.37	5	2
4	A	379	PX4	O3-C1-C2	2.76	122.92	109.65	11	2
4	A	401	PX4	C25-C24-C23	2.76	103.59	113.69	1	3
4	A	372	PX4	C32-C31-C30	2.75	100.44	114.37	3	3
4	A	424	PX4	C16-C15-C14	2.76	100.44	114.37	14	1
4	A	308	PX4	O4-P1-O2	2.75	119.84	108.94	12	2
4	A	317	PX4	C12-C11-C10	2.75	103.01	113.13	3	2
4	A	392	PX4	O1-P1-O4	2.75	120.05	107.57	11	1
4	A	398	PX4	O1-P1-O3	2.75	95.09	107.57	3	4
4	A	346	PX4	O5-C9-C10	2.75	120.23	111.83	6	1
4	A	362	PX4	C7-O7-C23	2.75	124.38	117.80	7	3
4	A	375	PX4	O4-P1-O2	2.75	98.03	108.94	3	2
4	A	386	PX4	C1-C2-N1	2.75	124.66	115.82	14	2
4	A	419	PX4	C26-C25-C24	2.75	103.02	113.13	13	2
4	A	327	PX4	C34-C33-C32	2.75	100.47	114.37	10	1
4	A	429	PX4	C5-N1-C3	2.75	101.75	108.98	3	6
4	A	419	PX4	C11-C10-C9	2.75	103.62	113.69	9	2
4	A	420	PX4	O1-P1-O3	2.75	95.11	107.57	1	2
4	A	330	PX4	C1-C2-N1	2.75	124.64	115.82	4	4
4	A	380	PX4	C4-N1-C3	2.75	101.76	108.98	6	2
4	A	326	PX4	C26-C25-C24	2.75	103.04	113.13	11	2
4	A	404	PX4	C29-C28-C27	2.75	100.48	114.37	2	1
4	A	321	PX4	O1-P1-O3	2.74	95.13	107.57	11	4
4	A	357	PX4	C11-C10-C9	2.74	103.64	113.69	4	3
4	A	378	PX4	O5-C9-O6	2.74	116.76	123.63	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	C5-N1-C4	2.75	101.77	108.98	11	2
4	A	381	PX4	O5-C9-C10	2.74	120.20	111.83	6	3
4	A	390	PX4	C12-C11-C10	2.74	103.04	113.13	8	3
4	A	407	PX4	O4-P1-O2	2.75	119.81	108.94	14	5
4	A	416	PX4	C19-C18-C17	2.74	100.49	114.37	8	1
4	A	334	PX4	C14-C13-C12	2.74	100.50	114.37	4	1
4	A	383	PX4	O3-C1-C2	2.74	122.84	109.65	2	2
4	A	384	PX4	C32-C31-C30	2.74	100.51	114.37	12	1
4	A	409	PX4	C4-N1-C3	2.74	101.77	108.98	9	2
4	A	419	PX4	C29-C28-C27	2.74	100.51	114.37	3	1
4	A	424	PX4	O7-C7-C6	2.74	118.18	108.34	6	1
4	A	411	PX4	O1-P1-O3	2.74	95.14	107.57	11	2
4	A	306	PX4	O4-P1-O2	2.74	119.79	108.94	5	5
4	A	358	PX4	O5-C9-O6	2.74	116.78	123.63	8	3
4	A	404	PX4	C4-N1-C2	2.74	120.80	109.91	1	1
4	A	314	PX4	C30-C29-C28	2.74	100.53	114.37	3	2
4	A	361	PX4	O4-P1-O2	2.74	119.79	108.94	9	2
4	A	371	PX4	O8-C23-C24	2.74	113.08	123.78	12	2
4	A	391	PX4	C33-C32-C31	2.74	100.53	114.37	1	3
4	A	416	PX4	C33-C32-C31	2.74	100.53	114.37	10	1
4	A	339	PX4	O5-C9-C10	2.74	120.18	111.83	11	2
4	A	363	PX4	C3-N1-C2	2.74	120.78	109.91	6	3
4	A	314	PX4	C8-O5-C9	2.73	107.12	117.12	3	4
4	A	322	PX4	C34-C33-C32	2.73	100.55	114.37	7	2
4	A	323	PX4	C32-C31-C30	2.73	100.55	114.37	11	1
4	A	376	PX4	C25-C24-C23	2.73	103.68	113.69	9	3
4	A	391	PX4	C5-N1-C3	2.73	101.79	108.98	13	2
4	A	413	PX4	C7-O7-C23	2.73	111.25	117.80	11	5
4	A	418	PX4	O3-C1-C2	2.73	122.81	109.65	6	3
4	A	338	PX4	C28-C27-C26	2.73	100.55	114.37	11	1
4	A	339	PX4	O7-C7-C8	2.73	118.14	108.34	5	3
4	A	364	PX4	C26-C25-C24	2.73	103.09	113.13	6	2
4	A	387	PX4	C4-N1-C3	2.73	101.80	108.98	5	2
4	A	416	PX4	O6-C9-C10	2.73	113.10	123.78	14	1
4	A	367	PX4	C32-C31-C30	2.73	100.57	114.37	11	1
4	A	419	PX4	C31-C30-C29	2.73	100.57	114.37	14	3
4	A	360	PX4	C19-C18-C17	2.73	100.58	114.37	10	2
4	A	378	PX4	C12-C11-C10	2.73	103.11	113.13	4	1
4	A	380	PX4	C8-O5-C9	2.73	107.15	117.12	1	1
4	A	398	PX4	C19-C18-C17	2.73	100.58	114.37	3	1
4	A	428	PX4	O5-C9-C10	2.73	120.15	111.83	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	418	PX4	C7-O7-C23	2.72	124.31	117.80	10	2
4	A	428	PX4	C7-O7-C23	2.72	124.32	117.80	12	4
4	A	317	PX4	O7-C7-C8	2.72	118.11	108.34	9	2
4	A	382	PX4	C5-N1-C3	2.72	116.13	108.98	5	1
4	A	421	PX4	C29-C28-C27	2.72	100.60	114.37	3	2
4	A	325	PX4	O1-P1-O3	2.72	95.23	107.57	5	2
4	A	311	PX4	C27-C26-C25	2.72	100.62	114.37	6	2
4	A	321	PX4	P1-O4-C6	2.72	105.77	121.35	13	5
4	A	338	PX4	O7-C7-C6	2.72	118.10	108.34	12	5
4	A	339	PX4	C33-C32-C31	2.72	100.62	114.37	3	3
4	A	387	PX4	O7-C7-C8	2.72	118.10	108.34	4	5
4	A	400	PX4	C5-N1-C3	2.72	116.12	108.98	4	2
4	A	308	PX4	C5-N1-C4	2.72	116.11	108.98	4	2
4	A	402	PX4	C26-C25-C24	2.72	103.14	113.13	2	3
4	A	327	PX4	C5-N1-C2	2.72	99.12	109.91	2	2
4	A	327	PX4	O4-P1-O2	2.72	98.17	108.94	8	3
4	A	355	PX4	C14-C13-C12	2.72	100.64	114.37	3	1
4	A	393	PX4	O1-P1-O4	2.71	119.87	107.57	14	2
4	A	394	PX4	C29-C28-C27	2.72	100.64	114.37	6	3
4	A	395	PX4	C11-C10-C9	2.71	103.75	113.69	1	2
4	A	405	PX4	C8-O5-C9	2.72	107.19	117.12	10	1
4	A	321	PX4	C13-C12-C11	2.71	100.66	114.37	7	3
4	A	382	PX4	C12-C11-C10	2.71	103.16	113.13	11	1
4	A	406	PX4	O4-P1-O2	2.71	119.69	108.94	14	4
4	A	338	PX4	C1-C2-N1	2.71	124.52	115.82	7	3
4	A	410	PX4	O1-P1-O4	2.71	119.85	107.57	7	2
4	A	365	PX4	O5-C9-O6	2.71	116.85	123.63	4	5
4	A	388	PX4	O3-C1-C2	2.71	122.69	109.65	2	2
4	A	341	PX4	C4-N1-C3	2.71	116.09	108.98	1	3
4	A	359	PX4	C4-N1-C3	2.71	101.86	108.98	7	1
4	A	381	PX4	O4-P1-O2	2.71	119.67	108.94	3	1
4	A	336	PX4	O3-P1-O2	2.71	98.21	108.94	13	3
4	A	406	PX4	C1-C2-N1	2.71	124.51	115.82	9	4
4	A	377	PX4	O7-C7-C6	2.70	118.05	108.34	6	5
4	A	319	PX4	C11-C10-C9	2.70	103.80	113.69	1	3
4	A	331	PX4	C32-C31-C30	2.70	100.71	114.37	7	1
4	A	351	PX4	O4-P1-O2	2.70	119.64	108.94	11	3
4	A	393	PX4	C5-N1-C4	2.70	101.88	108.98	10	2
4	A	361	PX4	C13-C12-C11	2.70	100.71	114.37	13	2
4	A	400	PX4	C12-C11-C10	2.70	103.20	113.13	11	1
4	A	404	PX4	O1-P1-O4	2.70	119.81	107.57	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	318	PX4	O5-C9-C10	2.70	120.06	111.83	10	2
4	A	323	PX4	O3-C1-C2	2.70	122.64	109.65	14	2
4	A	319	PX4	C14-C13-C12	2.70	100.73	114.37	1	2
4	A	347	PX4	C15-C14-C13	2.70	100.73	114.37	12	1
4	A	369	PX4	C12-C11-C10	2.70	123.04	113.13	8	2
4	A	402	PX4	O7-C7-C6	2.70	118.02	108.34	13	5
4	A	412	PX4	C16-C15-C14	2.70	100.73	114.37	14	1
4	A	414	PX4	C11-C10-C9	2.70	103.81	113.69	9	1
4	A	421	PX4	O7-C7-C6	2.70	118.02	108.34	7	2
4	A	340	PX4	O7-C7-C8	2.70	118.02	108.34	8	5
4	A	373	PX4	C12-C11-C10	2.70	103.22	113.13	4	1
4	A	424	PX4	C12-C11-C10	2.70	103.22	113.13	2	1
4	A	403	PX4	C4-N1-C3	2.70	101.90	108.98	8	4
4	A	406	PX4	O1-P1-O3	2.70	95.35	107.57	14	3
4	A	339	PX4	C5-N1-C4	2.69	116.05	108.98	13	1
4	A	385	PX4	C25-C24-C23	2.69	103.82	113.69	14	1
4	A	398	PX4	C12-C11-C10	2.69	103.23	113.13	6	2
4	A	399	PX4	C8-O5-C9	2.69	107.27	117.12	11	4
4	A	424	PX4	C1-C2-N1	2.69	124.47	115.82	5	3
4	A	377	PX4	C31-C30-C29	2.69	100.76	114.37	13	1
4	A	425	PX4	O4-P1-O2	2.69	119.61	108.94	10	3
4	A	428	PX4	O1-P1-O4	2.69	119.77	107.57	13	2
4	A	348	PX4	C5-N1-C2	2.69	120.61	109.91	2	1
4	A	407	PX4	C1-C2-N1	2.69	124.46	115.82	12	2
4	A	410	PX4	C34-C33-C32	2.69	100.76	114.37	4	1
4	A	341	PX4	O7-C7-C6	2.69	117.99	108.34	7	4
4	A	346	PX4	C14-C13-C12	2.69	100.78	114.37	3	1
4	A	355	PX4	C18-C17-C16	2.69	100.77	114.37	14	2
4	A	361	PX4	O1-P1-O2	2.69	124.96	112.44	14	7
4	A	328	PX4	O5-C9-O6	2.69	116.90	123.63	14	6
4	A	396	PX4	O3-C1-C2	2.69	122.59	109.65	10	2
4	A	397	PX4	C33-C32-C31	2.69	100.78	114.37	2	2
4	A	400	PX4	O8-C23-C24	2.69	113.26	123.78	13	1
4	A	414	PX4	C17-C16-C15	2.69	100.77	114.37	8	1
4	A	335	PX4	C8-O5-C9	2.69	107.29	117.12	5	3
4	A	403	PX4	C5-N1-C2	2.69	120.59	109.91	5	1
4	A	416	PX4	C11-C10-C9	2.69	103.84	113.69	8	2
4	A	319	PX4	C5-N1-C2	2.69	120.59	109.91	14	1
4	A	327	PX4	O5-C9-C10	2.69	120.02	111.83	13	5
4	A	358	PX4	C5-N1-C4	2.69	101.92	108.98	1	2
4	A	391	PX4	O4-P1-O2	2.69	119.58	108.94	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	397	PX4	O1-P1-O4	2.69	119.74	107.57	14	3
4	A	420	PX4	O7-C7-C6	2.69	117.98	108.34	11	5
4	A	310	PX4	C34-C33-C32	2.68	100.81	114.37	12	1
4	A	330	PX4	O5-C9-C10	2.68	120.02	111.83	6	2
4	A	376	PX4	C11-C10-C9	2.68	103.86	113.69	1	3
4	A	422	PX4	C14-C13-C12	2.68	100.80	114.37	14	2
4	A	384	PX4	C19-C18-C17	2.68	100.81	114.37	1	1
4	A	404	PX4	O5-C9-O6	2.68	116.92	123.63	2	2
4	A	308	PX4	C12-C11-C10	2.68	103.28	113.13	1	6
4	A	309	PX4	O1-P1-O3	2.68	95.42	107.57	3	3
4	A	341	PX4	O5-C9-C10	2.68	120.01	111.83	8	5
4	A	383	PX4	C16-C15-C14	2.68	100.81	114.37	4	1
4	A	404	PX4	C16-C15-C14	2.68	100.82	114.37	3	1
4	A	421	PX4	C19-C18-C17	2.68	100.82	114.37	6	1
4	A	353	PX4	C25-C24-C23	2.68	123.51	113.69	7	1
4	A	358	PX4	O1-P1-O3	2.68	95.42	107.57	11	2
4	A	409	PX4	C1-C2-N1	2.68	124.42	115.82	8	6
4	A	425	PX4	O3-C1-C2	2.68	122.55	109.65	9	1
4	A	367	PX4	C12-C11-C10	2.68	103.28	113.13	6	2
4	A	382	PX4	C11-C10-C9	2.68	103.89	113.69	10	2
4	A	430	PX4	C14-C13-C12	2.68	100.83	114.37	8	3
4	A	343	PX4	C5-N1-C4	2.68	101.95	108.98	3	1
4	A	359	PX4	C1-C2-N1	2.67	124.41	115.82	12	3
4	A	320	PX4	C26-C25-C24	2.67	103.30	113.13	10	1
4	A	356	PX4	O7-C7-C6	2.67	117.93	108.34	8	5
4	A	368	PX4	C14-C13-C12	2.67	100.86	114.37	7	3
4	A	384	PX4	O6-C9-C10	2.67	113.33	123.78	7	1
4	A	406	PX4	C4-N1-C2	2.67	120.54	109.91	13	2
4	A	318	PX4	C12-C11-C10	2.67	103.31	113.13	5	2
4	A	338	PX4	C5-N1-C4	2.67	101.96	108.98	13	2
4	A	372	PX4	C31-C30-C29	2.67	100.86	114.37	14	1
4	A	404	PX4	C27-C26-C25	2.67	100.86	114.37	2	2
4	A	329	PX4	C30-C29-C28	2.67	100.87	114.37	4	2
4	A	330	PX4	O4-P1-O2	2.67	119.52	108.94	8	2
4	A	374	PX4	C29-C28-C27	2.67	100.87	114.37	1	1
4	A	384	PX4	C5-N1-C2	2.67	120.53	109.91	3	3
4	A	400	PX4	C5-N1-C2	2.67	120.53	109.91	2	3
4	A	311	PX4	C7-O7-C23	2.67	111.41	117.80	5	1
4	A	324	PX4	O1-P1-O3	2.67	95.47	107.57	5	2
4	A	337	PX4	C3-N1-C2	2.67	99.30	109.91	3	1
4	A	333	PX4	O3-C1-C2	2.67	122.49	109.65	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	370	PX4	O7-C7-C6	2.67	117.91	108.34	14	2
4	A	390	PX4	O1-P1-O2	2.67	124.85	112.44	10	7
4	A	392	PX4	O3-C1-C2	2.67	122.49	109.65	8	2
4	A	395	PX4	O8-C23-C24	2.67	113.35	123.78	14	1
4	A	327	PX4	O1-P1-O4	2.67	119.66	107.57	3	5
4	A	370	PX4	O4-P1-O2	2.67	119.50	108.94	11	1
4	A	372	PX4	C5-N1-C4	2.67	101.97	108.98	3	2
4	A	382	PX4	C3-N1-C2	2.67	99.31	109.91	5	2
4	A	397	PX4	C31-C30-C29	2.67	100.89	114.37	10	4
4	A	408	PX4	C28-C27-C26	2.67	100.88	114.37	7	1
4	A	422	PX4	C4-N1-C2	2.67	99.31	109.91	7	3
4	A	346	PX4	O3-P1-O2	2.67	98.37	108.94	8	2
4	A	367	PX4	O1-P1-O4	2.66	119.64	107.57	11	2
4	A	389	PX4	C26-C25-C24	2.66	103.34	113.13	12	3
4	A	311	PX4	O5-C9-C10	2.66	119.95	111.83	9	4
4	A	376	PX4	C17-C16-C15	2.66	100.91	114.37	14	1
4	A	400	PX4	O3-P1-O2	2.66	98.38	108.94	13	4
4	A	370	PX4	C5-N1-C3	2.66	115.96	108.98	9	4
4	A	371	PX4	O3-P1-O2	2.66	98.39	108.94	6	5
4	A	390	PX4	O1-P1-O4	2.66	119.63	107.57	2	1
4	A	393	PX4	O1-P1-O3	2.66	95.50	107.57	5	2
4	A	398	PX4	O3-C1-C2	2.66	122.46	109.65	14	1
4	A	400	PX4	C1-C2-N1	2.66	124.36	115.82	10	2
4	A	322	PX4	C5-N1-C3	2.66	101.99	108.98	14	4
4	A	363	PX4	C13-C12-C11	2.66	100.92	114.37	14	1
4	A	373	PX4	O4-P1-O2	2.66	119.48	108.94	7	6
4	A	382	PX4	C31-C30-C29	2.66	100.92	114.37	13	2
4	A	386	PX4	C11-C10-C9	2.66	103.95	113.69	7	2
4	A	392	PX4	P1-O4-C6	2.66	106.12	121.35	10	5
4	A	428	PX4	C20-C19-C18	2.66	100.93	114.37	3	2
4	A	321	PX4	C5-N1-C2	2.66	120.47	109.91	11	1
4	A	370	PX4	O1-P1-O3	2.66	119.60	107.57	14	1
4	A	379	PX4	C5-N1-C4	2.66	102.00	108.98	11	2
4	A	396	PX4	C20-C19-C18	2.66	100.94	114.37	2	2
4	A	321	PX4	O4-P1-O2	2.65	98.41	108.94	8	2
4	A	332	PX4	C29-C28-C27	2.65	100.95	114.37	11	3
4	A	318	PX4	C5-N1-C4	2.65	102.01	108.98	6	1
4	A	327	PX4	C16-C15-C14	2.65	100.96	114.37	4	1
4	A	335	PX4	C31-C30-C29	2.65	100.97	114.37	13	1
4	A	366	PX4	C8-O5-C9	2.65	107.42	117.12	10	2
4	A	399	PX4	C16-C15-C14	2.65	100.96	114.37	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	323	PX4	C12-C11-C10	2.65	103.39	113.13	4	3
4	A	389	PX4	C1-C2-N1	2.65	124.33	115.82	2	2
4	A	401	PX4	C34-C33-C32	2.65	100.98	114.37	8	1
4	A	402	PX4	C13-C12-C11	2.65	100.98	114.37	2	2
4	A	412	PX4	C28-C27-C26	2.65	100.97	114.37	14	2
4	A	320	PX4	C25-C24-C23	2.65	104.00	113.69	5	2
4	A	324	PX4	C8-O5-C9	2.65	107.44	117.12	14	3
4	A	340	PX4	C27-C26-C25	2.65	100.99	114.37	9	2
4	A	365	PX4	C3-N1-C2	2.65	99.39	109.91	5	1
4	A	394	PX4	C17-C16-C15	2.65	100.99	114.37	10	1
4	A	421	PX4	P1-O4-C6	2.65	106.18	121.35	2	10
4	A	340	PX4	O6-C9-C10	2.65	113.44	123.78	14	4
4	A	347	PX4	C12-C11-C10	2.65	103.41	113.13	12	5
4	A	398	PX4	C20-C19-C18	2.65	100.99	114.37	7	1
4	A	387	PX4	O8-C23-C24	2.64	113.44	123.78	2	1
4	A	399	PX4	C26-C25-C24	2.65	103.41	113.13	9	2
4	A	391	PX4	C26-C25-C24	2.64	103.41	113.13	9	2
4	A	415	PX4	O5-C9-O6	2.65	117.01	123.63	8	1
4	A	314	PX4	C20-C19-C18	2.64	101.00	114.37	8	4
4	A	316	PX4	C14-C13-C12	2.64	101.01	114.37	5	2
4	A	325	PX4	O3-C1-C2	2.64	122.37	109.65	3	2
4	A	397	PX4	O6-C9-C10	2.64	113.44	123.78	11	2
4	A	317	PX4	C16-C15-C14	2.64	101.02	114.37	5	2
4	A	345	PX4	C1-C2-N1	2.64	124.30	115.82	9	1
4	A	383	PX4	O3-P1-O2	2.64	98.47	108.94	10	2
4	A	342	PX4	O1-P1-O4	2.64	119.53	107.57	3	2
4	A	310	PX4	C8-O5-C9	2.64	107.47	117.12	14	2
4	A	326	PX4	C34-C33-C32	2.64	101.03	114.37	7	2
4	A	334	PX4	C11-C10-C9	2.64	104.03	113.69	6	1
4	A	417	PX4	C1-C2-N1	2.64	124.29	115.82	2	2
4	A	425	PX4	C12-C11-C10	2.64	122.82	113.13	12	1
4	A	399	PX4	C13-C12-C11	2.63	101.05	114.37	2	1
4	A	410	PX4	C5-N1-C4	2.63	102.06	108.98	2	3
4	A	429	PX4	C3-N1-C2	2.64	99.43	109.91	10	3
4	A	353	PX4	O3-P1-O2	2.63	98.49	108.94	4	4
4	A	366	PX4	C12-C11-C10	2.63	103.45	113.13	3	1
4	A	403	PX4	O3-C1-C2	2.63	122.32	109.65	5	1
4	A	422	PX4	C12-C11-C10	2.63	103.45	113.13	4	2
4	A	326	PX4	C17-C16-C15	2.63	101.07	114.37	5	2
4	A	375	PX4	C12-C11-C10	2.63	103.46	113.13	10	3
4	A	393	PX4	C11-C10-C9	2.63	104.05	113.69	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	404	PX4	C17-C16-C15	2.63	101.06	114.37	1	1
4	A	426	PX4	C5-N1-C2	2.63	99.45	109.91	4	2
4	A	311	PX4	C18-C17-C16	2.63	101.07	114.37	12	3
4	A	312	PX4	C18-C17-C16	2.63	101.08	114.37	2	2
4	A	314	PX4	C33-C32-C31	2.63	101.08	114.37	4	3
4	A	318	PX4	C11-C10-C9	2.63	104.06	113.69	10	3
4	A	331	PX4	C1-C2-N1	2.63	124.26	115.82	1	1
4	A	380	PX4	C11-C10-C9	2.63	104.06	113.69	4	3
4	A	417	PX4	C11-C10-C9	2.63	104.07	113.69	3	1
4	A	314	PX4	C28-C27-C26	2.62	101.11	114.37	11	1
4	A	415	PX4	C1-C2-N1	2.62	124.24	115.82	1	4
4	A	426	PX4	O3-C1-C2	2.62	122.28	109.65	9	2
4	A	310	PX4	C4-N1-C3	2.62	102.09	108.98	11	4
4	A	333	PX4	C25-C24-C23	2.62	104.09	113.69	11	1
4	A	370	PX4	C16-C15-C14	2.62	101.12	114.37	4	1
4	A	396	PX4	C29-C28-C27	2.62	101.12	114.37	9	1
4	A	410	PX4	C25-C24-C23	2.62	104.09	113.69	12	2
4	A	393	PX4	C4-N1-C3	2.62	115.86	108.98	11	2
4	A	411	PX4	C7-O7-C23	2.62	124.07	117.80	12	1
4	A	424	PX4	O5-C9-C10	2.62	119.83	111.83	8	3
4	A	312	PX4	O1-P1-O2	2.62	124.63	112.44	6	5
4	A	359	PX4	C30-C29-C28	2.62	101.13	114.37	5	1
4	A	390	PX4	O5-C9-C10	2.62	119.82	111.83	5	3
4	A	330	PX4	C19-C18-C17	2.62	101.14	114.37	13	1
4	A	417	PX4	C5-N1-C3	2.62	102.10	108.98	4	2
4	A	313	PX4	C3-N1-C2	2.61	120.30	109.91	10	1
4	A	386	PX4	O4-P1-O2	2.61	119.30	108.94	1	3
4	A	325	PX4	C19-C18-C17	2.61	101.16	114.37	8	2
4	A	360	PX4	C5-N1-C3	2.61	102.11	108.98	7	2
4	A	367	PX4	O7-C7-C8	2.61	117.72	108.34	8	2
4	A	388	PX4	C4-N1-C3	2.61	102.11	108.98	13	2
4	A	398	PX4	C33-C32-C31	2.61	101.16	114.37	9	2
4	A	399	PX4	C1-C2-N1	2.61	124.21	115.82	12	2
4	A	407	PX4	C28-C27-C26	2.61	101.16	114.37	9	2
4	A	412	PX4	C14-C13-C12	2.61	101.16	114.37	3	1
4	A	414	PX4	O4-P1-O2	2.61	119.29	108.94	1	3
4	A	357	PX4	O3-P1-O2	2.61	98.59	108.94	2	2
4	A	379	PX4	C20-C19-C18	2.61	101.17	114.37	5	2
4	A	399	PX4	O3-C1-C2	2.61	122.21	109.65	9	2
4	A	409	PX4	C18-C17-C16	2.61	101.17	114.37	1	1
4	A	414	PX4	C3-N1-C2	2.61	120.29	109.91	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	422	PX4	C7-O7-C23	2.61	124.04	117.80	11	2
4	A	312	PX4	C28-C27-C26	2.61	101.18	114.37	5	4
4	A	317	PX4	C31-C30-C29	2.61	101.19	114.37	1	2
4	A	322	PX4	C1-C2-N1	2.61	124.19	115.82	14	2
4	A	306	PX4	O1-P1-O3	2.60	95.76	107.57	1	3
4	A	337	PX4	C1-C2-N1	2.61	124.18	115.82	10	4
4	A	398	PX4	C29-C28-C27	2.61	101.20	114.37	10	1
4	A	321	PX4	O7-C7-C6	2.60	117.68	108.34	8	2
4	A	377	PX4	O4-P1-O2	2.60	98.61	108.94	1	2
4	A	320	PX4	O1-P1-O3	2.60	95.77	107.57	8	3
4	A	330	PX4	C4-N1-C3	2.60	115.81	108.98	4	1
4	A	404	PX4	C28-C27-C26	2.60	101.21	114.37	9	2
4	A	406	PX4	C26-C25-C24	2.60	103.56	113.13	4	3
4	A	399	PX4	C19-C18-C17	2.60	101.22	114.37	9	3
4	A	408	PX4	O3-P1-O2	2.60	98.62	108.94	1	4
4	A	309	PX4	C8-O5-C9	2.60	107.61	117.12	7	3
4	A	332	PX4	O7-C7-C6	2.60	117.67	108.34	6	7
4	A	320	PX4	C12-C11-C10	2.60	103.58	113.13	2	2
4	A	327	PX4	C11-C10-C9	2.60	104.17	113.69	4	1
4	A	333	PX4	C8-O5-C9	2.60	126.62	117.12	8	3
4	A	362	PX4	C30-C29-C28	2.60	101.22	114.37	11	1
4	A	365	PX4	C4-N1-C3	2.60	115.81	108.98	10	2
4	A	405	PX4	C13-C12-C11	2.60	101.22	114.37	4	1
4	A	411	PX4	C1-C2-N1	2.60	124.17	115.82	9	4
4	A	319	PX4	C12-C11-C10	2.60	103.58	113.13	5	3
4	A	347	PX4	C4-N1-C3	2.60	102.15	108.98	11	2
4	A	397	PX4	O4-P1-O2	2.60	119.23	108.94	11	2
4	A	317	PX4	O5-C9-O6	2.59	117.14	123.63	1	1
4	A	330	PX4	C3-N1-C2	2.60	99.59	109.91	1	2
4	A	378	PX4	C20-C19-C18	2.60	101.24	114.37	14	1
4	A	407	PX4	O3-P1-O2	2.60	98.64	108.94	2	3
4	A	414	PX4	C26-C25-C24	2.60	103.59	113.13	13	1
4	A	344	PX4	O1-P1-O3	2.59	95.81	107.57	1	2
4	A	347	PX4	C1-C2-N1	2.60	124.15	115.82	9	3
4	A	394	PX4	C1-C2-N1	2.60	124.15	115.82	12	2
4	A	324	PX4	C11-C10-C9	2.59	104.19	113.69	5	2
4	A	387	PX4	O3-C1-C2	2.59	122.12	109.65	7	2
4	A	404	PX4	O3-C1-C2	2.59	122.13	109.65	8	2
4	A	317	PX4	C11-C10-C9	2.59	123.19	113.69	6	4
4	A	318	PX4	C3-N1-C2	2.59	120.21	109.91	9	1
4	A	348	PX4	C34-C33-C32	2.59	101.27	114.37	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	372	PX4	O3-C1-C2	2.59	122.11	109.65	3	2
4	A	376	PX4	O7-C7-C6	2.59	117.64	108.34	7	4
4	A	407	PX4	O6-C9-C10	2.59	113.65	123.78	8	1
4	A	425	PX4	C13-C12-C11	2.59	101.27	114.37	3	2
4	A	327	PX4	C3-N1-C2	2.59	120.20	109.91	13	1
4	A	340	PX4	C3-N1-C2	2.59	99.62	109.91	9	2
4	A	353	PX4	C5-N1-C3	2.59	102.18	108.98	14	3
4	A	361	PX4	C34-C33-C32	2.59	101.28	114.37	11	2
4	A	389	PX4	C7-O7-C23	2.59	123.99	117.80	14	2
4	A	413	PX4	C34-C33-C32	2.59	101.28	114.37	3	3
4	A	423	PX4	C31-C30-C29	2.59	101.28	114.37	12	2
4	A	425	PX4	C28-C27-C26	2.59	101.28	114.37	9	2
4	A	426	PX4	C27-C26-C25	2.59	101.28	114.37	7	2
4	A	332	PX4	C5-N1-C2	2.59	99.63	109.91	11	1
4	A	360	PX4	O3-C1-C2	2.59	122.10	109.65	10	2
4	A	311	PX4	C8-O5-C9	2.59	107.67	117.12	6	2
4	A	347	PX4	C26-C25-C24	2.59	103.63	113.13	7	3
4	A	369	PX4	C5-N1-C3	2.59	102.18	108.98	11	3
4	A	401	PX4	O1-P1-O4	2.59	119.29	107.57	2	3
4	A	421	PX4	C15-C14-C13	2.59	101.30	114.37	14	2
4	A	317	PX4	O3-P1-O2	2.58	98.69	108.94	9	1
4	A	349	PX4	C12-C11-C10	2.58	103.63	113.13	1	1
4	A	419	PX4	O1-P1-O4	2.58	119.28	107.57	7	2
4	A	428	PX4	O1-P1-O3	2.59	119.28	107.57	7	2
4	A	307	PX4	C11-C10-C9	2.58	104.23	113.69	4	2
4	A	313	PX4	C25-C24-C23	2.58	104.23	113.69	3	1
4	A	390	PX4	C30-C29-C28	2.58	101.31	114.37	6	1
4	A	418	PX4	O1-P1-O3	2.58	119.27	107.57	3	1
4	A	419	PX4	O7-C23-O8	2.58	117.67	123.70	2	2
4	A	310	PX4	C26-C25-C24	2.58	103.64	113.13	2	2
4	A	333	PX4	C26-C25-C24	2.58	103.64	113.13	8	1
4	A	371	PX4	C28-C27-C26	2.58	101.32	114.37	1	1
4	A	374	PX4	C5-N1-C4	2.58	115.76	108.98	14	3
4	A	408	PX4	C34-C33-C32	2.58	101.32	114.37	5	1
4	A	408	PX4	C18-C17-C16	2.58	101.32	114.37	6	1
4	A	412	PX4	O1-P1-O4	2.58	119.27	107.57	4	2
4	A	317	PX4	C5-N1-C4	2.58	102.20	108.98	13	4
4	A	330	PX4	O3-P1-O2	2.58	98.71	108.94	9	1
4	A	373	PX4	O7-C7-C6	2.58	117.60	108.34	4	6
4	A	384	PX4	O1-P1-O3	2.58	95.88	107.57	13	3
4	A	385	PX4	O3-P1-O2	2.58	98.71	108.94	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	405	PX4	O5-C9-C10	2.58	119.70	111.83	1	5
4	A	326	PX4	C20-C19-C18	2.58	101.33	114.37	12	1
4	A	312	PX4	C3-N1-C2	2.58	99.67	109.91	9	2
4	A	340	PX4	C31-C30-C29	2.58	101.34	114.37	10	2
4	A	357	PX4	O3-C1-C2	2.58	122.05	109.65	2	2
4	A	353	PX4	O1-P1-O4	2.58	119.25	107.57	9	1
4	A	359	PX4	O5-C9-C10	2.58	119.69	111.83	3	2
4	A	364	PX4	C5-N1-C2	2.58	120.15	109.91	13	2
4	A	372	PX4	C1-C2-N1	2.58	124.09	115.82	13	6
4	A	397	PX4	C19-C18-C17	2.58	101.34	114.37	3	2
4	A	331	PX4	C13-C12-C11	2.57	101.35	114.37	3	1
4	A	414	PX4	C8-O5-C9	2.58	107.70	117.12	4	2
4	A	372	PX4	C26-C25-C24	2.57	103.67	113.13	7	1
4	A	409	PX4	C12-C11-C10	2.57	103.67	113.13	13	2
4	A	334	PX4	C1-C2-N1	2.57	124.08	115.82	7	4
4	A	337	PX4	C18-C17-C16	2.57	101.37	114.37	7	2
4	A	358	PX4	C26-C25-C24	2.57	103.67	113.13	4	1
4	A	313	PX4	O1-P1-O3	2.57	95.92	107.57	12	3
4	A	332	PX4	C14-C13-C12	2.57	101.38	114.37	9	2
4	A	339	PX4	O5-C9-O6	2.57	130.06	123.63	10	2
4	A	428	PX4	O3-P1-O2	2.57	98.74	108.94	9	1
4	A	364	PX4	O8-C23-C24	2.57	133.83	123.78	11	2
4	A	331	PX4	C29-C28-C27	2.57	101.39	114.37	3	1
4	A	368	PX4	C5-N1-C2	2.57	99.70	109.91	14	1
4	A	382	PX4	C34-C33-C32	2.57	101.38	114.37	8	1
4	A	396	PX4	C33-C32-C31	2.57	101.38	114.37	13	2
4	A	412	PX4	C31-C30-C29	2.57	101.39	114.37	4	1
4	A	415	PX4	C29-C28-C27	2.57	101.39	114.37	6	3
4	A	417	PX4	C3-N1-C2	2.57	99.70	109.91	9	1
4	A	421	PX4	C12-C11-C10	2.57	103.69	113.13	5	1
4	A	317	PX4	C15-C14-C13	2.57	101.39	114.37	9	2
4	A	307	PX4	C16-C15-C14	2.56	101.40	114.37	9	1
4	A	309	PX4	C27-C26-C25	2.57	101.40	114.37	5	1
4	A	340	PX4	C4-N1-C2	2.57	120.11	109.91	10	4
4	A	313	PX4	C15-C14-C13	2.56	101.41	114.37	13	1
4	A	345	PX4	C34-C33-C32	2.56	101.40	114.37	3	3
4	A	348	PX4	C32-C31-C30	2.56	101.40	114.37	10	1
4	A	351	PX4	C1-C2-N1	2.56	124.05	115.82	13	3
4	A	372	PX4	C33-C32-C31	2.57	101.40	114.37	7	1
4	A	352	PX4	C3-N1-C2	2.56	99.72	109.91	6	2
4	A	318	PX4	O5-C9-O6	2.56	117.22	123.63	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	325	PX4	C18-C17-C16	2.56	101.41	114.37	13	3
4	A	352	PX4	C15-C14-C13	2.56	101.41	114.37	6	1
4	A	357	PX4	C30-C29-C28	2.56	101.41	114.37	11	2
4	A	359	PX4	C5-N1-C3	2.56	102.24	108.98	12	5
4	A	363	PX4	C31-C30-C29	2.56	101.41	114.37	3	1
4	A	364	PX4	C17-C16-C15	2.56	101.41	114.37	8	1
4	A	372	PX4	O7-C7-C6	2.56	117.54	108.34	5	3
4	A	397	PX4	O5-C9-O6	2.56	117.22	123.63	13	3
4	A	408	PX4	C14-C13-C12	2.56	101.41	114.37	9	1
4	A	309	PX4	C30-C29-C28	2.56	101.42	114.37	11	1
4	A	320	PX4	C32-C31-C30	2.56	101.42	114.37	9	1
4	A	336	PX4	O3-C1-C2	2.56	121.97	109.65	4	4
4	A	370	PX4	C12-C11-C10	2.56	103.72	113.13	5	2
4	A	412	PX4	O4-P1-O2	2.56	119.09	108.94	5	2
4	A	417	PX4	O5-C9-O6	2.56	117.22	123.63	12	6
4	A	430	PX4	C26-C25-C24	2.56	122.54	113.13	12	2
4	A	334	PX4	C5-N1-C2	2.56	120.08	109.91	3	1
4	A	343	PX4	C27-C26-C25	2.56	101.43	114.37	2	1
4	A	359	PX4	O3-C1-C2	2.56	121.96	109.65	14	2
4	A	412	PX4	C20-C19-C18	2.56	101.43	114.37	1	2
4	A	415	PX4	C17-C16-C15	2.56	101.43	114.37	8	1
4	A	315	PX4	C33-C32-C31	2.56	101.44	114.37	6	1
4	A	348	PX4	C4-N1-C3	2.56	102.26	108.98	6	2
4	A	402	PX4	C3-N1-C2	2.56	99.75	109.91	2	1
4	A	319	PX4	C27-C26-C25	2.56	101.45	114.37	1	1
4	A	390	PX4	O3-C1-C2	2.56	121.94	109.65	11	2
4	A	397	PX4	O8-C23-C24	2.55	113.79	123.78	3	2
4	A	312	PX4	C34-C33-C32	2.55	101.47	114.37	5	4
4	A	314	PX4	O7-C23-O8	2.55	117.74	123.70	14	3
4	A	358	PX4	O7-C7-C6	2.55	117.50	108.34	6	4
4	A	323	PX4	C29-C28-C27	2.55	101.47	114.37	4	2
4	A	345	PX4	C7-O7-C23	2.55	111.69	117.80	14	4
4	A	358	PX4	C11-C10-C9	2.55	104.34	113.69	12	2
4	A	360	PX4	O4-P1-O2	2.55	119.05	108.94	9	4
4	A	391	PX4	O8-C23-C24	2.55	113.80	123.78	3	2
4	A	406	PX4	C34-C33-C32	2.55	101.47	114.37	5	2
4	A	420	PX4	O3-P1-O2	2.55	98.82	108.94	10	3
4	A	424	PX4	O3-P1-O2	2.55	98.82	108.94	11	5
4	A	427	PX4	C8-O5-C9	2.55	107.79	117.12	14	1
4	A	428	PX4	C34-C33-C32	2.55	101.47	114.37	12	3
4	A	319	PX4	O3-C1-C2	2.55	121.92	109.65	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	321	PX4	C4-N1-C2	2.55	120.05	109.91	13	1
4	A	377	PX4	C12-C11-C10	2.55	122.50	113.13	7	2
4	A	335	PX4	C1-C2-N1	2.55	124.00	115.82	11	5
4	A	385	PX4	C34-C33-C32	2.55	101.48	114.37	1	1
4	A	390	PX4	C28-C27-C26	2.55	101.48	114.37	3	1
4	A	328	PX4	C16-C15-C14	2.55	101.49	114.37	3	2
4	A	359	PX4	C12-C11-C10	2.55	103.76	113.13	8	2
4	A	390	PX4	C4-N1-C3	2.55	102.28	108.98	3	2
4	A	411	PX4	O7-C7-C6	2.55	117.48	108.34	4	4
4	A	419	PX4	C4-N1-C2	2.55	99.78	109.91	8	1
4	A	306	PX4	C4-N1-C3	2.55	102.29	108.98	8	1
4	A	325	PX4	C1-C2-N1	2.54	123.99	115.82	14	4
4	A	348	PX4	C7-O7-C23	2.55	111.70	117.80	10	2
4	A	349	PX4	C13-C12-C11	2.55	101.50	114.37	3	2
4	A	370	PX4	C15-C14-C13	2.55	101.50	114.37	8	1
4	A	405	PX4	O3-P1-O2	2.55	98.84	108.94	14	2
4	A	338	PX4	C8-O5-C9	2.54	107.82	117.12	2	2
4	A	375	PX4	O3-C1-C2	2.54	121.89	109.65	8	1
4	A	375	PX4	C1-C2-N1	2.54	123.99	115.82	13	2
4	A	388	PX4	C19-C18-C17	2.54	101.51	114.37	8	1
4	A	419	PX4	O3-C1-C2	2.54	121.89	109.65	1	3
4	A	332	PX4	C25-C24-C23	2.54	104.38	113.69	4	1
4	A	365	PX4	C15-C14-C13	2.54	101.51	114.37	7	1
4	A	410	PX4	C28-C27-C26	2.54	101.52	114.37	5	1
4	A	421	PX4	C13-C12-C11	2.54	101.51	114.37	10	1
4	A	322	PX4	C19-C18-C17	2.54	101.52	114.37	9	2
4	A	340	PX4	O5-C9-C10	2.54	119.58	111.83	11	2
4	A	360	PX4	C15-C14-C13	2.54	101.52	114.37	6	2
4	A	390	PX4	C3-N1-C2	2.54	99.80	109.91	5	2
4	A	365	PX4	C26-C25-C24	2.54	103.79	113.13	1	2
4	A	411	PX4	C25-C24-C23	2.54	104.38	113.69	6	3
4	A	389	PX4	C3-N1-C2	2.54	120.00	109.91	14	1
4	A	405	PX4	C5-N1-C2	2.54	120.00	109.91	10	1
4	A	412	PX4	O3-P1-O2	2.54	98.87	108.94	5	3
4	A	345	PX4	O1-P1-O3	2.54	96.06	107.57	4	4
4	A	400	PX4	C4-N1-C2	2.54	120.00	109.91	13	2
4	A	315	PX4	C4-N1-C2	2.54	119.99	109.91	5	1
4	A	369	PX4	C17-C16-C15	2.54	101.55	114.37	10	1
4	A	371	PX4	C25-C24-C23	2.54	104.40	113.69	10	2
4	A	388	PX4	O5-C9-O6	2.54	117.28	123.63	13	1
4	A	414	PX4	C4-N1-C2	2.54	99.83	109.91	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	336	PX4	C13-C12-C11	2.54	101.55	114.37	13	1
4	A	415	PX4	O3-C1-C2	2.54	121.85	109.65	5	2
4	A	422	PX4	C11-C10-C9	2.54	104.40	113.69	8	1
4	A	309	PX4	O5-C9-C10	2.53	119.56	111.83	13	5
4	A	343	PX4	O5-C9-O6	2.53	117.29	123.63	5	5
4	A	349	PX4	C31-C30-C29	2.53	101.56	114.37	5	1
4	A	376	PX4	C28-C27-C26	2.53	101.56	114.37	2	2
4	A	397	PX4	C26-C25-C24	2.53	103.82	113.13	13	1
4	A	401	PX4	C28-C27-C26	2.53	101.56	114.37	10	2
4	A	421	PX4	C3-N1-C2	2.53	99.84	109.91	12	2
4	A	321	PX4	C5-N1-C4	2.53	115.63	108.98	5	2
4	A	331	PX4	C12-C11-C10	2.53	103.82	113.13	13	3
4	A	349	PX4	O1-P1-O4	2.53	119.05	107.57	7	1
4	A	376	PX4	C18-C17-C16	2.53	101.58	114.37	11	2
4	A	379	PX4	C31-C30-C29	2.53	101.57	114.37	1	1
4	A	392	PX4	C31-C30-C29	2.53	101.57	114.37	12	1
4	A	422	PX4	C28-C27-C26	2.53	101.56	114.37	4	1
4	A	367	PX4	C17-C16-C15	2.53	101.58	114.37	13	3
4	A	385	PX4	C4-N1-C2	2.53	119.97	109.91	11	1
4	A	350	PX4	C19-C18-C17	2.53	101.58	114.37	11	1
4	A	389	PX4	O4-P1-O2	2.53	118.96	108.94	7	4
4	A	319	PX4	C17-C16-C15	2.53	101.59	114.37	11	1
4	A	364	PX4	O6-C9-C10	2.53	113.89	123.78	13	3
4	A	430	PX4	C30-C29-C28	2.53	101.59	114.37	9	1
4	A	309	PX4	O1-P1-O4	2.53	119.02	107.57	5	3
4	A	312	PX4	C4-N1-C2	2.53	119.95	109.91	12	1
4	A	334	PX4	C25-C24-C23	2.53	104.44	113.69	13	2
4	A	365	PX4	O7-C23-O8	2.53	117.80	123.70	3	2
4	A	367	PX4	C3-N1-C2	2.53	99.87	109.91	5	2
4	A	395	PX4	C31-C30-C29	2.53	101.60	114.37	9	2
4	A	366	PX4	O7-C23-O8	2.52	117.80	123.70	7	5
4	A	398	PX4	C11-C10-C9	2.52	104.44	113.69	1	2
4	A	416	PX4	O3-C1-C2	2.52	121.80	109.65	11	5
4	A	351	PX4	O5-C9-C10	2.52	119.53	111.83	8	2
4	A	392	PX4	O1-P1-O3	2.52	96.13	107.57	11	1
4	A	319	PX4	C4-N1-C2	2.52	119.93	109.91	13	1
4	A	306	PX4	O3-P1-O2	2.52	98.95	108.94	8	3
4	A	307	PX4	O4-P1-O2	2.52	118.92	108.94	12	1
4	A	312	PX4	C17-C16-C15	2.52	101.63	114.37	12	3
4	A	353	PX4	C12-C11-C10	2.52	122.39	113.13	10	1
4	A	354	PX4	C27-C26-C25	2.52	101.63	114.37	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	408	PX4	C33-C32-C31	2.52	101.63	114.37	6	1
4	A	422	PX4	C17-C16-C15	2.52	101.63	114.37	11	1
4	A	313	PX4	C27-C26-C25	2.52	101.64	114.37	9	2
4	A	371	PX4	C14-C13-C12	2.52	101.64	114.37	5	3
4	A	378	PX4	C7-O7-C23	2.52	111.77	117.80	4	2
4	A	384	PX4	O7-C7-C6	2.52	117.38	108.34	13	2
4	A	374	PX4	O3-P1-O2	2.52	98.96	108.94	12	1
4	A	386	PX4	C20-C19-C18	2.52	101.64	114.37	6	2
4	A	392	PX4	O8-C23-C24	2.52	113.93	123.78	2	1
4	A	419	PX4	C12-C11-C10	2.52	103.87	113.13	8	1
4	A	322	PX4	O5-C9-C10	2.52	119.51	111.83	10	4
4	A	342	PX4	C14-C13-C12	2.52	101.65	114.37	14	1
4	A	321	PX4	O1-P1-O4	2.51	118.96	107.57	9	3
4	A	368	PX4	C11-C10-C9	2.51	104.48	113.69	5	1
4	A	398	PX4	O8-C23-C24	2.51	113.95	123.78	4	2
4	A	405	PX4	O1-P1-O4	2.51	118.96	107.57	4	2
4	A	419	PX4	C3-N1-C2	2.51	119.91	109.91	4	3
4	A	324	PX4	O5-C9-O6	2.51	117.34	123.63	13	1
4	A	374	PX4	O1-P1-O4	2.51	118.96	107.57	14	1
4	A	315	PX4	O6-C9-C10	2.51	113.96	123.78	3	1
4	A	331	PX4	C3-N1-C2	2.51	119.89	109.91	2	3
4	A	353	PX4	O7-C7-C6	2.51	117.36	108.34	6	2
4	A	356	PX4	C13-C12-C11	2.51	101.67	114.37	8	1
4	A	399	PX4	C17-C16-C15	2.51	101.67	114.37	13	2
4	A	326	PX4	C25-C24-C23	2.51	104.50	113.69	13	2
4	A	368	PX4	O8-C23-C24	2.51	113.96	123.78	13	2
4	A	374	PX4	C27-C26-C25	2.51	101.68	114.37	12	3
4	A	385	PX4	C33-C32-C31	2.51	101.68	114.37	6	1
4	A	386	PX4	C31-C30-C29	2.51	101.68	114.37	7	2
4	A	399	PX4	C15-C14-C13	2.51	101.68	114.37	9	1
4	A	324	PX4	C15-C14-C13	2.51	101.69	114.37	10	1
4	A	328	PX4	C17-C16-C15	2.51	101.69	114.37	13	1
4	A	350	PX4	O5-C9-O6	2.51	117.35	123.63	1	2
4	A	387	PX4	C19-C18-C17	2.51	101.68	114.37	5	2
4	A	392	PX4	C14-C13-C12	2.51	101.69	114.37	9	1
4	A	395	PX4	C5-N1-C2	2.51	99.94	109.91	12	2
4	A	415	PX4	C16-C15-C14	2.51	101.68	114.37	3	2
4	A	355	PX4	C13-C12-C11	2.51	101.69	114.37	11	1
4	A	315	PX4	C11-C10-C9	2.51	104.51	113.69	7	1
4	A	360	PX4	C13-C12-C11	2.51	101.69	114.37	13	1
4	A	406	PX4	C4-N1-C3	2.51	102.39	108.98	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	408	PX4	C5-N1-C3	2.51	102.39	108.98	9	2
4	A	365	PX4	C30-C29-C28	2.51	101.70	114.37	1	1
4	A	365	PX4	C11-C10-C9	2.51	122.88	113.69	12	2
4	A	329	PX4	C28-C27-C26	2.50	101.71	114.37	6	1
4	A	334	PX4	O1-P1-O4	2.50	118.92	107.57	8	2
4	A	343	PX4	C29-C28-C27	2.50	101.71	114.37	5	1
4	A	428	PX4	O6-C9-C10	2.51	113.98	123.78	3	2
4	A	389	PX4	C16-C15-C14	2.50	101.71	114.37	6	1
4	A	394	PX4	C8-O5-C9	2.50	107.97	117.12	12	4
4	A	396	PX4	C30-C29-C28	2.50	101.71	114.37	5	1
4	A	324	PX4	C20-C19-C18	2.50	101.72	114.37	2	4
4	A	397	PX4	C29-C28-C27	2.50	101.72	114.37	6	4
4	A	410	PX4	C8-O5-C9	2.50	107.97	117.12	1	1
4	A	315	PX4	C15-C14-C13	2.50	101.72	114.37	3	1
4	A	319	PX4	C20-C19-C18	2.50	101.72	114.37	7	1
4	A	346	PX4	C3-N1-C2	2.50	99.97	109.91	9	1
4	A	361	PX4	C17-C16-C15	2.50	101.72	114.37	5	1
4	A	407	PX4	C19-C18-C17	2.50	101.72	114.37	4	1
4	A	408	PX4	C11-C10-C9	2.50	104.53	113.69	1	1
4	A	408	PX4	C17-C16-C15	2.50	101.72	114.37	4	2
4	A	411	PX4	C33-C32-C31	2.50	101.72	114.37	8	2
4	A	419	PX4	C15-C14-C13	2.50	101.72	114.37	8	1
4	A	428	PX4	C25-C24-C23	2.50	104.52	113.69	10	1
4	A	311	PX4	O3-C1-C2	2.50	121.68	109.65	2	2
4	A	356	PX4	C34-C33-C32	2.50	101.73	114.37	12	1
4	A	335	PX4	C27-C26-C25	2.50	101.74	114.37	14	1
4	A	360	PX4	O1-P1-O4	2.50	118.89	107.57	5	1
4	A	370	PX4	C33-C32-C31	2.50	101.73	114.37	10	3
4	A	389	PX4	O3-P1-O2	2.50	99.04	108.94	6	3
4	A	331	PX4	C4-N1-C2	2.50	119.83	109.91	13	1
4	A	402	PX4	C18-C17-C16	2.50	101.75	114.37	6	2
4	A	308	PX4	C34-C33-C32	2.49	101.76	114.37	11	2
4	A	316	PX4	C5-N1-C3	2.49	102.42	108.98	8	3
4	A	312	PX4	C27-C26-C25	2.49	101.77	114.37	2	1
4	A	321	PX4	C3-N1-C2	2.49	100.00	109.91	13	2
4	A	323	PX4	C1-C2-N1	2.49	123.82	115.82	10	3
4	A	351	PX4	C27-C26-C25	2.49	101.76	114.37	4	2
4	A	324	PX4	C5-N1-C3	2.49	102.43	108.98	12	3
4	A	330	PX4	C4-N1-C2	2.49	100.00	109.91	4	3
4	A	318	PX4	C20-C19-C18	2.49	101.78	114.37	14	2
4	A	330	PX4	C34-C33-C32	2.49	101.77	114.37	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	345	PX4	C19-C18-C17	2.49	101.77	114.37	11	2
4	A	346	PX4	C31-C30-C29	2.49	101.77	114.37	7	1
4	A	360	PX4	C18-C17-C16	2.49	101.77	114.37	1	1
4	A	376	PX4	C12-C11-C10	2.49	103.97	113.13	8	1
4	A	392	PX4	C17-C16-C15	2.49	101.77	114.37	5	1
4	A	311	PX4	O8-C23-C24	2.49	114.05	123.78	1	3
4	A	333	PX4	O7-C23-O8	2.49	117.88	123.70	10	2
4	A	356	PX4	C14-C13-C12	2.49	101.78	114.37	5	2
4	A	352	PX4	O3-P1-O2	2.49	99.07	108.94	5	2
4	A	407	PX4	C34-C33-C32	2.49	101.78	114.37	1	1
4	A	416	PX4	C16-C15-C14	2.49	101.79	114.37	1	1
4	A	430	PX4	C4-N1-C2	2.49	100.01	109.91	4	2
4	A	336	PX4	C4-N1-C2	2.49	119.80	109.91	4	4
4	A	343	PX4	C32-C31-C30	2.49	101.79	114.37	2	1
4	A	414	PX4	C19-C18-C17	2.49	101.79	114.37	8	1
4	A	339	PX4	O8-C23-C24	2.49	114.06	123.78	3	3
4	A	341	PX4	C33-C32-C31	2.49	101.80	114.37	5	1
4	A	340	PX4	O3-P1-O2	2.49	99.08	108.94	5	1
4	A	364	PX4	C32-C31-C30	2.49	101.80	114.37	8	1
4	A	311	PX4	O7-C7-C8	2.48	117.25	108.34	7	4
4	A	316	PX4	C5-N1-C4	2.48	102.45	108.98	4	3
4	A	349	PX4	O4-P1-O2	2.48	99.09	108.94	10	2
4	A	367	PX4	C28-C27-C26	2.48	101.81	114.37	5	1
4	A	370	PX4	C26-C25-C24	2.49	104.00	113.13	14	3
4	A	384	PX4	C34-C33-C32	2.49	101.81	114.37	3	2
4	A	395	PX4	C4-N1-C2	2.48	119.78	109.91	6	3
4	A	396	PX4	O4-P1-O2	2.48	118.78	108.94	1	2
4	A	403	PX4	C11-C10-C9	2.48	104.59	113.69	14	2
4	A	421	PX4	C33-C32-C31	2.48	101.82	114.37	2	1
4	A	311	PX4	C5-N1-C4	2.48	102.46	108.98	14	4
4	A	322	PX4	C3-N1-C2	2.48	119.77	109.91	8	4
4	A	339	PX4	C13-C12-C11	2.48	101.83	114.37	13	2
4	A	386	PX4	C27-C26-C25	2.48	101.83	114.37	14	2
4	A	360	PX4	C30-C29-C28	2.48	101.83	114.37	11	1
4	A	389	PX4	C5-N1-C4	2.48	115.49	108.98	8	3
4	A	343	PX4	O3-C1-C2	2.48	121.57	109.65	10	2
4	A	385	PX4	C13-C12-C11	2.48	101.85	114.37	9	2
4	A	411	PX4	C19-C18-C17	2.48	101.85	114.37	9	1
4	A	424	PX4	C33-C32-C31	2.48	101.85	114.37	7	2
4	A	317	PX4	O1-P1-O3	2.48	118.79	107.57	14	2
4	A	319	PX4	C31-C30-C29	2.48	101.85	114.37	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	334	PX4	C15-C14-C13	2.48	101.86	114.37	11	1
4	A	323	PX4	O1-P1-O3	2.47	96.35	107.57	8	2
4	A	332	PX4	O3-P1-O2	2.47	99.13	108.94	2	2
4	A	336	PX4	C25-C24-C23	2.47	104.63	113.69	11	1
4	A	352	PX4	C8-O5-C9	2.47	108.07	117.12	1	3
4	A	358	PX4	C18-C17-C16	2.47	101.86	114.37	4	2
4	A	382	PX4	C20-C19-C18	2.47	101.86	114.37	1	2
4	A	405	PX4	C33-C32-C31	2.48	101.86	114.37	5	2
4	A	413	PX4	O1-P1-O4	2.47	118.78	107.57	5	1
4	A	370	PX4	C18-C17-C16	2.47	101.87	114.37	14	1
4	A	371	PX4	C15-C14-C13	2.47	101.87	114.37	10	3
4	A	416	PX4	O7-C23-O8	2.47	117.92	123.70	7	5
4	A	307	PX4	C19-C18-C17	2.47	101.88	114.37	14	2
4	A	317	PX4	C25-C24-C23	2.47	104.64	113.69	13	3
4	A	322	PX4	C25-C24-C23	2.47	104.64	113.69	6	1
4	A	333	PX4	O1-P1-O4	2.47	118.78	107.57	12	3
4	A	355	PX4	C1-C2-N1	2.47	123.76	115.82	11	6
4	A	361	PX4	C19-C18-C17	2.47	101.87	114.37	10	1
4	A	382	PX4	C27-C26-C25	2.47	101.87	114.37	13	2
4	A	390	PX4	O7-C7-C8	2.47	117.21	108.34	3	5
4	A	416	PX4	C17-C16-C15	2.47	101.87	114.37	8	2
4	A	426	PX4	O3-P1-O2	2.47	99.14	108.94	10	3
4	A	402	PX4	C15-C14-C13	2.47	101.88	114.37	14	1
4	A	393	PX4	C3-N1-C2	2.47	100.09	109.91	5	1
4	A	410	PX4	C31-C30-C29	2.47	101.88	114.37	5	3
4	A	420	PX4	O5-C9-O6	2.47	117.45	123.63	2	4
4	A	423	PX4	O1-P1-O4	2.47	118.77	107.57	1	4
4	A	314	PX4	C34-C33-C32	2.47	101.89	114.37	3	1
4	A	361	PX4	C31-C30-C29	2.47	101.89	114.37	9	1
4	A	347	PX4	C33-C32-C31	2.47	101.89	114.37	11	1
4	A	390	PX4	C11-C10-C9	2.47	104.65	113.69	12	4
4	A	308	PX4	C29-C28-C27	2.47	101.90	114.37	10	1
4	A	363	PX4	C16-C15-C14	2.47	101.90	114.37	13	2
4	A	395	PX4	C29-C28-C27	2.47	101.90	114.37	4	1
4	A	398	PX4	C13-C12-C11	2.47	101.90	114.37	7	3
4	A	425	PX4	C26-C25-C24	2.47	104.06	113.13	4	1
4	A	359	PX4	O4-P1-O2	2.47	118.71	108.94	11	1
4	A	403	PX4	C20-C19-C18	2.47	101.90	114.37	11	2
4	A	396	PX4	O5-C9-O6	2.46	117.46	123.63	14	5
4	A	425	PX4	O8-C23-C24	2.47	114.14	123.78	10	2
4	A	329	PX4	O3-C1-C2	2.46	121.51	109.65	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	C19-C18-C17	2.46	101.91	114.37	2	1
4	A	362	PX4	C18-C17-C16	2.46	101.92	114.37	9	3
4	A	404	PX4	C25-C24-C23	2.46	104.67	113.69	14	2
4	A	430	PX4	C31-C30-C29	2.46	101.91	114.37	12	1
4	A	396	PX4	C16-C15-C14	2.46	101.92	114.37	4	2
4	A	308	PX4	C5-N1-C2	2.46	119.70	109.91	9	1
4	A	317	PX4	C8-O5-C9	2.46	108.12	117.12	3	4
4	A	378	PX4	O4-P1-O2	2.46	118.69	108.94	4	1
4	A	404	PX4	C32-C31-C30	2.46	101.92	114.37	1	1
4	A	417	PX4	C5-N1-C4	2.46	102.51	108.98	10	2
4	A	323	PX4	C13-C12-C11	2.46	101.93	114.37	10	2
4	A	325	PX4	C32-C31-C30	2.46	101.93	114.37	5	1
4	A	385	PX4	C12-C11-C10	2.46	104.08	113.13	13	4
4	A	429	PX4	C4-N1-C3	2.46	115.44	108.98	11	2
4	A	367	PX4	C20-C19-C18	2.46	101.93	114.37	9	2
4	A	340	PX4	C17-C16-C15	2.46	101.94	114.37	8	1
4	A	369	PX4	O5-C9-O6	2.46	117.48	123.63	5	4
4	A	404	PX4	C34-C33-C32	2.46	101.93	114.37	7	1
4	A	410	PX4	O1-P1-O3	2.46	96.42	107.57	11	1
4	A	401	PX4	O6-C9-C10	2.46	114.17	123.78	14	1
4	A	411	PX4	C30-C29-C28	2.46	101.94	114.37	13	1
4	A	430	PX4	C20-C19-C18	2.46	101.94	114.37	13	3
4	A	326	PX4	C4-N1-C2	2.46	119.68	109.91	6	2
4	A	314	PX4	C4-N1-C2	2.46	119.68	109.91	11	1
4	A	315	PX4	O4-P1-O2	2.46	118.67	108.94	13	1
4	A	322	PX4	C33-C32-C31	2.46	101.95	114.37	7	4
4	A	333	PX4	C12-C11-C10	2.46	104.10	113.13	6	1
4	A	336	PX4	C34-C33-C32	2.46	101.95	114.37	3	2
4	A	372	PX4	C3-N1-C2	2.46	119.68	109.91	3	1
4	A	323	PX4	C26-C25-C24	2.46	104.11	113.13	2	2
4	A	355	PX4	C12-C11-C10	2.46	104.10	113.13	2	1
4	A	381	PX4	O3-C1-C2	2.45	121.46	109.65	3	2
4	A	396	PX4	O3-P1-O2	2.46	99.20	108.94	12	1
4	A	411	PX4	C27-C26-C25	2.46	101.95	114.37	7	2
4	A	421	PX4	C8-O5-C9	2.46	108.14	117.12	1	3
4	A	421	PX4	C25-C24-C23	2.46	104.70	113.69	13	1
4	A	422	PX4	C18-C17-C16	2.46	101.95	114.37	2	2
4	A	398	PX4	C26-C25-C24	2.45	104.11	113.13	12	2
4	A	418	PX4	C15-C14-C13	2.45	101.96	114.37	5	2
4	A	307	PX4	O1-P1-O3	2.45	96.45	107.57	6	1
4	A	356	PX4	O1-P1-O3	2.45	118.69	107.57	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	323	PX4	C5-N1-C4	2.45	102.54	108.98	5	3
4	A	361	PX4	C27-C26-C25	2.45	101.98	114.37	13	1
4	A	375	PX4	C5-N1-C2	2.45	119.65	109.91	2	2
4	A	377	PX4	C19-C18-C17	2.45	101.98	114.37	5	2
4	A	387	PX4	C8-O5-C9	2.45	108.16	117.12	3	3
4	A	399	PX4	C29-C28-C27	2.45	101.98	114.37	5	2
4	A	421	PX4	C5-N1-C4	2.45	102.54	108.98	6	4
4	A	375	PX4	C29-C28-C27	2.45	101.99	114.37	2	2
4	A	387	PX4	O7-C7-C6	2.45	117.13	108.34	2	3
4	A	417	PX4	O7-C7-C6	2.45	117.13	108.34	5	5
4	A	313	PX4	O3-C1-C2	2.45	121.43	109.65	11	2
4	A	385	PX4	C27-C26-C25	2.45	102.00	114.37	7	2
4	A	374	PX4	C15-C14-C13	2.45	102.01	114.37	6	1
4	A	376	PX4	C30-C29-C28	2.45	102.00	114.37	14	2
4	A	378	PX4	C16-C15-C14	2.45	102.00	114.37	6	3
4	A	424	PX4	O8-C23-C24	2.45	114.21	123.78	10	1
4	A	318	PX4	O4-P1-O2	2.45	99.24	108.94	10	2
4	A	339	PX4	C30-C29-C28	2.44	102.01	114.37	5	2
4	A	341	PX4	C12-C11-C10	2.45	122.11	113.13	11	2
4	A	393	PX4	C4-N1-C2	2.45	119.63	109.91	5	3
4	A	398	PX4	C34-C33-C32	2.45	102.01	114.37	11	1
4	A	325	PX4	O8-C23-C24	2.44	114.23	123.78	6	1
4	A	326	PX4	O4-P1-O2	2.44	118.62	108.94	1	1
4	A	329	PX4	C13-C12-C11	2.44	102.02	114.37	14	3
4	A	340	PX4	C34-C33-C32	2.44	102.02	114.37	7	2
4	A	345	PX4	C30-C29-C28	2.44	102.02	114.37	14	1
4	A	381	PX4	C30-C29-C28	2.44	102.02	114.37	5	1
4	A	391	PX4	C16-C15-C14	2.44	102.02	114.37	2	1
4	A	405	PX4	C11-C10-C9	2.44	104.74	113.69	1	4
4	A	392	PX4	C3-N1-C2	2.44	119.61	109.91	8	2
4	A	394	PX4	C16-C15-C14	2.44	102.03	114.37	11	1
4	A	404	PX4	C11-C10-C9	2.44	104.75	113.69	6	1
4	A	405	PX4	C18-C17-C16	2.44	102.03	114.37	8	3
4	A	415	PX4	C25-C24-C23	2.44	104.75	113.69	5	1
4	A	415	PX4	O8-C23-C24	2.44	114.23	123.78	7	2
4	A	421	PX4	C5-N1-C3	2.44	102.56	108.98	5	1
4	A	423	PX4	C30-C29-C28	2.44	102.02	114.37	1	1
4	A	360	PX4	C14-C13-C12	2.44	102.03	114.37	9	1
4	A	315	PX4	O3-P1-O2	2.44	99.27	108.94	4	3
4	A	348	PX4	C8-O5-C9	2.44	108.20	117.12	9	3
4	A	370	PX4	C14-C13-C12	2.44	102.03	114.37	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	413	PX4	O4-P1-O2	2.44	118.61	108.94	14	4
4	A	348	PX4	O1-P1-O2	2.44	123.79	112.44	14	5
4	A	332	PX4	C26-C25-C24	2.44	104.17	113.13	5	3
4	A	356	PX4	C3-N1-C2	2.44	119.60	109.91	3	1
4	A	414	PX4	O3-P1-O2	2.44	99.27	108.94	1	2
4	A	370	PX4	C8-O5-C9	2.44	108.21	117.12	6	2
4	A	389	PX4	C27-C26-C25	2.44	102.05	114.37	3	1
4	A	395	PX4	C22-C21-C20	2.44	96.91	113.36	6	1
4	A	397	PX4	C30-C29-C28	2.44	102.05	114.37	6	1
4	A	334	PX4	C3-N1-C2	2.44	100.23	109.91	12	1
4	A	384	PX4	C11-C10-C9	2.43	104.77	113.69	3	3
4	A	395	PX4	C5-N1-C3	2.43	102.58	108.98	13	1
4	A	387	PX4	C34-C33-C32	2.43	102.06	114.37	12	2
4	A	425	PX4	C15-C14-C13	2.43	102.06	114.37	8	1
4	A	326	PX4	C13-C12-C11	2.43	102.07	114.37	4	2
4	A	361	PX4	O1-P1-O3	2.43	118.60	107.57	12	1
4	A	333	PX4	C20-C19-C18	2.43	102.08	114.37	3	1
4	A	334	PX4	C19-C18-C17	2.43	102.08	114.37	4	1
4	A	363	PX4	O3-P1-O2	2.43	99.29	108.94	10	2
4	A	372	PX4	C28-C27-C26	2.43	102.07	114.37	4	1
4	A	392	PX4	C32-C31-C30	2.43	102.07	114.37	12	1
4	A	401	PX4	C19-C18-C17	2.43	102.07	114.37	2	2
4	A	362	PX4	C16-C15-C14	2.43	102.08	114.37	1	2
4	A	363	PX4	C33-C32-C31	2.43	102.08	114.37	8	1
4	A	364	PX4	C25-C24-C23	2.43	104.78	113.69	3	3
4	A	365	PX4	C22-C21-C20	2.43	96.94	113.36	13	1
4	A	373	PX4	O1-P1-O4	2.43	96.55	107.57	13	3
4	A	375	PX4	O5-C9-O6	2.43	117.55	123.63	6	1
4	A	377	PX4	C29-C28-C27	2.43	102.08	114.37	10	1
4	A	393	PX4	C30-C29-C28	2.43	102.08	114.37	8	1
4	A	423	PX4	C8-O5-C9	2.43	108.23	117.12	13	1
4	A	307	PX4	O5-C9-C10	2.43	119.24	111.83	4	1
4	A	354	PX4	C31-C30-C29	2.43	102.09	114.37	1	1
4	A	314	PX4	O4-P1-O2	2.43	118.56	108.94	13	1
4	A	318	PX4	C25-C24-C23	2.43	104.80	113.69	7	3
4	A	348	PX4	O4-P1-O2	2.43	118.56	108.94	8	3
4	A	380	PX4	C5-N1-C4	2.43	102.59	108.98	3	1
4	A	404	PX4	O6-C9-C10	2.43	114.29	123.78	3	1
4	A	416	PX4	C5-N1-C2	2.43	119.56	109.91	11	2
4	A	307	PX4	C5-N1-C2	2.43	119.55	109.91	3	1
4	A	313	PX4	O5-C9-C10	2.43	119.23	111.83	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	346	PX4	C5-N1-C2	2.43	100.27	109.91	3	1
4	A	412	PX4	C4-N1-C2	2.43	119.55	109.91	1	1
4	A	425	PX4	C20-C19-C18	2.43	102.11	114.37	4	1
4	A	427	PX4	C34-C33-C32	2.42	102.11	114.37	1	1
4	A	310	PX4	C27-C26-C25	2.42	102.12	114.37	7	1
4	A	314	PX4	O7-C7-C8	2.42	117.03	108.34	12	2
4	A	308	PX4	C32-C31-C30	2.42	102.13	114.37	5	1
4	A	322	PX4	C14-C13-C12	2.42	102.13	114.37	8	1
4	A	324	PX4	C26-C25-C24	2.42	104.23	113.13	11	2
4	A	330	PX4	C17-C16-C15	2.42	102.13	114.37	13	1
4	A	397	PX4	C5-N1-C3	2.42	115.34	108.98	10	4
4	A	411	PX4	C31-C30-C29	2.42	102.13	114.37	5	2
4	A	415	PX4	O5-C9-C10	2.42	119.22	111.83	6	2
4	A	336	PX4	C8-O5-C9	2.42	108.27	117.12	3	2
4	A	391	PX4	C17-C16-C15	2.42	102.14	114.37	1	1
4	A	309	PX4	C5-N1-C2	2.42	100.30	109.91	4	3
4	A	314	PX4	C13-C12-C11	2.42	102.14	114.37	13	1
4	A	351	PX4	C31-C30-C29	2.42	102.15	114.37	4	1
4	A	428	PX4	C30-C29-C28	2.42	102.14	114.37	4	2
4	A	318	PX4	O7-C23-O8	2.42	118.06	123.70	14	4
4	A	353	PX4	C26-C25-C24	2.42	104.25	113.13	7	2
4	A	369	PX4	C15-C14-C13	2.42	102.15	114.37	7	1
4	A	413	PX4	C27-C26-C25	2.42	102.15	114.37	11	2
4	A	402	PX4	C31-C30-C29	2.42	102.16	114.37	7	1
4	A	407	PX4	C14-C13-C12	2.42	102.15	114.37	9	1
4	A	417	PX4	C28-C27-C26	2.42	102.15	114.37	6	1
4	A	321	PX4	C15-C14-C13	2.41	102.16	114.37	7	1
4	A	367	PX4	O3-C1-C2	2.42	121.27	109.65	8	2
4	A	371	PX4	C30-C29-C28	2.42	102.16	114.37	14	1
4	A	373	PX4	C18-C17-C16	2.42	102.16	114.37	10	1
4	A	426	PX4	C33-C32-C31	2.42	102.16	114.37	11	2
4	A	306	PX4	C8-O5-C9	2.41	108.30	117.12	1	3
4	A	354	PX4	O4-P1-O2	2.41	118.50	108.94	9	1
4	A	370	PX4	C30-C29-C28	2.41	102.17	114.37	12	1
4	A	377	PX4	O1-P1-O4	2.41	118.51	107.57	11	2
4	A	388	PX4	C16-C15-C14	2.41	102.17	114.37	9	1
4	A	341	PX4	C18-C17-C16	2.41	102.17	114.37	1	2
4	A	344	PX4	O3-C1-C2	2.41	121.26	109.65	12	2
4	A	408	PX4	C25-C24-C23	2.41	104.85	113.69	13	2
4	A	413	PX4	O6-C9-C10	2.41	114.34	123.78	6	1
4	A	337	PX4	C8-O5-C9	2.41	108.30	117.12	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	C27-C26-C25	2.41	102.18	114.37	14	3
4	A	348	PX4	O6-C9-C10	2.41	114.35	123.78	13	1
4	A	370	PX4	C7-O7-C23	2.41	123.57	117.80	9	3
4	A	390	PX4	C4-N1-C2	2.41	119.49	109.91	2	1
4	A	393	PX4	C25-C24-C23	2.41	104.86	113.69	3	1
4	A	406	PX4	C19-C18-C17	2.41	102.18	114.37	7	2
4	A	342	PX4	C5-N1-C2	2.41	119.49	109.91	9	1
4	A	359	PX4	C16-C15-C14	2.41	102.18	114.37	7	1
4	A	399	PX4	O3-P1-O2	2.41	99.38	108.94	5	2
4	A	414	PX4	C15-C14-C13	2.41	102.19	114.37	14	1
4	A	427	PX4	C29-C28-C27	2.41	102.18	114.37	13	2
4	A	306	PX4	P1-O4-C6	2.41	107.55	121.35	11	4
4	A	377	PX4	C17-C16-C15	2.41	102.19	114.37	7	2
4	A	394	PX4	C5-N1-C2	2.41	100.34	109.91	2	3
4	A	319	PX4	C29-C28-C27	2.41	102.20	114.37	11	1
4	A	402	PX4	C34-C33-C32	2.41	102.20	114.37	9	1
4	A	402	PX4	C4-N1-C3	2.41	102.65	108.98	12	2
4	A	328	PX4	C30-C29-C28	2.41	102.21	114.37	1	2
4	A	348	PX4	C16-C15-C14	2.41	102.21	114.37	9	3
4	A	380	PX4	C5-N1-C3	2.41	102.66	108.98	1	1
4	A	386	PX4	C17-C16-C15	2.41	102.21	114.37	5	2
4	A	407	PX4	O1-P1-O3	2.41	96.67	107.57	2	2
4	A	416	PX4	C25-C24-C23	2.41	104.88	113.69	5	2
4	A	430	PX4	C15-C14-C13	2.41	102.21	114.37	13	1
4	A	327	PX4	C17-C16-C15	2.40	102.22	114.37	5	2
4	A	311	PX4	C25-C24-C23	2.40	104.89	113.69	7	2
4	A	361	PX4	C12-C11-C10	2.40	104.30	113.13	7	1
4	A	333	PX4	C15-C14-C13	2.40	102.23	114.37	1	1
4	A	383	PX4	C33-C32-C31	2.40	102.23	114.37	5	2
4	A	386	PX4	C25-C24-C23	2.40	104.89	113.69	5	2
4	A	402	PX4	C32-C31-C30	2.40	102.22	114.37	12	1
4	A	418	PX4	C17-C16-C15	2.40	102.22	114.37	8	1
4	A	355	PX4	C26-C25-C24	2.40	104.30	113.13	6	1
4	A	379	PX4	C33-C32-C31	2.40	102.23	114.37	2	1
4	A	386	PX4	C28-C27-C26	2.40	102.23	114.37	3	2
4	A	392	PX4	C26-C25-C24	2.40	104.30	113.13	5	2
4	A	423	PX4	C17-C16-C15	2.40	102.23	114.37	6	4
4	A	426	PX4	O5-C8-C7	2.40	115.32	108.40	3	5
4	A	387	PX4	C30-C29-C28	2.40	102.24	114.37	5	1
4	A	388	PX4	O1-P1-O4	2.40	118.44	107.57	6	2
4	A	313	PX4	O1-P1-O4	2.40	118.44	107.57	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	335	PX4	C25-C24-C23	2.40	104.91	113.69	14	1
4	A	419	PX4	C8-O5-C9	2.40	108.35	117.12	13	1
4	A	365	PX4	C27-C26-C25	2.40	102.25	114.37	4	3
4	A	348	PX4	C27-C26-C25	2.40	102.25	114.37	13	1
4	A	376	PX4	O1-P1-O4	2.40	118.43	107.57	10	1
4	A	428	PX4	C13-C12-C11	2.40	102.25	114.37	12	2
4	A	352	PX4	C33-C32-C31	2.40	102.25	114.37	2	1
4	A	354	PX4	C34-C33-C32	2.40	102.26	114.37	8	1
4	A	356	PX4	C20-C19-C18	2.40	102.26	114.37	7	2
4	A	366	PX4	C19-C18-C17	2.40	102.25	114.37	12	2
4	A	405	PX4	C25-C24-C23	2.40	104.91	113.69	5	1
4	A	314	PX4	C11-C10-C9	2.40	122.47	113.69	10	1
4	A	396	PX4	C27-C26-C25	2.40	102.26	114.37	13	1
4	A	357	PX4	C5-N1-C2	2.39	119.42	109.91	5	1
4	A	366	PX4	O1-P1-O3	2.39	118.42	107.57	10	1
4	A	330	PX4	C31-C30-C29	2.39	102.28	114.37	9	3
4	A	401	PX4	C15-C14-C13	2.39	102.27	114.37	1	2
4	A	342	PX4	C8-O5-C9	2.39	108.38	117.12	1	1
4	A	375	PX4	C16-C15-C14	2.39	102.28	114.37	13	2
4	A	391	PX4	C29-C28-C27	2.39	102.28	114.37	7	1
4	A	328	PX4	C13-C12-C11	2.39	102.29	114.37	10	2
4	A	330	PX4	O3-C1-C2	2.39	121.15	109.65	6	1
4	A	345	PX4	C17-C16-C15	2.39	102.28	114.37	6	2
4	A	345	PX4	C28-C27-C26	2.39	102.29	114.37	13	3
4	A	364	PX4	C3-N1-C2	2.39	100.41	109.91	13	1
4	A	376	PX4	C15-C14-C13	2.39	102.28	114.37	8	1
4	A	412	PX4	C27-C26-C25	2.39	102.28	114.37	7	1
4	A	399	PX4	O8-C23-C24	2.39	114.43	123.78	7	1
4	A	425	PX4	C5-N1-C2	2.39	119.41	109.91	4	1
4	A	358	PX4	O3-C1-C2	2.39	121.14	109.65	12	1
4	A	365	PX4	O1-P1-O3	2.39	96.74	107.57	2	1
4	A	386	PX4	O6-C9-C10	2.39	114.44	123.78	3	1
4	A	425	PX4	C30-C29-C28	2.39	102.29	114.37	7	1
4	A	426	PX4	O6-C9-C10	2.39	114.44	123.78	12	1
4	A	307	PX4	C13-C12-C11	2.39	102.30	114.37	9	1
4	A	344	PX4	C28-C27-C26	2.39	102.30	114.37	10	1
4	A	351	PX4	C5-N1-C4	2.39	115.25	108.98	1	2
4	A	308	PX4	O5-C9-O6	2.39	117.66	123.63	13	3
4	A	355	PX4	O1-P1-O3	2.39	96.75	107.57	6	1
4	A	382	PX4	O3-C1-C2	2.39	121.14	109.65	9	2
4	A	316	PX4	C16-C15-C14	2.39	102.31	114.37	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	326	PX4	O7-C23-O8	2.38	118.13	123.70	12	3
4	A	357	PX4	C4-N1-C3	2.38	102.71	108.98	4	5
4	A	377	PX4	C25-C24-C23	2.39	122.43	113.69	6	2
4	A	414	PX4	C30-C29-C28	2.38	102.31	114.37	7	3
4	A	355	PX4	C27-C26-C25	2.38	102.33	114.37	2	3
4	A	363	PX4	O5-C9-C10	2.38	119.10	111.83	3	1
4	A	374	PX4	C19-C18-C17	2.38	102.32	114.37	3	2
4	A	401	PX4	C3-N1-C2	2.38	100.44	109.91	2	2
4	A	401	PX4	O4-P1-O2	2.38	118.38	108.94	6	1
4	A	369	PX4	C20-C19-C18	2.38	102.33	114.37	7	1
4	A	429	PX4	C5-N1-C2	2.38	119.38	109.91	5	1
4	A	429	PX4	C26-C25-C24	2.38	104.37	113.13	8	2
4	A	430	PX4	C17-C16-C15	2.38	102.32	114.37	10	1
4	A	322	PX4	C8-O5-C9	2.38	108.41	117.12	9	2
4	A	373	PX4	C28-C27-C26	2.38	102.33	114.37	6	1
4	A	374	PX4	C5-N1-C2	2.38	119.38	109.91	10	2
4	A	391	PX4	C8-O5-C9	2.38	108.41	117.12	13	1
4	A	306	PX4	C12-C11-C10	2.38	104.38	113.13	10	3
4	A	333	PX4	O8-C23-C24	2.38	114.47	123.78	8	1
4	A	418	PX4	C29-C28-C27	2.38	102.33	114.37	7	1
4	A	420	PX4	C28-C27-C26	2.38	102.34	114.37	7	2
4	A	424	PX4	C32-C31-C30	2.38	102.33	114.37	7	1
4	A	407	PX4	C12-C11-C10	2.38	104.38	113.13	9	3
4	A	425	PX4	C4-N1-C3	2.38	102.72	108.98	5	3
4	A	313	PX4	C16-C15-C14	2.38	102.35	114.37	12	2
4	A	387	PX4	C18-C17-C16	2.38	102.35	114.37	5	2
4	A	389	PX4	O7-C7-C6	2.38	116.87	108.34	13	2
4	A	397	PX4	C13-C12-C11	2.38	102.34	114.37	4	4
4	A	403	PX4	C29-C28-C27	2.38	102.35	114.37	10	2
4	A	413	PX4	C26-C25-C24	2.38	104.39	113.13	6	1
4	A	428	PX4	C12-C11-C10	2.38	104.39	113.13	4	1
4	A	326	PX4	C32-C31-C30	2.38	102.35	114.37	14	1
4	A	368	PX4	C3-N1-C2	2.38	119.36	109.91	1	1
4	A	376	PX4	C27-C26-C25	2.38	102.35	114.37	11	1
4	A	361	PX4	C26-C25-C24	2.38	104.40	113.13	2	2
4	A	423	PX4	C4-N1-C2	2.38	100.47	109.91	6	2
4	A	380	PX4	O4-P1-O2	2.37	118.35	108.94	10	4
4	A	392	PX4	C15-C14-C13	2.37	102.36	114.37	4	2
4	A	399	PX4	C33-C32-C31	2.37	102.36	114.37	10	2
4	A	375	PX4	C8-O5-C9	2.37	108.44	117.12	12	1
4	A	402	PX4	O4-P1-O2	2.37	118.34	108.94	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	310	PX4	C29-C28-C27	2.37	102.38	114.37	6	1
4	A	332	PX4	C15-C14-C13	2.37	102.38	114.37	5	1
4	A	375	PX4	O8-C23-C24	2.37	133.06	123.78	8	2
4	A	387	PX4	C1-C2-N1	2.37	123.44	115.82	3	4
4	A	390	PX4	C1-C2-N1	2.37	123.44	115.82	2	5
4	A	390	PX4	C19-C18-C17	2.37	102.38	114.37	11	2
4	A	405	PX4	C34-C33-C32	2.37	102.38	114.37	2	1
4	A	307	PX4	C20-C19-C18	2.37	102.39	114.37	9	1
4	A	312	PX4	O6-C9-C10	2.37	114.52	123.78	10	1
4	A	365	PX4	C12-C11-C10	2.37	104.42	113.13	6	2
4	A	370	PX4	C28-C27-C26	2.37	102.40	114.37	2	1
4	A	373	PX4	C34-C33-C32	2.37	102.39	114.37	11	1
4	A	381	PX4	C28-C27-C26	2.37	102.39	114.37	10	2
4	A	387	PX4	C11-C10-C9	2.37	105.01	113.69	4	1
4	A	427	PX4	C11-C10-C9	2.37	122.38	113.69	14	1
4	A	430	PX4	C25-C24-C23	2.37	105.01	113.69	7	1
4	A	393	PX4	C26-C25-C24	2.37	104.42	113.13	7	1
4	A	306	PX4	O3-C1-C2	2.37	121.04	109.65	5	1
4	A	364	PX4	C15-C14-C13	2.37	102.40	114.37	14	1
4	A	373	PX4	C14-C13-C12	2.37	102.40	114.37	5	1
4	A	385	PX4	C5-N1-C2	2.37	119.32	109.91	4	3
4	A	388	PX4	C18-C17-C16	2.37	102.40	114.37	5	1
4	A	392	PX4	O5-C9-C10	2.37	119.05	111.83	3	3
4	A	405	PX4	C3-N1-C2	2.37	100.50	109.91	4	3
4	A	424	PX4	C5-N1-C4	2.37	102.76	108.98	12	2
4	A	399	PX4	O4-P1-O2	2.37	99.56	108.94	1	1
4	A	415	PX4	C34-C33-C32	2.37	102.41	114.37	6	2
4	A	308	PX4	C8-O5-C9	2.36	108.48	117.12	1	1
4	A	345	PX4	C15-C14-C13	2.36	102.42	114.37	13	2
4	A	425	PX4	O5-C9-O6	2.36	117.71	123.63	5	2
4	A	429	PX4	C29-C28-C27	2.37	102.41	114.37	8	1
4	A	307	PX4	C32-C31-C30	2.36	102.43	114.37	5	1
4	A	316	PX4	O5-C9-C10	2.36	119.04	111.83	8	2
4	A	351	PX4	C11-C10-C9	2.36	105.04	113.69	7	2
4	A	379	PX4	O8-C23-C24	2.36	114.54	123.78	14	2
4	A	392	PX4	C19-C18-C17	2.36	102.43	114.37	7	1
4	A	428	PX4	C32-C31-C30	2.36	102.43	114.37	11	3
4	A	306	PX4	C34-C33-C32	2.36	102.44	114.37	4	1
4	A	316	PX4	O7-C7-C8	2.36	116.81	108.34	9	2
4	A	320	PX4	C13-C12-C11	2.36	102.44	114.37	5	1
4	A	334	PX4	O4-P1-O2	2.36	99.59	108.94	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	335	PX4	C16-C15-C14	2.36	126.29	114.37	4	2
4	A	337	PX4	C33-C32-C31	2.36	102.44	114.37	5	2
4	A	322	PX4	O6-C9-C10	2.36	114.56	123.78	3	1
4	A	370	PX4	O5-C9-O6	2.36	117.73	123.63	2	2
4	A	387	PX4	O1-P1-O4	2.36	118.25	107.57	12	1
4	A	320	PX4	O7-C23-O8	2.36	118.20	123.70	2	1
4	A	321	PX4	C18-C17-C16	2.36	102.46	114.37	4	1
4	A	414	PX4	C14-C13-C12	2.36	102.45	114.37	6	2
4	A	317	PX4	O7-C23-O8	2.35	118.20	123.70	13	2
4	A	354	PX4	O5-C9-C10	2.36	119.02	111.83	11	3
4	A	420	PX4	O3-C1-C2	2.36	120.98	109.65	10	2
4	A	313	PX4	C5-N1-C3	2.35	102.80	108.98	2	1
4	A	350	PX4	C3-N1-C2	2.35	119.27	109.91	2	1
4	A	358	PX4	C29-C28-C27	2.35	102.47	114.37	6	2
4	A	384	PX4	O1-P1-O4	2.35	118.24	107.57	8	2
4	A	347	PX4	C34-C33-C32	2.35	102.48	114.37	10	2
4	A	329	PX4	C19-C18-C17	2.35	102.48	114.37	6	1
4	A	350	PX4	C16-C15-C14	2.35	102.48	114.37	5	1
4	A	404	PX4	C30-C29-C28	2.35	102.48	114.37	12	1
4	A	360	PX4	C11-C10-C9	2.35	105.08	113.69	1	2
4	A	384	PX4	C29-C28-C27	2.35	102.49	114.37	10	1
4	A	409	PX4	C8-O5-C9	2.35	108.53	117.12	1	1
4	A	310	PX4	C28-C27-C26	2.35	102.49	114.37	13	1
4	A	340	PX4	C32-C31-C30	2.35	102.50	114.37	5	1
4	A	348	PX4	C17-C16-C15	2.35	102.49	114.37	4	1
4	A	411	PX4	O3-P1-O2	2.35	99.62	108.94	5	4
4	A	351	PX4	C5-N1-C3	2.35	102.81	108.98	12	2
4	A	352	PX4	C16-C15-C14	2.35	102.51	114.37	1	1
4	A	402	PX4	C5-N1-C2	2.35	100.58	109.91	13	1
4	A	390	PX4	C20-C19-C18	2.35	102.51	114.37	4	1
4	A	423	PX4	C13-C12-C11	2.35	102.51	114.37	9	1
4	A	309	PX4	C26-C25-C24	2.34	104.51	113.13	14	1
4	A	315	PX4	C8-O5-C9	2.34	108.55	117.12	4	1
4	A	360	PX4	C32-C31-C30	2.34	102.52	114.37	6	1
4	A	388	PX4	C25-C24-C23	2.34	105.11	113.69	9	1
4	A	306	PX4	C3-N1-C2	2.34	100.60	109.91	9	3
4	A	314	PX4	C14-C13-C12	2.34	102.54	114.37	7	1
4	A	325	PX4	O6-C9-C10	2.34	114.63	123.78	9	1
4	A	329	PX4	C15-C14-C13	2.34	102.53	114.37	12	3
4	A	356	PX4	C19-C18-C17	2.34	102.53	114.37	3	2
4	A	362	PX4	C32-C31-C30	2.34	102.53	114.37	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	363	PX4	C1-C2-N1	2.34	123.33	115.82	6	2
4	A	425	PX4	C32-C31-C30	2.34	102.53	114.37	7	1
4	A	312	PX4	C32-C31-C30	2.34	102.55	114.37	12	1
4	A	402	PX4	O1-P1-O4	2.34	118.17	107.57	9	2
4	A	387	PX4	C29-C28-C27	2.34	102.55	114.37	6	2
4	A	418	PX4	C31-C30-C29	2.34	102.54	114.37	6	1
4	A	307	PX4	C34-C33-C32	2.34	102.55	114.37	3	1
4	A	331	PX4	O4-P1-O2	2.34	118.20	108.94	6	1
4	A	357	PX4	C14-C13-C12	2.34	102.55	114.37	2	1
4	A	392	PX4	C8-O5-C9	2.34	108.58	117.12	1	1
4	A	417	PX4	C17-C16-C15	2.34	102.55	114.37	6	2
4	A	353	PX4	C19-C18-C17	2.34	102.56	114.37	14	1
4	A	394	PX4	C34-C33-C32	2.34	102.56	114.37	3	2
4	A	400	PX4	O6-C9-C10	2.34	114.64	123.78	12	2
4	A	405	PX4	C12-C11-C10	2.34	104.54	113.13	5	2
4	A	342	PX4	C33-C32-C31	2.33	102.57	114.37	4	1
4	A	354	PX4	C32-C31-C30	2.33	102.57	114.37	6	2
4	A	363	PX4	C28-C27-C26	2.33	102.57	114.37	6	1
4	A	391	PX4	O5-C9-C10	2.33	118.95	111.83	6	2
4	A	309	PX4	C4-N1-C2	2.33	119.18	109.91	1	3
4	A	318	PX4	C31-C30-C29	2.33	102.58	114.37	13	1
4	A	373	PX4	C5-N1-C2	2.33	100.64	109.91	4	1
4	A	376	PX4	C26-C25-C24	2.33	104.56	113.13	7	2
4	A	385	PX4	C14-C13-C12	2.33	102.58	114.37	11	1
4	A	309	PX4	C12-C11-C10	2.33	104.56	113.13	6	2
4	A	335	PX4	C28-C27-C26	2.33	102.58	114.37	6	1
4	A	424	PX4	C17-C16-C15	2.33	102.58	114.37	7	1
4	A	351	PX4	C13-C12-C11	2.33	126.15	114.37	11	3
4	A	348	PX4	C1-C2-N1	2.33	123.30	115.82	10	1
4	A	349	PX4	C3-N1-C2	2.33	119.17	109.91	8	2
4	A	365	PX4	O4-P1-O2	2.33	118.17	108.94	3	1
4	A	371	PX4	C32-C31-C30	2.33	102.59	114.37	2	1
4	A	378	PX4	C17-C16-C15	2.33	102.59	114.37	14	1
4	A	398	PX4	C3-N1-C2	2.33	119.17	109.91	4	1
4	A	313	PX4	C30-C29-C28	2.33	102.61	114.37	1	2
4	A	343	PX4	C20-C19-C18	2.33	102.61	114.37	14	1
4	A	358	PX4	O5-C9-C10	2.33	118.93	111.83	8	3
4	A	370	PX4	C29-C28-C27	2.33	102.61	114.37	10	1
4	A	370	PX4	C3-N1-C2	2.33	100.66	109.91	13	1
4	A	328	PX4	C33-C32-C31	2.33	102.61	114.37	9	1
4	A	334	PX4	C7-O7-C23	2.33	123.36	117.80	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	C27-C26-C25	2.33	102.61	114.37	10	2
4	A	314	PX4	C19-C18-C17	2.32	102.62	114.37	14	1
4	A	341	PX4	O3-C1-C2	2.32	120.84	109.65	13	2
4	A	322	PX4	C28-C27-C26	2.32	102.62	114.37	5	2
4	A	327	PX4	C36-C35-C34	2.32	97.67	113.36	10	1
4	A	336	PX4	C3-N1-C2	2.32	119.15	109.91	5	1
4	A	343	PX4	C3-N1-C2	2.32	119.15	109.91	6	1
4	A	363	PX4	O3-C1-C2	2.32	120.83	109.65	5	1
4	A	407	PX4	C26-C25-C24	2.33	104.58	113.13	6	2
4	A	328	PX4	C18-C17-C16	2.32	102.63	114.37	13	1
4	A	329	PX4	C26-C25-C24	2.32	104.59	113.13	10	4
4	A	334	PX4	C26-C25-C24	2.32	104.60	113.13	5	1
4	A	361	PX4	O3-C1-C2	2.32	120.82	109.65	10	1
4	A	362	PX4	C33-C32-C31	2.32	102.63	114.37	7	2
4	A	379	PX4	C12-C11-C10	2.32	104.59	113.13	10	2
4	A	406	PX4	C18-C17-C16	2.32	102.63	114.37	3	1
4	A	409	PX4	C5-N1-C2	2.32	119.14	109.91	9	1
4	A	415	PX4	C15-C14-C13	2.32	102.63	114.37	14	3
4	A	337	PX4	O3-P1-O2	2.32	99.74	108.94	3	1
4	A	348	PX4	C4-N1-C2	2.32	119.14	109.91	5	2
4	A	349	PX4	C11-C10-C9	2.32	105.19	113.69	10	2
4	A	408	PX4	O4-P1-O2	2.32	118.13	108.94	6	1
4	A	369	PX4	C5-N1-C2	2.32	119.13	109.91	14	1
4	A	374	PX4	C8-O5-C9	2.32	108.64	117.12	4	3
4	A	391	PX4	C25-C24-C23	2.32	105.19	113.69	11	2
4	A	423	PX4	C33-C32-C31	2.32	102.65	114.37	12	1
4	A	312	PX4	O3-C1-C2	2.32	120.79	109.65	3	1
4	A	348	PX4	C33-C32-C31	2.32	102.66	114.37	3	1
4	A	371	PX4	C26-C25-C24	2.32	104.61	113.13	14	2
4	A	393	PX4	C20-C19-C18	2.32	102.65	114.37	3	2
4	A	363	PX4	C8-O5-C9	2.32	108.65	117.12	7	1
4	A	382	PX4	C29-C28-C27	2.32	102.66	114.37	11	2
4	A	395	PX4	C12-C11-C10	2.32	104.61	113.13	10	2
4	A	403	PX4	C34-C33-C32	2.32	102.66	114.37	4	1
4	A	401	PX4	O8-C23-C24	2.32	114.72	123.78	5	1
4	A	411	PX4	C15-C14-C13	2.32	102.66	114.37	2	1
4	A	420	PX4	O4-P1-O2	2.32	118.12	108.94	1	2
4	A	425	PX4	C3-N1-C2	2.32	119.12	109.91	2	1
4	A	331	PX4	C25-C24-C23	2.31	122.18	113.69	1	1
4	A	335	PX4	O5-C9-C10	2.31	118.89	111.83	9	3
4	A	337	PX4	O1-P1-O4	2.31	118.06	107.57	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	368	PX4	O4-P1-O2	2.31	99.76	108.94	14	2
4	A	352	PX4	C18-C17-C16	2.31	102.67	114.37	9	1
4	A	380	PX4	O3-C1-C2	2.31	120.78	109.65	3	2
4	A	396	PX4	C11-C10-C9	2.31	105.22	113.69	7	3
4	A	339	PX4	C17-C16-C15	2.31	102.69	114.37	2	1
4	A	341	PX4	C4-N1-C2	2.31	119.10	109.91	14	1
4	A	346	PX4	C30-C29-C28	2.31	102.68	114.37	8	2
4	A	422	PX4	C34-C33-C32	2.31	102.68	114.37	2	1
4	A	347	PX4	C5-N1-C3	2.31	115.05	108.98	10	1
4	A	352	PX4	C14-C13-C12	2.31	102.69	114.37	11	1
4	A	335	PX4	O1-P1-O4	2.31	97.11	107.57	11	1
4	A	342	PX4	C34-C33-C32	2.31	102.70	114.37	14	2
4	A	423	PX4	C32-C31-C30	2.31	102.69	114.37	12	1
4	A	359	PX4	C33-C32-C31	2.31	102.70	114.37	4	2
4	A	394	PX4	C14-C13-C12	2.31	102.70	114.37	11	1
4	A	379	PX4	O4-P1-O2	2.31	118.07	108.94	11	1
4	A	383	PX4	C19-C18-C17	2.31	102.71	114.37	3	1
4	A	404	PX4	C5-N1-C2	2.31	119.08	109.91	9	3
4	A	409	PX4	O4-P1-O2	2.31	118.07	108.94	11	1
4	A	310	PX4	C13-C12-C11	2.30	102.72	114.37	5	2
4	A	316	PX4	O3-C1-C2	2.30	120.74	109.65	7	2
4	A	332	PX4	C4-N1-C3	2.30	102.92	108.98	3	1
4	A	418	PX4	C27-C26-C25	2.30	102.72	114.37	11	1
4	A	427	PX4	O3-C1-C2	2.31	120.74	109.65	12	1
4	A	353	PX4	C11-C10-C9	2.30	105.25	113.69	6	1
4	A	371	PX4	C11-C10-C9	2.30	105.25	113.69	5	1
4	A	392	PX4	C16-C15-C14	2.30	102.73	114.37	4	1
4	A	392	PX4	O4-P1-O2	2.30	118.07	108.94	7	1
4	A	409	PX4	C14-C13-C12	2.30	102.72	114.37	4	2
4	A	349	PX4	C32-C31-C30	2.30	102.73	114.37	9	1
4	A	363	PX4	C4-N1-C2	2.30	100.76	109.91	14	1
4	A	371	PX4	O6-C9-C10	2.30	114.78	123.78	12	2
4	A	405	PX4	C27-C26-C25	2.30	102.73	114.37	12	1
4	A	326	PX4	O5-C9-O6	2.30	117.87	123.63	6	2
4	A	421	PX4	C14-C13-C12	2.30	102.74	114.37	7	1
4	A	424	PX4	O6-C9-C10	2.30	114.78	123.78	13	1
4	A	314	PX4	O5-C9-C10	2.30	118.85	111.83	14	1
4	A	335	PX4	C4-N1-C2	2.30	100.76	109.91	8	1
4	A	341	PX4	C31-C30-C29	2.30	102.74	114.37	4	1
4	A	325	PX4	C11-C10-C9	2.30	105.27	113.69	12	1
4	A	364	PX4	O1-P1-O4	2.30	117.99	107.57	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	328	PX4	O6-C9-C10	2.30	114.79	123.78	6	1
4	A	342	PX4	C16-C15-C14	2.30	102.75	114.37	14	2
4	A	381	PX4	C17-C16-C15	2.30	102.74	114.37	10	1
4	A	358	PX4	O7-C7-C8	2.30	116.59	108.34	1	4
4	A	328	PX4	O1-P1-O3	2.30	117.98	107.57	11	2
4	A	332	PX4	O3-C1-C2	2.30	120.70	109.65	3	1
4	A	388	PX4	C14-C13-C12	2.30	102.75	114.37	14	2
4	A	415	PX4	C8-O5-C9	2.30	108.72	117.12	11	2
4	A	417	PX4	C15-C14-C13	2.30	102.75	114.37	8	1
4	A	343	PX4	C16-C15-C14	2.30	102.76	114.37	14	1
4	A	346	PX4	C32-C31-C30	2.30	102.77	114.37	4	1
4	A	351	PX4	C3-N1-C2	2.30	119.03	109.91	3	2
4	A	375	PX4	O6-C9-C10	2.30	114.80	123.78	7	1
4	A	386	PX4	C3-N1-C2	2.30	100.79	109.91	8	1
4	A	396	PX4	C14-C13-C12	2.30	102.76	114.37	2	1
4	A	416	PX4	C34-C33-C32	2.30	102.77	114.37	11	3
4	A	341	PX4	O8-C23-C24	2.29	114.81	123.78	10	2
4	A	348	PX4	C26-C25-C24	2.29	104.70	113.13	5	3
4	A	364	PX4	C30-C29-C28	2.29	102.77	114.37	11	1
4	A	375	PX4	C27-C26-C25	2.29	102.78	114.37	1	1
4	A	394	PX4	C20-C19-C18	2.29	102.77	114.37	7	1
4	A	381	PX4	C12-C11-C10	2.29	104.70	113.13	1	2
4	A	383	PX4	C17-C16-C15	2.29	102.78	114.37	5	3
4	A	418	PX4	C19-C18-C17	2.29	102.78	114.37	3	1
4	A	428	PX4	C33-C32-C31	2.29	102.77	114.37	1	1
4	A	344	PX4	C27-C26-C25	2.29	102.78	114.37	7	2
4	A	320	PX4	C5-N1-C2	2.29	119.02	109.91	9	1
4	A	350	PX4	C34-C33-C32	2.29	102.79	114.37	11	1
4	A	366	PX4	O3-C1-C2	2.29	120.68	109.65	5	1
4	A	378	PX4	O1-P1-O4	2.29	117.95	107.57	7	2
4	A	388	PX4	C5-N1-C3	2.29	102.95	108.98	4	4
4	A	315	PX4	O1-P1-O4	2.29	117.95	107.57	11	2
4	A	336	PX4	C19-C18-C17	2.29	102.80	114.37	2	2
4	A	347	PX4	C5-N1-C2	2.29	119.01	109.91	14	2
4	A	323	PX4	C14-C13-C12	2.29	102.81	114.37	3	1
4	A	329	PX4	O8-C23-C24	2.29	114.83	123.78	4	1
4	A	354	PX4	C19-C18-C17	2.29	102.80	114.37	13	1
4	A	371	PX4	C33-C32-C31	2.29	102.79	114.37	11	2
4	A	394	PX4	C3-N1-C2	2.29	100.81	109.91	13	2
4	A	418	PX4	C5-N1-C2	2.29	119.01	109.91	4	1
4	A	425	PX4	C1-C2-N1	2.29	123.17	115.82	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	359	PX4	C8-O5-C9	2.29	108.76	117.12	13	1
4	A	388	PX4	C17-C16-C15	2.29	102.81	114.37	2	1
4	A	390	PX4	O8-C23-C24	2.29	114.83	123.78	9	2
4	A	394	PX4	C33-C32-C31	2.29	102.81	114.37	5	1
4	A	371	PX4	C18-C17-C16	2.29	102.81	114.37	13	1
4	A	390	PX4	O7-C7-C6	2.28	116.54	108.34	10	3
4	A	397	PX4	C27-C26-C25	2.29	102.82	114.37	8	1
4	A	402	PX4	C19-C18-C17	2.29	102.81	114.37	13	1
4	A	425	PX4	C31-C30-C29	2.28	102.82	114.37	2	2
4	A	427	PX4	O1-P1-O4	2.28	117.92	107.57	7	2
4	A	428	PX4	C28-C27-C26	2.29	102.81	114.37	2	1
4	A	317	PX4	C14-C13-C12	2.28	102.83	114.37	14	1
4	A	319	PX4	C33-C32-C31	2.28	102.82	114.37	2	1
4	A	347	PX4	C13-C12-C11	2.28	102.83	114.37	13	1
4	A	364	PX4	O1-P1-O3	2.28	97.22	107.57	8	2
4	A	408	PX4	C13-C12-C11	2.28	102.83	114.37	3	2
4	A	320	PX4	C4-N1-C2	2.28	100.84	109.91	14	1
4	A	358	PX4	C5-N1-C2	2.28	118.98	109.91	5	1
4	A	338	PX4	O1-P1-O4	2.28	117.90	107.57	8	2
4	A	385	PX4	O1-P1-O4	2.28	117.91	107.57	4	1
4	A	388	PX4	C4-N1-C2	2.28	118.97	109.91	7	2
4	A	396	PX4	C12-C11-C10	2.28	104.75	113.13	7	1
4	A	420	PX4	C26-C25-C24	2.28	104.75	113.13	1	1
4	A	310	PX4	C16-C15-C14	2.28	102.85	114.37	13	2
4	A	312	PX4	C11-C10-C9	2.28	105.35	113.69	7	2
4	A	333	PX4	C30-C29-C28	2.28	102.85	114.37	10	1
4	A	352	PX4	C28-C27-C26	2.28	102.85	114.37	12	1
4	A	365	PX4	O7-C7-C6	2.28	116.52	108.34	5	5
4	A	383	PX4	C31-C30-C29	2.28	102.84	114.37	13	1
4	A	371	PX4	C20-C19-C18	2.28	102.85	114.37	12	3
4	A	413	PX4	C33-C32-C31	2.28	102.85	114.37	1	1
4	A	330	PX4	C5-N1-C3	2.28	114.96	108.98	12	1
4	A	349	PX4	O8-C23-C24	2.28	114.87	123.78	8	1
4	A	405	PX4	C20-C19-C18	2.28	102.86	114.37	1	2
4	A	426	PX4	C26-C25-C24	2.28	121.50	113.13	3	1
4	A	376	PX4	C16-C15-C14	2.28	102.87	114.37	5	1
4	A	410	PX4	C27-C26-C25	2.28	102.86	114.37	3	1
4	A	421	PX4	O3-C1-C2	2.28	120.60	109.65	6	1
4	A	316	PX4	C34-C33-C32	2.27	102.88	114.37	9	1
4	A	334	PX4	O7-C7-C8	2.27	116.50	108.34	12	2
4	A	345	PX4	O6-C9-C10	2.27	114.89	123.78	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	O3-C1-C2	2.27	120.59	109.65	5	1
4	A	353	PX4	C18-C17-C16	2.27	102.87	114.37	7	1
4	A	316	PX4	C29-C28-C27	2.27	102.88	114.37	3	1
4	A	347	PX4	C14-C13-C12	2.27	102.88	114.37	2	2
4	A	362	PX4	C25-C24-C23	2.27	105.37	113.69	4	1
4	A	368	PX4	O3-P1-O2	2.27	99.93	108.94	11	1
4	A	406	PX4	C12-C11-C10	2.27	104.78	113.13	4	1
4	A	308	PX4	C18-C17-C16	2.27	102.89	114.37	10	1
4	A	315	PX4	C5-N1-C2	2.27	118.94	109.91	14	1
4	A	409	PX4	C29-C28-C27	2.27	102.89	114.37	13	1
4	A	378	PX4	C30-C29-C28	2.27	102.89	114.37	13	1
4	A	415	PX4	C14-C13-C12	2.27	102.89	114.37	2	2
4	A	358	PX4	C31-C30-C29	2.27	102.90	114.37	10	2
4	A	364	PX4	C31-C30-C29	2.27	102.90	114.37	4	1
4	A	421	PX4	C32-C31-C30	2.27	102.90	114.37	11	1
4	A	425	PX4	O1-P1-O4	2.27	117.85	107.57	7	1
4	A	320	PX4	C20-C19-C18	2.27	102.90	114.37	1	1
4	A	362	PX4	O6-C9-C10	2.27	114.91	123.78	11	1
4	A	339	PX4	C16-C15-C14	2.27	102.92	114.37	13	1
4	A	343	PX4	C5-N1-C2	2.27	100.90	109.91	7	2
4	A	386	PX4	C32-C31-C30	2.27	102.91	114.37	7	1
4	A	397	PX4	C11-C10-C9	2.27	105.39	113.69	8	1
4	A	306	PX4	C29-C28-C27	2.26	102.92	114.37	9	2
4	A	317	PX4	C20-C19-C18	2.26	102.92	114.37	9	1
4	A	341	PX4	C8-O5-C9	2.26	108.84	117.12	6	2
4	A	345	PX4	C18-C17-C16	2.26	102.92	114.37	7	2
4	A	360	PX4	O1-P1-O3	2.26	97.30	107.57	13	1
4	A	384	PX4	C30-C29-C28	2.26	102.92	114.37	2	1
4	A	387	PX4	C33-C32-C31	2.26	102.93	114.37	5	3
4	A	388	PX4	C32-C31-C30	2.26	102.93	114.37	2	1
4	A	391	PX4	C11-C10-C9	2.26	105.40	113.69	5	2
4	A	427	PX4	C20-C19-C18	2.26	102.92	114.37	2	2
4	A	331	PX4	O3-C1-C2	2.26	120.54	109.65	2	1
4	A	334	PX4	C27-C26-C25	2.26	102.93	114.37	7	1
4	A	350	PX4	C25-C24-C23	2.26	105.40	113.69	9	3
4	A	430	PX4	C1-C2-N1	2.26	123.08	115.82	6	4
4	A	357	PX4	C12-C11-C10	2.26	104.82	113.13	5	1
4	A	362	PX4	C14-C13-C12	2.26	102.94	114.37	7	1
4	A	380	PX4	C1-C2-N1	2.26	123.08	115.82	3	3
4	A	389	PX4	C15-C14-C13	2.26	102.94	114.37	3	1
4	A	392	PX4	C20-C19-C18	2.26	102.94	114.37	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	328	PX4	C20-C19-C18	2.26	102.94	114.37	13	1
4	A	315	PX4	C13-C12-C11	2.26	102.95	114.37	9	1
4	A	345	PX4	C33-C32-C31	2.26	102.95	114.37	14	1
4	A	358	PX4	C7-O7-C23	2.26	112.39	117.80	3	4
4	A	363	PX4	C14-C13-C12	2.26	102.95	114.37	8	1
4	A	367	PX4	C18-C17-C16	2.26	102.95	114.37	4	2
4	A	336	PX4	C28-C27-C26	2.26	102.96	114.37	1	2
4	A	368	PX4	O3-C1-C2	2.26	120.51	109.65	5	1
4	A	397	PX4	C4-N1-C2	2.26	100.94	109.91	2	1
4	A	418	PX4	C20-C19-C18	2.26	102.96	114.37	5	1
4	A	421	PX4	C5-N1-C2	2.26	118.89	109.91	11	1
4	A	357	PX4	C3-N1-C2	2.26	118.88	109.91	1	2
4	A	359	PX4	C13-C12-C11	2.26	102.96	114.37	11	1
4	A	312	PX4	C5-N1-C4	2.25	103.06	108.98	14	2
4	A	315	PX4	C25-C24-C23	2.25	105.44	113.69	8	1
4	A	329	PX4	C16-C15-C14	2.25	102.97	114.37	13	1
4	A	341	PX4	C19-C18-C17	2.26	102.97	114.37	7	2
4	A	352	PX4	C5-N1-C4	2.26	114.90	108.98	3	2
4	A	364	PX4	O7-C7-C8	2.26	116.44	108.34	8	3
4	A	406	PX4	C32-C31-C30	2.26	102.96	114.37	5	2
4	A	407	PX4	C18-C17-C16	2.26	102.96	114.37	7	1
4	A	409	PX4	O5-C9-C10	2.26	118.72	111.83	2	1
4	A	386	PX4	C30-C29-C28	2.26	102.97	114.37	10	2
4	A	422	PX4	C32-C31-C30	2.26	102.97	114.37	10	1
4	A	345	PX4	C32-C31-C30	2.25	102.98	114.37	4	2
4	A	350	PX4	C5-N1-C4	2.25	103.06	108.98	12	2
4	A	378	PX4	C5-N1-C2	2.25	100.95	109.91	1	1
4	A	388	PX4	O6-C9-C10	2.25	114.97	123.78	5	1
4	A	397	PX4	C32-C31-C30	2.25	102.98	114.37	11	1
4	A	400	PX4	C19-C18-C17	2.25	102.97	114.37	4	1
4	A	377	PX4	C32-C31-C30	2.25	102.99	114.37	14	2
4	A	399	PX4	C12-C11-C10	2.25	104.85	113.13	10	1
4	A	403	PX4	C13-C12-C11	2.25	102.99	114.37	11	2
4	A	405	PX4	C19-C18-C17	2.25	102.99	114.37	7	1
4	A	417	PX4	C14-C13-C12	2.25	102.98	114.37	3	1
4	A	367	PX4	O8-C23-C24	2.25	114.98	123.78	9	1
4	A	384	PX4	O3-C1-C2	2.25	120.48	109.65	5	1
4	A	385	PX4	C20-C19-C18	2.25	102.99	114.37	6	1
4	A	319	PX4	C4-N1-C3	2.25	103.07	108.98	3	1
4	A	326	PX4	C28-C27-C26	2.25	103.00	114.37	2	1
4	A	330	PX4	C12-C11-C10	2.25	104.86	113.13	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	C20-C19-C18	2.25	103.00	114.37	9	1
4	A	384	PX4	C27-C26-C25	2.25	103.00	114.37	12	3
4	A	373	PX4	C32-C31-C30	2.25	103.00	114.37	6	1
4	A	407	PX4	O1-P1-O4	2.25	117.75	107.57	5	1
4	A	420	PX4	C8-O5-C9	2.25	108.90	117.12	1	2
4	A	307	PX4	C8-O5-C9	2.25	108.91	117.12	8	1
4	A	362	PX4	O8-C23-C24	2.25	115.00	123.78	9	1
4	A	427	PX4	C16-C15-C14	2.25	103.01	114.37	12	1
4	A	306	PX4	C5-N1-C2	2.25	118.83	109.91	13	1
4	A	325	PX4	C5-N1-C4	2.25	103.08	108.98	12	1
4	A	351	PX4	C28-C27-C26	2.24	103.02	114.37	1	1
4	A	355	PX4	C4-N1-C2	2.24	118.83	109.91	12	1
4	A	338	PX4	C30-C29-C28	2.24	103.03	114.37	5	2
4	A	364	PX4	O3-P1-O2	2.24	100.04	108.94	4	2
4	A	364	PX4	C13-C12-C11	2.24	103.02	114.37	10	2
4	A	335	PX4	C5-N1-C2	2.24	118.83	109.91	12	1
4	A	406	PX4	C16-C15-C14	2.24	103.03	114.37	10	2
4	A	313	PX4	C28-C27-C26	2.24	103.04	114.37	5	1
4	A	333	PX4	C4-N1-C2	2.24	118.82	109.91	3	1
4	A	337	PX4	C16-C15-C14	2.24	103.04	114.37	14	1
4	A	392	PX4	C5-N1-C2	2.24	101.00	109.91	14	1
4	A	398	PX4	C4-N1-C2	2.24	118.82	109.91	7	1
4	A	412	PX4	C26-C25-C24	2.24	104.89	113.13	2	3
4	A	408	PX4	O3-C1-C2	2.24	120.43	109.65	2	1
4	A	406	PX4	C27-C26-C25	2.24	103.05	114.37	4	1
4	A	412	PX4	C18-C17-C16	2.24	103.04	114.37	10	2
4	A	422	PX4	O8-C23-C24	2.24	115.02	123.78	11	1
4	A	349	PX4	C15-C14-C13	2.24	103.04	114.37	8	3
4	A	358	PX4	C25-C24-C23	2.24	105.48	113.69	7	1
4	A	384	PX4	C18-C17-C16	2.24	103.04	114.37	2	1
4	A	332	PX4	C11-C10-C9	2.24	105.49	113.69	14	1
4	A	353	PX4	C30-C29-C28	2.24	103.06	114.37	13	2
4	A	360	PX4	C4-N1-C2	2.24	118.81	109.91	10	1
4	A	365	PX4	C25-C24-C23	2.24	105.49	113.69	9	3
4	A	376	PX4	C5-N1-C2	2.24	118.81	109.91	3	2
4	A	399	PX4	C27-C26-C25	2.24	103.05	114.37	14	1
4	A	311	PX4	O6-C9-C10	2.24	115.03	123.78	4	1
4	A	319	PX4	C32-C31-C30	2.24	103.06	114.37	13	1
4	A	360	PX4	C5-N1-C2	2.24	101.02	109.91	6	1
4	A	407	PX4	C5-N1-C3	2.24	114.85	108.98	11	1
4	A	326	PX4	C15-C14-C13	2.24	103.07	114.37	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	328	PX4	C31-C30-C29	2.24	103.07	114.37	8	1
4	A	383	PX4	C34-C33-C32	2.24	103.07	114.37	1	1
4	A	425	PX4	C17-C16-C15	2.24	103.06	114.37	14	1
4	A	319	PX4	C1-C2-N1	2.23	122.99	115.82	10	4
4	A	321	PX4	C5-N1-C3	2.23	103.11	108.98	5	2
4	A	331	PX4	C17-C16-C15	2.23	103.08	114.37	11	1
4	A	334	PX4	C18-C17-C16	2.23	103.07	114.37	8	1
4	A	337	PX4	C29-C28-C27	2.23	103.08	114.37	4	2
4	A	343	PX4	C18-C17-C16	2.23	103.07	114.37	10	2
4	A	383	PX4	C5-N1-C2	2.23	118.79	109.91	12	1
4	A	384	PX4	C8-O5-C9	2.23	108.95	117.12	7	1
4	A	323	PX4	C31-C30-C29	2.23	103.09	114.37	7	2
4	A	329	PX4	C12-C11-C10	2.23	104.93	113.13	6	1
4	A	372	PX4	C13-C12-C11	2.23	103.09	114.37	5	1
4	A	383	PX4	C1-C2-N1	2.23	122.99	115.82	9	2
4	A	384	PX4	C13-C12-C11	2.23	103.09	114.37	13	2
4	A	391	PX4	O1-P1-O3	2.23	97.45	107.57	11	1
4	A	404	PX4	C18-C17-C16	2.23	103.08	114.37	8	1
4	A	321	PX4	C28-C27-C26	2.23	103.10	114.37	8	1
4	A	355	PX4	C29-C28-C27	2.23	103.09	114.37	11	1
4	A	412	PX4	C32-C31-C30	2.23	103.09	114.37	12	1
4	A	401	PX4	O3-C1-C2	2.23	120.38	109.65	7	1
4	A	382	PX4	O1-P1-O3	2.23	97.47	107.57	13	1
4	A	420	PX4	C14-C13-C12	2.23	103.10	114.37	12	1
4	A	310	PX4	O6-C9-C10	2.23	115.07	123.78	6	1
4	A	325	PX4	C4-N1-C2	2.23	118.77	109.91	7	1
4	A	329	PX4	C18-C17-C16	2.23	103.11	114.37	3	2
4	A	346	PX4	C16-C15-C14	2.23	103.10	114.37	14	1
4	A	356	PX4	C32-C31-C30	2.23	103.11	114.37	2	1
4	A	400	PX4	O1-P1-O3	2.23	97.47	107.57	3	1
4	A	320	PX4	C18-C17-C16	2.23	103.12	114.37	7	1
4	A	325	PX4	C17-C16-C15	2.23	103.12	114.37	11	2
4	A	338	PX4	C13-C12-C11	2.23	103.12	114.37	5	1
4	A	341	PX4	O1-P1-O3	2.23	97.47	107.57	14	1
4	A	393	PX4	C16-C15-C14	2.23	103.11	114.37	11	1
4	A	400	PX4	C20-C19-C18	2.23	103.11	114.37	9	1
4	A	325	PX4	C33-C32-C31	2.23	103.12	114.37	14	1
4	A	421	PX4	C28-C27-C26	2.23	103.11	114.37	10	3
4	A	383	PX4	C32-C31-C30	2.23	103.12	114.37	13	1
4	A	403	PX4	C12-C11-C10	2.23	104.95	113.13	13	1
4	A	315	PX4	O3-C1-C2	2.22	120.35	109.65	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	318	PX4	C17-C16-C15	2.22	103.13	114.37	7	2
4	A	343	PX4	C15-C14-C13	2.22	103.13	114.37	3	1
4	A	351	PX4	C17-C16-C15	2.22	103.13	114.37	4	1
4	A	379	PX4	C34-C33-C32	2.22	103.13	114.37	12	2
4	A	337	PX4	C4-N1-C3	2.22	103.14	108.98	9	1
4	A	338	PX4	C20-C19-C18	2.22	103.14	114.37	10	1
4	A	319	PX4	C25-C24-C23	2.22	105.56	113.69	3	1
4	A	355	PX4	C30-C29-C28	2.22	103.14	114.37	12	1
4	A	392	PX4	C34-C33-C32	2.22	103.14	114.37	2	2
4	A	402	PX4	C16-C15-C14	2.22	103.13	114.37	8	2
4	A	412	PX4	C33-C32-C31	2.22	103.13	114.37	6	1
4	A	350	PX4	O1-P1-O3	2.22	117.63	107.57	13	1
4	A	364	PX4	C11-C10-C9	2.22	105.56	113.69	7	2
4	A	417	PX4	O3-C1-C2	2.22	120.34	109.65	1	1
4	A	321	PX4	C14-C13-C12	2.22	103.15	114.37	6	1
4	A	389	PX4	C18-C17-C16	2.22	103.14	114.37	14	1
4	A	420	PX4	C34-C33-C32	2.22	103.14	114.37	11	1
4	A	422	PX4	C27-C26-C25	2.22	103.15	114.37	1	1
4	A	310	PX4	C11-C10-C9	2.22	121.82	113.69	2	1
4	A	309	PX4	C34-C33-C32	2.22	103.16	114.37	2	1
4	A	371	PX4	C12-C11-C10	2.22	104.98	113.13	9	1
4	A	340	PX4	C33-C32-C31	2.22	103.16	114.37	10	1
4	A	339	PX4	C14-C13-C12	2.22	103.17	114.37	13	1
4	A	354	PX4	C29-C28-C27	2.22	103.17	114.37	3	1
4	A	398	PX4	C25-C24-C23	2.22	105.57	113.69	1	2
4	A	419	PX4	C16-C15-C14	2.22	103.16	114.37	11	2
4	A	326	PX4	C5-N1-C2	2.22	101.11	109.91	8	2
4	A	395	PX4	C3-N1-C2	2.22	118.72	109.91	7	1
4	A	329	PX4	C17-C16-C15	2.21	103.18	114.37	12	1
4	A	339	PX4	C1-C2-N1	2.21	122.92	115.82	9	3
4	A	344	PX4	C30-C29-C28	2.21	103.18	114.37	8	1
4	A	349	PX4	C28-C27-C26	2.21	103.17	114.37	9	3
4	A	413	PX4	C14-C13-C12	2.21	103.17	114.37	8	1
4	A	308	PX4	C15-C14-C13	2.21	103.19	114.37	11	1
4	A	352	PX4	C12-C11-C10	2.21	105.00	113.13	13	1
4	A	368	PX4	C32-C31-C30	2.21	103.18	114.37	13	1
4	A	400	PX4	C29-C28-C27	2.21	103.19	114.37	10	1
4	A	412	PX4	C11-C10-C9	2.21	105.59	113.69	4	1
4	A	308	PX4	O3-C1-C2	2.21	120.28	109.65	10	1
4	A	330	PX4	C11-C10-C9	2.21	105.60	113.69	13	1
4	A	352	PX4	C29-C28-C27	2.21	103.20	114.37	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	355	PX4	C33-C32-C31	2.21	103.20	114.37	3	2
4	A	355	PX4	C16-C15-C14	2.21	103.20	114.37	7	1
4	A	375	PX4	C7-O7-C23	2.21	112.51	117.80	12	4
4	A	393	PX4	O4-P1-O2	2.21	117.69	108.94	9	1
4	A	417	PX4	C31-C30-C29	2.21	103.20	114.37	11	3
4	A	420	PX4	C16-C15-C14	2.21	103.20	114.37	1	4
4	A	306	PX4	C26-C25-C24	2.21	105.02	113.13	11	4
4	A	359	PX4	C26-C25-C24	2.21	105.02	113.13	10	1
4	A	381	PX4	C13-C12-C11	2.21	103.21	114.37	1	1
4	A	407	PX4	C33-C32-C31	2.21	103.21	114.37	7	1
4	A	421	PX4	O1-P1-O3	2.21	117.58	107.57	5	2
4	A	321	PX4	C22-C21-C20	2.21	98.47	113.36	9	1
4	A	409	PX4	C30-C29-C28	2.21	103.21	114.37	11	1
4	A	412	PX4	C19-C18-C17	2.21	103.21	114.37	1	1
4	A	413	PX4	O3-P1-O2	2.21	117.68	108.94	10	2
4	A	422	PX4	C3-N1-C2	2.21	118.68	109.91	3	1
4	A	422	PX4	C20-C19-C18	2.21	103.22	114.37	9	1
4	A	429	PX4	C1-C2-N1	2.21	122.90	115.82	11	2
4	A	316	PX4	C1-C2-N1	2.20	122.90	115.82	12	1
4	A	384	PX4	C20-C19-C18	2.20	125.51	114.37	13	1
4	A	306	PX4	C25-C24-C23	2.20	105.62	113.69	7	1
4	A	320	PX4	C8-O5-C9	2.20	109.07	117.12	6	1
4	A	322	PX4	C11-C10-C9	2.20	105.62	113.69	2	1
4	A	324	PX4	C30-C29-C28	2.20	103.23	114.37	8	1
4	A	343	PX4	C17-C16-C15	2.20	103.23	114.37	2	1
4	A	351	PX4	O3-C1-C2	2.20	120.25	109.65	10	1
4	A	389	PX4	O6-C9-C10	2.20	115.17	123.78	9	1
4	A	394	PX4	C27-C26-C25	2.20	103.23	114.37	5	2
4	A	422	PX4	C13-C12-C11	2.20	103.23	114.37	4	1
4	A	306	PX4	C18-C17-C16	2.20	103.25	114.37	6	1
4	A	344	PX4	C8-O5-C9	2.20	125.16	117.12	13	3
4	A	403	PX4	C14-C13-C12	2.20	103.25	114.37	1	2
4	A	316	PX4	C8-O5-C9	2.20	109.08	117.12	8	1
4	A	373	PX4	C19-C18-C17	2.20	103.25	114.37	6	2
4	A	400	PX4	C15-C14-C13	2.20	103.25	114.37	5	1
4	A	415	PX4	O6-C9-C10	2.20	115.18	123.78	9	1
4	A	428	PX4	C4-N1-C2	2.20	118.65	109.91	4	2
4	A	329	PX4	C32-C31-C30	2.20	103.25	114.37	12	1
4	A	411	PX4	C17-C16-C15	2.20	103.26	114.37	3	1
4	A	331	PX4	C20-C19-C18	2.20	103.27	114.37	6	1
4	A	341	PX4	O4-P1-O2	2.20	117.64	108.94	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	361	PX4	C1-C2-N1	2.20	122.87	115.82	8	1
4	A	375	PX4	C34-C33-C32	2.20	103.26	114.37	5	2
4	A	413	PX4	C18-C17-C16	2.20	103.26	114.37	3	1
4	A	379	PX4	C11-C10-C9	2.20	105.65	113.69	11	1
4	A	390	PX4	C34-C33-C32	2.20	103.27	114.37	1	2
4	A	407	PX4	C36-C35-C34	2.20	98.54	113.36	8	1
4	A	337	PX4	C34-C33-C32	2.19	103.28	114.37	7	1
4	A	322	PX4	C20-C19-C18	2.19	103.29	114.37	10	1
4	A	339	PX4	C29-C28-C27	2.19	103.29	114.37	9	1
4	A	361	PX4	C30-C29-C28	2.19	103.29	114.37	6	1
4	A	320	PX4	O6-C9-C10	2.19	115.22	123.78	14	1
4	A	322	PX4	C12-C11-C10	2.19	105.08	113.13	6	1
4	A	335	PX4	C5-N1-C4	2.19	114.73	108.98	14	2
4	A	354	PX4	C14-C13-C12	2.19	103.30	114.37	3	1
4	A	348	PX4	C3-N1-C2	2.19	101.21	109.91	2	2
4	A	349	PX4	C8-O5-C9	2.19	125.12	117.12	14	1
4	A	359	PX4	C5-N1-C2	2.19	118.61	109.91	13	1
4	A	402	PX4	O3-C1-C2	2.19	120.19	109.65	7	1
4	A	327	PX4	O3-C1-C2	2.19	120.18	109.65	2	3
4	A	334	PX4	C30-C29-C28	2.19	103.31	114.37	7	1
4	A	334	PX4	O8-C23-C24	2.19	115.22	123.78	14	2
4	A	428	PX4	C8-O5-C9	2.19	109.12	117.12	9	1
4	A	320	PX4	C19-C18-C17	2.19	103.32	114.37	1	2
4	A	328	PX4	C29-C28-C27	2.19	103.31	114.37	10	2
4	A	373	PX4	C3-N1-C2	2.19	118.60	109.91	8	1
4	A	380	PX4	C30-C29-C28	2.19	103.32	114.37	10	1
4	A	406	PX4	C5-N1-C4	2.19	103.23	108.98	2	2
4	A	321	PX4	C16-C15-C14	2.18	103.33	114.37	8	3
4	A	330	PX4	C25-C24-C23	2.18	105.69	113.69	5	1
4	A	386	PX4	C5-N1-C2	2.18	118.59	109.91	12	2
4	A	411	PX4	O4-P1-O2	2.19	117.60	108.94	6	1
4	A	417	PX4	C32-C31-C30	2.18	103.33	114.37	2	1
4	A	427	PX4	C27-C26-C25	2.19	103.32	114.37	1	1
4	A	309	PX4	C3-N1-C2	2.18	118.59	109.91	4	1
4	A	338	PX4	O6-C9-C10	2.18	115.24	123.78	1	1
4	A	335	PX4	C29-C28-C27	2.18	103.34	114.37	13	2
4	A	353	PX4	C29-C28-C27	2.18	103.34	114.37	4	1
4	A	356	PX4	C5-N1-C2	2.18	101.23	109.91	7	1
4	A	395	PX4	C8-O5-C9	2.18	109.14	117.12	11	2
4	A	376	PX4	C20-C19-C18	2.18	103.34	114.37	13	1
4	A	429	PX4	C28-C27-C26	2.18	103.34	114.37	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	430	PX4	O1-P1-O3	2.18	97.68	107.57	8	1
4	A	314	PX4	O3-P1-O2	2.18	100.30	108.94	13	1
4	A	312	PX4	C31-C30-C29	2.18	103.36	114.37	5	1
4	A	315	PX4	C30-C29-C28	2.18	103.35	114.37	7	2
4	A	337	PX4	C12-C11-C10	2.18	105.12	113.13	13	4
4	A	407	PX4	C11-C10-C9	2.18	105.71	113.69	12	1
4	A	427	PX4	C17-C16-C15	2.18	103.35	114.37	12	2
4	A	353	PX4	C14-C13-C12	2.18	103.36	114.37	14	1
4	A	383	PX4	C28-C27-C26	2.18	103.36	114.37	14	1
4	A	419	PX4	C20-C19-C18	2.18	103.36	114.37	10	1
4	A	309	PX4	C14-C13-C12	2.18	103.37	114.37	4	1
4	A	317	PX4	C19-C18-C17	2.17	103.38	114.37	4	1
4	A	323	PX4	C20-C19-C18	2.17	103.38	114.37	3	1
4	A	328	PX4	C27-C26-C25	2.18	103.37	114.37	4	1
4	A	335	PX4	O3-C1-C2	2.18	120.12	109.65	14	1
4	A	341	PX4	C30-C29-C28	2.18	103.37	114.37	6	2
4	A	345	PX4	C13-C12-C11	2.18	103.37	114.37	6	1
4	A	424	PX4	C26-C25-C24	2.18	105.13	113.13	5	1
4	A	341	PX4	C27-C26-C25	2.17	103.38	114.37	10	1
4	A	345	PX4	C4-N1-C2	2.17	101.27	109.91	8	1
4	A	350	PX4	C14-C13-C12	2.17	103.38	114.37	6	1
4	A	360	PX4	O8-C23-C24	2.17	115.28	123.78	7	1
4	A	368	PX4	C4-N1-C3	2.17	114.69	108.98	14	2
4	A	375	PX4	C14-C13-C12	2.17	103.38	114.37	3	1
4	A	341	PX4	C29-C28-C27	2.17	103.39	114.37	4	2
4	A	348	PX4	C31-C30-C29	2.17	103.38	114.37	10	1
4	A	319	PX4	O1-P1-O4	2.17	97.72	107.57	14	1
4	A	324	PX4	C13-C12-C11	2.17	103.39	114.37	14	2
4	A	351	PX4	C34-C33-C32	2.17	103.39	114.37	14	1
4	A	380	PX4	O1-P1-O4	2.17	117.41	107.57	9	1
4	A	402	PX4	C14-C13-C12	2.17	103.39	114.37	7	2
4	A	323	PX4	C17-C16-C15	2.17	103.40	114.37	14	1
4	A	327	PX4	C5-N1-C4	2.17	103.28	108.98	14	1
4	A	345	PX4	C29-C28-C27	2.17	103.40	114.37	4	2
4	A	362	PX4	C15-C14-C13	2.17	103.40	114.37	12	1
4	A	416	PX4	C3-N1-C2	2.17	101.28	109.91	12	2
4	A	424	PX4	C18-C17-C16	2.17	103.39	114.37	9	1
4	A	319	PX4	O6-C9-C10	2.17	115.30	123.78	12	1
4	A	322	PX4	C4-N1-C2	2.17	101.29	109.91	13	1
4	A	341	PX4	O6-C9-C10	2.17	115.31	123.78	7	1
4	A	377	PX4	C5-N1-C2	2.17	118.53	109.91	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	327	PX4	C26-C25-C24	2.17	121.08	113.13	2	2
4	A	335	PX4	C20-C19-C18	2.17	103.42	114.37	7	1
4	A	347	PX4	C8-O5-C9	2.17	109.20	117.12	7	2
4	A	349	PX4	O6-C9-C10	2.17	115.31	123.78	14	1
4	A	356	PX4	O4-P1-O2	2.17	117.52	108.94	4	2
4	A	352	PX4	C20-C19-C18	2.16	103.43	114.37	8	1
4	A	366	PX4	C33-C32-C31	2.16	103.42	114.37	12	2
4	A	368	PX4	C16-C15-C14	2.17	103.42	114.37	14	2
4	A	422	PX4	C25-C24-C23	2.17	105.75	113.69	6	1
4	A	400	PX4	C11-C10-C9	2.17	105.76	113.69	2	2
4	A	430	PX4	O3-C1-C2	2.17	120.07	109.65	13	1
4	A	315	PX4	C14-C13-C12	2.16	103.43	114.37	13	2
4	A	374	PX4	C3-N1-C2	2.16	118.51	109.91	11	2
4	A	390	PX4	C8-O5-C9	2.16	109.21	117.12	5	1
4	A	416	PX4	C20-C19-C18	2.16	103.43	114.37	1	1
4	A	424	PX4	C4-N1-C3	2.16	114.66	108.98	8	2
4	A	425	PX4	C8-O5-C9	2.16	109.21	117.12	14	2
4	A	313	PX4	C8-O5-C9	2.16	109.22	117.12	12	2
4	A	318	PX4	C36-C35-C34	2.16	98.77	113.36	13	1
4	A	325	PX4	C34-C33-C32	2.16	103.44	114.37	8	1
4	A	335	PX4	C11-C10-C9	2.16	105.78	113.69	2	2
4	A	355	PX4	O6-C9-C10	2.16	115.33	123.78	2	2
4	A	359	PX4	C28-C27-C26	2.16	103.45	114.37	5	1
4	A	408	PX4	C26-C25-C24	2.16	105.19	113.13	13	1
4	A	403	PX4	C25-C24-C23	2.16	105.78	113.69	11	1
4	A	404	PX4	C26-C25-C24	2.16	105.19	113.13	7	2
4	A	344	PX4	C5-N1-C2	2.16	118.49	109.91	11	1
4	A	350	PX4	C12-C11-C10	2.16	105.19	113.13	5	1
4	A	369	PX4	C29-C28-C27	2.16	103.46	114.37	13	2
4	A	386	PX4	O1-P1-O3	2.16	117.35	107.57	12	1
4	A	336	PX4	C33-C32-C31	2.16	103.46	114.37	1	2
4	A	350	PX4	C28-C27-C26	2.16	103.46	114.37	13	1
4	A	365	PX4	C20-C19-C18	2.16	103.46	114.37	3	1
4	A	378	PX4	C19-C18-C17	2.16	103.46	114.37	4	1
4	A	395	PX4	C20-C19-C18	2.16	103.46	114.37	10	1
4	A	416	PX4	C30-C29-C28	2.16	103.46	114.37	7	1
4	A	365	PX4	C34-C33-C32	2.16	103.46	114.37	7	1
4	A	351	PX4	O3-P1-O2	2.16	100.39	108.94	9	1
4	A	355	PX4	O3-C1-C2	2.16	120.02	109.65	9	1
4	A	367	PX4	C15-C14-C13	2.16	103.47	114.37	10	1
4	A	396	PX4	C26-C25-C24	2.16	105.20	113.13	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	423	PX4	C5-N1-C2	2.16	101.34	109.91	13	2
4	A	339	PX4	C8-O5-C9	2.15	109.25	117.12	4	1
4	A	378	PX4	C15-C14-C13	2.15	103.48	114.37	11	1
4	A	357	PX4	C26-C25-C24	2.15	121.04	113.13	11	1
4	A	310	PX4	C4-N1-C2	2.15	118.47	109.91	11	2
4	A	359	PX4	C17-C16-C15	2.15	103.49	114.37	14	1
4	A	419	PX4	C30-C29-C28	2.15	103.48	114.37	8	1
4	A	332	PX4	C3-N1-C2	2.15	118.46	109.91	14	1
4	A	338	PX4	O8-C23-C24	2.15	115.37	123.78	4	2
4	A	341	PX4	C14-C13-C12	2.15	103.49	114.37	10	2
4	A	346	PX4	O1-P1-O4	2.15	117.32	107.57	3	4
4	A	398	PX4	C30-C29-C28	2.15	103.49	114.37	5	1
4	A	331	PX4	C31-C30-C29	2.15	103.50	114.37	6	3
4	A	353	PX4	C5-N1-C2	2.15	118.46	109.91	11	2
4	A	343	PX4	O1-P1-O4	2.15	97.82	107.57	1	1
4	A	427	PX4	C18-C17-C16	2.15	103.50	114.37	12	1
4	A	423	PX4	C25-C24-C23	2.15	121.57	113.69	8	2
4	A	424	PX4	O1-P1-O4	2.15	117.31	107.57	5	1
4	A	429	PX4	C4-N1-C2	2.15	118.46	109.91	6	1
4	A	324	PX4	C36-C35-C34	2.15	98.85	113.36	6	2
4	A	325	PX4	C16-C15-C14	2.15	103.51	114.37	1	1
4	A	357	PX4	C17-C16-C15	2.15	103.50	114.37	12	1
4	A	388	PX4	C3-N1-C2	2.15	101.37	109.91	8	1
4	A	400	PX4	C26-C25-C24	2.15	105.23	113.13	3	1
4	A	349	PX4	C18-C17-C16	2.15	103.52	114.37	12	1
4	A	357	PX4	O8-C23-C24	2.15	115.39	123.78	9	1
4	A	361	PX4	C18-C17-C16	2.15	103.52	114.37	5	1
4	A	363	PX4	O1-P1-O3	2.15	97.83	107.57	12	1
4	A	366	PX4	C5-N1-C2	2.15	118.44	109.91	1	1
4	A	370	PX4	C19-C18-C17	2.15	103.52	114.37	12	1
4	A	403	PX4	C31-C30-C29	2.15	103.52	114.37	13	2
4	A	429	PX4	C16-C15-C14	2.15	103.52	114.37	10	1
4	A	377	PX4	C26-C25-C24	2.15	121.01	113.13	2	1
4	A	376	PX4	O8-C23-C24	2.14	115.39	123.78	2	1
4	A	380	PX4	C15-C14-C13	2.15	103.53	114.37	5	1
4	A	385	PX4	C1-C2-N1	2.14	108.94	115.82	11	2
4	A	394	PX4	C12-C11-C10	2.14	105.25	113.13	11	2
4	A	319	PX4	C7-O7-C23	2.14	112.67	117.80	14	2
4	A	415	PX4	C18-C17-C16	2.14	103.53	114.37	8	1
4	A	326	PX4	O1-P1-O4	2.14	117.28	107.57	5	2
4	A	339	PX4	C5-N1-C3	2.14	103.35	108.98	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	C28-C27-C26	2.14	103.53	114.37	4	1
4	A	355	PX4	C34-C33-C32	2.14	103.54	114.37	14	1
4	A	416	PX4	O8-C23-C24	2.14	115.41	123.78	9	1
4	A	429	PX4	C30-C29-C28	2.14	103.54	114.37	10	1
4	A	330	PX4	C35-C34-C33	2.14	96.48	115.25	13	1
4	A	353	PX4	O5-C9-O6	2.14	118.27	123.63	11	2
4	A	366	PX4	C27-C26-C25	2.14	103.55	114.37	11	2
4	A	399	PX4	C20-C19-C18	2.14	103.55	114.37	1	1
4	A	401	PX4	C31-C30-C29	2.14	103.55	114.37	6	2
4	A	423	PX4	C18-C17-C16	2.14	103.54	114.37	8	3
4	A	324	PX4	C3-N1-C2	2.14	101.41	109.91	2	1
4	A	328	PX4	C19-C18-C17	2.14	103.56	114.37	4	1
4	A	366	PX4	C4-N1-C2	2.14	118.41	109.91	4	1
4	A	395	PX4	C13-C12-C11	2.14	103.56	114.37	10	2
4	A	389	PX4	C32-C31-C30	2.14	103.56	114.37	11	1
4	A	420	PX4	C33-C32-C31	2.14	103.57	114.37	11	1
4	A	424	PX4	C11-C10-C9	2.14	105.86	113.69	12	1
4	A	325	PX4	C15-C14-C13	2.14	103.58	114.37	7	1
4	A	333	PX4	O6-C9-C10	2.14	132.13	123.78	11	1
4	A	369	PX4	O1-P1-O3	2.14	97.89	107.57	3	1
4	A	402	PX4	C25-C24-C23	2.14	105.86	113.69	12	2
4	A	360	PX4	C29-C28-C27	2.13	103.58	114.37	2	1
4	A	360	PX4	C16-C15-C14	2.14	103.57	114.37	5	1
4	A	369	PX4	C27-C26-C25	2.13	103.58	114.37	6	1
4	A	375	PX4	C33-C32-C31	2.13	103.58	114.37	14	2
4	A	394	PX4	C26-C25-C24	2.13	105.28	113.13	11	2
4	A	409	PX4	C17-C16-C15	2.13	103.58	114.37	11	1
4	A	419	PX4	C32-C31-C30	2.14	103.57	114.37	9	1
4	A	315	PX4	C31-C30-C29	2.13	103.59	114.37	12	2
4	A	367	PX4	C33-C32-C31	2.13	103.58	114.37	5	1
4	A	368	PX4	C18-C17-C16	2.13	103.58	114.37	5	1
4	A	424	PX4	C31-C30-C29	2.13	103.58	114.37	12	1
4	A	311	PX4	C16-C15-C14	2.13	103.59	114.37	6	2
4	A	317	PX4	C34-C33-C32	2.13	103.59	114.37	6	1
4	A	403	PX4	C15-C14-C13	2.13	103.60	114.37	8	1
4	A	415	PX4	C4-N1-C2	2.13	118.38	109.91	1	1
4	A	419	PX4	C25-C24-C23	2.13	105.88	113.69	1	1
4	A	425	PX4	C18-C17-C16	2.13	103.59	114.37	9	1
4	A	427	PX4	C14-C13-C12	2.13	103.59	114.37	10	1
4	A	344	PX4	C11-C10-C9	2.13	105.89	113.69	3	1
4	A	430	PX4	C33-C32-C31	2.13	103.59	114.37	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	363	PX4	C11-C10-C9	2.13	105.89	113.69	11	2
4	A	382	PX4	C18-C17-C16	2.13	103.60	114.37	8	3
4	A	389	PX4	C4-N1-C2	2.13	118.38	109.91	14	1
4	A	306	PX4	C31-C30-C29	2.13	103.61	114.37	10	1
4	A	322	PX4	C17-C16-C15	2.13	103.61	114.37	12	1
4	A	340	PX4	C13-C12-C11	2.13	103.61	114.37	14	1
4	A	342	PX4	C18-C17-C16	2.13	103.61	114.37	5	2
4	A	409	PX4	C4-N1-C2	2.13	118.38	109.91	14	2
4	A	373	PX4	C36-C35-C34	2.13	98.99	113.36	5	1
4	A	396	PX4	C13-C12-C11	2.13	103.61	114.37	6	1
4	A	404	PX4	C12-C11-C10	2.13	120.95	113.13	13	1
4	A	351	PX4	C30-C29-C28	2.13	103.62	114.37	8	2
4	A	366	PX4	C25-C24-C23	2.13	105.90	113.69	5	1
4	A	387	PX4	C32-C31-C30	2.13	103.62	114.37	8	1
4	A	392	PX4	C27-C26-C25	2.13	103.62	114.37	9	1
4	A	413	PX4	C17-C16-C15	2.13	103.61	114.37	5	1
4	A	374	PX4	C25-C24-C23	2.13	105.91	113.69	2	1
4	A	409	PX4	C16-C15-C14	2.13	103.62	114.37	10	1
4	A	340	PX4	C20-C19-C18	2.12	103.63	114.37	2	1
4	A	407	PX4	C17-C16-C15	2.12	103.63	114.37	4	1
4	A	412	PX4	C5-N1-C2	2.12	118.35	109.91	5	1
4	A	307	PX4	C25-C24-C23	2.12	105.92	113.69	10	3
4	A	332	PX4	C32-C31-C30	2.12	103.64	114.37	9	1
4	A	355	PX4	O1-P1-O4	2.12	117.19	107.57	2	1
4	A	339	PX4	C31-C30-C29	2.12	103.64	114.37	6	2
4	A	362	PX4	C28-C27-C26	2.12	103.64	114.37	9	1
4	A	362	PX4	C11-C10-C9	2.12	105.92	113.69	13	1
4	A	336	PX4	C14-C13-C12	2.12	103.64	114.37	3	2
4	A	368	PX4	C19-C18-C17	2.12	103.64	114.37	6	2
4	A	377	PX4	C13-C12-C11	2.12	103.64	114.37	8	1
4	A	350	PX4	O6-C9-C10	2.12	115.49	123.78	10	1
4	A	406	PX4	C5-N1-C3	2.12	114.55	108.98	2	1
4	A	397	PX4	C5-N1-C2	2.12	118.34	109.91	12	1
4	A	409	PX4	O6-C9-C10	2.12	115.49	123.78	1	2
4	A	411	PX4	O3-C1-C2	2.12	119.86	109.65	6	1
4	A	315	PX4	O1-P1-O3	2.12	97.96	107.57	13	1
4	A	324	PX4	C28-C27-C26	2.12	103.65	114.37	13	1
4	A	334	PX4	C32-C31-C30	2.12	103.65	114.37	1	1
4	A	336	PX4	C27-C26-C25	2.12	103.65	114.37	2	2
4	A	369	PX4	C34-C33-C32	2.12	103.66	114.37	2	1
4	A	385	PX4	C19-C18-C17	2.12	103.66	114.37	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	394	PX4	O3-C1-C2	2.12	119.85	109.65	14	1
4	A	395	PX4	C17-C16-C15	2.12	103.65	114.37	14	1
4	A	311	PX4	C31-C30-C29	2.12	103.66	114.37	10	1
4	A	335	PX4	O8-C23-C24	2.12	115.50	123.78	7	1
4	A	366	PX4	O8-C23-C24	2.12	115.50	123.78	4	1
4	A	355	PX4	C8-O5-C9	2.12	109.38	117.12	8	1
4	A	375	PX4	C11-C10-C9	2.12	105.94	113.69	9	1
4	A	390	PX4	C25-C24-C23	2.12	105.94	113.69	14	1
4	A	310	PX4	C20-C19-C18	2.12	103.67	114.37	13	1
4	A	357	PX4	C32-C31-C30	2.12	103.67	114.37	2	1
4	A	396	PX4	C8-O5-C9	2.12	109.38	117.12	3	1
4	A	372	PX4	C5-N1-C2	2.12	118.32	109.91	6	1
4	A	425	PX4	C33-C32-C31	2.12	103.67	114.37	10	1
4	A	311	PX4	O1-P1-O3	2.11	117.15	107.57	11	1
4	A	320	PX4	C31-C30-C29	2.11	103.68	114.37	1	2
4	A	362	PX4	O3-P1-O2	2.12	100.55	108.94	3	1
4	A	310	PX4	C25-C24-C23	2.11	121.44	113.69	7	1
4	A	320	PX4	C15-C14-C13	2.11	103.68	114.37	6	1
4	A	338	PX4	C3-N1-C2	2.11	101.51	109.91	11	1
4	A	351	PX4	C20-C19-C18	2.11	103.69	114.37	1	1
4	A	365	PX4	O8-C23-C24	2.11	115.51	123.78	14	1
4	A	418	PX4	C4-N1-C2	2.11	101.51	109.91	14	1
4	A	423	PX4	C5-N1-C4	2.11	114.53	108.98	11	1
4	A	318	PX4	O3-C1-C2	2.11	119.81	109.65	9	1
4	A	353	PX4	C17-C16-C15	2.11	103.69	114.37	7	1
4	A	366	PX4	C5-N1-C4	2.11	103.43	108.98	5	2
4	A	376	PX4	C19-C18-C17	2.11	103.69	114.37	12	1
4	A	406	PX4	C25-C24-C23	2.11	105.96	113.69	10	1
4	A	407	PX4	C15-C14-C13	2.11	103.70	114.37	6	1
4	A	409	PX4	C27-C26-C25	2.11	103.70	114.37	6	2
4	A	411	PX4	C28-C27-C26	2.11	103.69	114.37	9	1
4	A	419	PX4	C33-C32-C31	2.11	103.69	114.37	2	1
4	A	323	PX4	C28-C27-C26	2.11	103.70	114.37	1	1
4	A	349	PX4	C14-C13-C12	2.11	103.70	114.37	6	1
4	A	349	PX4	C4-N1-C2	2.11	101.52	109.91	7	1
4	A	362	PX4	O1-P1-O4	2.11	117.14	107.57	1	2
4	A	358	PX4	C33-C32-C31	2.11	103.70	114.37	13	1
4	A	362	PX4	C31-C30-C29	2.11	103.70	114.37	8	1
4	A	396	PX4	C18-C17-C16	2.11	103.70	114.37	12	1
4	A	399	PX4	O1-P1-O4	2.11	117.14	107.57	8	1
4	A	424	PX4	O4-P1-O2	2.11	117.30	108.94	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	344	PX4	C19-C18-C17	2.11	103.71	114.37	6	1
4	A	428	PX4	C1-C2-N1	2.11	122.59	115.82	7	1
4	A	308	PX4	C3-N1-C2	2.11	118.28	109.91	6	3
4	A	322	PX4	C5-N1-C4	2.11	103.44	108.98	8	1
4	A	322	PX4	C15-C14-C13	2.11	103.72	114.37	11	1
4	A	323	PX4	O8-C23-C24	2.11	115.54	123.78	10	1
4	A	314	PX4	O1-P1-O4	2.11	117.11	107.57	13	1
4	A	316	PX4	C13-C12-C11	2.11	103.73	114.37	10	1
4	A	334	PX4	C29-C28-C27	2.11	103.72	114.37	11	2
4	A	351	PX4	C5-N1-C2	2.11	118.28	109.91	9	2
4	A	352	PX4	C19-C18-C17	2.11	103.72	114.37	9	1
4	A	379	PX4	C17-C16-C15	2.11	103.72	114.37	13	3
4	A	357	PX4	C33-C32-C31	2.11	103.72	114.37	7	3
4	A	365	PX4	C36-C35-C34	2.11	99.14	113.36	5	1
4	A	427	PX4	C19-C18-C17	2.11	103.72	114.37	12	1
4	A	320	PX4	C17-C16-C15	2.10	103.74	114.37	10	1
4	A	366	PX4	C34-C33-C32	2.10	103.73	114.37	10	1
4	A	426	PX4	C13-C12-C11	2.10	103.74	114.37	13	1
4	A	343	PX4	C33-C32-C31	2.10	103.75	114.37	10	2
4	A	374	PX4	C13-C12-C11	2.10	103.75	114.37	10	1
4	A	378	PX4	C8-O5-C9	2.10	109.44	117.12	2	1
4	A	416	PX4	O1-P1-O3	2.10	98.05	107.57	4	2
4	A	418	PX4	C1-C2-N1	2.10	122.56	115.82	5	2
4	A	313	PX4	C34-C33-C32	2.10	103.75	114.37	10	2
4	A	426	PX4	C11-C10-C9	2.10	106.00	113.69	14	1
4	A	317	PX4	O6-C9-C10	2.10	115.58	123.78	3	1
4	A	347	PX4	C30-C29-C28	2.10	103.77	114.37	14	1
4	A	365	PX4	C4-N1-C2	2.10	118.25	109.91	5	1
4	A	366	PX4	C26-C25-C24	2.10	105.42	113.13	4	1
4	A	372	PX4	C18-C17-C16	2.10	103.78	114.37	11	1
4	A	381	PX4	C32-C31-C30	2.10	103.78	114.37	13	1
4	A	382	PX4	C32-C31-C30	2.10	103.77	114.37	1	1
4	A	410	PX4	O8-C23-C24	2.10	115.58	123.78	10	1
4	A	423	PX4	O3-C1-C2	2.10	119.74	109.65	2	1
4	A	320	PX4	C33-C32-C31	2.09	103.78	114.37	4	1
4	A	321	PX4	C20-C19-C18	2.09	103.78	114.37	1	2
4	A	402	PX4	C8-O5-C9	2.10	124.78	117.12	8	1
4	A	342	PX4	C25-C24-C23	2.09	106.02	113.69	2	1
4	A	387	PX4	C14-C13-C12	2.09	103.78	114.37	14	3
4	A	401	PX4	C30-C29-C28	2.09	103.78	114.37	10	2
4	A	412	PX4	O8-C23-C24	2.09	115.59	123.78	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	314	PX4	C5-N1-C2	2.09	118.23	109.91	1	1
4	A	328	PX4	C5-N1-C2	2.09	118.23	109.91	5	1
4	A	353	PX4	C27-C26-C25	2.09	103.79	114.37	4	1
4	A	354	PX4	O6-C9-C10	2.09	115.60	123.78	11	1
4	A	394	PX4	C18-C17-C16	2.09	103.79	114.37	11	1
4	A	404	PX4	C33-C32-C31	2.09	103.79	114.37	2	2
4	A	393	PX4	C31-C30-C29	2.09	103.80	114.37	2	1
4	A	397	PX4	C16-C15-C14	2.09	103.79	114.37	8	1
4	A	412	PX4	C3-N1-C2	2.09	118.23	109.91	8	1
4	A	334	PX4	C4-N1-C2	2.09	118.22	109.91	7	1
4	A	427	PX4	C31-C30-C29	2.09	103.79	114.37	10	1
4	A	306	PX4	C14-C13-C12	2.09	103.81	114.37	10	1
4	A	312	PX4	C5-N1-C2	2.09	118.21	109.91	10	1
4	A	325	PX4	C28-C27-C26	2.09	103.81	114.37	7	1
4	A	350	PX4	C26-C25-C24	2.09	105.45	113.13	3	2
4	A	366	PX4	C18-C17-C16	2.09	103.81	114.37	5	1
4	A	308	PX4	C19-C18-C17	2.09	103.82	114.37	9	1
4	A	310	PX4	O4-P1-O2	2.09	117.21	108.94	12	1
4	A	321	PX4	C4-N1-C3	2.09	103.49	108.98	2	2
4	A	391	PX4	C13-C12-C11	2.09	103.81	114.37	14	1
4	A	337	PX4	C11-C10-C9	2.09	106.05	113.69	8	1
4	A	358	PX4	C32-C31-C30	2.09	103.83	114.37	4	1
4	A	366	PX4	C14-C13-C12	2.09	103.82	114.37	5	1
4	A	380	PX4	C14-C13-C12	2.09	103.82	114.37	8	1
4	A	373	PX4	C29-C28-C27	2.09	103.83	114.37	12	2
4	A	400	PX4	C13-C12-C11	2.09	103.83	114.37	8	1
4	A	426	PX4	O1-P1-O4	2.09	117.02	107.57	6	1
4	A	360	PX4	C3-N1-C2	2.08	118.20	109.91	8	1
4	A	416	PX4	C32-C31-C30	2.08	103.83	114.37	1	1
4	A	424	PX4	C20-C19-C18	2.08	103.83	114.37	12	1
4	A	316	PX4	O8-C23-C24	2.08	115.64	123.78	3	1
4	A	326	PX4	C19-C18-C17	2.08	103.84	114.37	8	1
4	A	353	PX4	O1-P1-O3	2.08	98.13	107.57	2	2
4	A	369	PX4	C28-C27-C26	2.08	103.84	114.37	1	1
4	A	393	PX4	O5-C9-C10	2.08	118.19	111.83	12	2
4	A	401	PX4	C8-O5-C9	2.08	124.73	117.12	1	1
4	A	325	PX4	C25-C24-C23	2.08	106.07	113.69	3	1
4	A	381	PX4	C31-C30-C29	2.08	103.85	114.37	9	1
4	A	395	PX4	C25-C24-C23	2.08	121.32	113.69	11	1
4	A	423	PX4	C27-C26-C25	2.08	103.85	114.37	13	1
4	A	337	PX4	C20-C19-C18	2.08	103.85	114.37	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	338	PX4	C16-C15-C14	2.08	103.86	114.37	8	1
4	A	360	PX4	C28-C27-C26	2.08	103.86	114.37	3	1
4	A	376	PX4	C14-C13-C12	2.08	103.86	114.37	12	1
4	A	384	PX4	C4-N1-C2	2.08	101.65	109.91	9	1
4	A	418	PX4	C11-C10-C9	2.08	106.08	113.69	6	1
4	A	323	PX4	O5-C9-C10	2.08	118.17	111.83	7	1
4	A	349	PX4	C19-C18-C17	2.08	103.87	114.37	13	1
4	A	352	PX4	C27-C26-C25	2.08	103.86	114.37	8	1
4	A	420	PX4	O8-C23-C24	2.08	115.65	123.78	13	1
4	A	306	PX4	C15-C14-C13	2.07	103.88	114.37	4	1
4	A	311	PX4	C29-C28-C27	2.08	103.88	114.37	9	1
4	A	352	PX4	O4-P1-O2	2.08	117.17	108.94	2	1
4	A	386	PX4	C34-C33-C32	2.08	103.87	114.37	14	1
4	A	389	PX4	C13-C12-C11	2.08	103.87	114.37	4	1
4	A	333	PX4	C34-C33-C32	2.08	124.86	114.37	2	1
4	A	383	PX4	C14-C13-C12	2.08	103.88	114.37	11	1
4	A	310	PX4	C3-N1-C2	2.07	101.67	109.91	3	1
4	A	334	PX4	C33-C32-C31	2.07	103.89	114.37	8	1
4	A	345	PX4	C12-C11-C10	2.07	120.75	113.13	2	1
4	A	378	PX4	C11-C10-C9	2.07	106.09	113.69	5	1
4	A	378	PX4	C14-C13-C12	2.07	103.89	114.37	7	1
4	A	378	PX4	C18-C17-C16	2.07	103.89	114.37	10	1
4	A	415	PX4	O1-P1-O4	2.07	116.96	107.57	1	1
4	A	418	PX4	C33-C32-C31	2.07	103.89	114.37	12	2
4	A	362	PX4	C5-N1-C2	2.07	118.14	109.91	2	1
4	A	421	PX4	O1-P1-O4	2.07	116.95	107.57	7	1
4	A	426	PX4	C3-N1-C2	2.07	101.68	109.91	12	1
4	A	429	PX4	C20-C19-C18	2.07	103.90	114.37	6	1
4	A	347	PX4	O6-C9-C10	2.07	115.69	123.78	2	1
4	A	395	PX4	C28-C27-C26	2.07	103.91	114.37	11	2
4	A	358	PX4	C8-O5-C9	2.07	109.56	117.12	6	1
4	A	359	PX4	C34-C33-C32	2.07	103.92	114.37	5	1
4	A	406	PX4	C29-C28-C27	2.07	103.91	114.37	10	2
4	A	366	PX4	C32-C31-C30	2.07	103.93	114.37	13	2
4	A	383	PX4	C15-C14-C13	2.07	103.93	114.37	1	1
4	A	421	PX4	C20-C19-C18	2.07	103.93	114.37	4	1
4	A	315	PX4	C19-C18-C17	2.06	103.93	114.37	12	2
4	A	320	PX4	C29-C28-C27	2.06	103.93	114.37	7	1
4	A	354	PX4	C16-C15-C14	2.06	103.94	114.37	10	1
4	A	358	PX4	C12-C11-C10	2.06	105.54	113.13	8	1
4	A	359	PX4	O1-P1-O3	2.06	98.21	107.57	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	379	PX4	O6-C9-C10	2.06	115.71	123.78	5	1
4	A	399	PX4	C31-C30-C29	2.06	103.94	114.37	2	1
4	A	430	PX4	C16-C15-C14	2.06	103.94	114.37	14	1
4	A	317	PX4	O4-P1-O2	2.06	117.11	108.94	12	1
4	A	338	PX4	C15-C14-C13	2.06	103.94	114.37	6	1
4	A	342	PX4	C29-C28-C27	2.06	103.95	114.37	5	1
4	A	364	PX4	C27-C26-C25	2.06	103.94	114.37	7	3
4	A	323	PX4	C22-C21-C20	2.06	99.44	113.36	13	1
4	A	318	PX4	C27-C26-C25	2.06	103.95	114.37	12	2
4	A	327	PX4	C4-N1-C2	2.06	118.10	109.91	10	1
4	A	389	PX4	C19-C18-C17	2.06	103.95	114.37	14	1
4	A	408	PX4	C15-C14-C13	2.06	103.96	114.37	2	1
4	A	410	PX4	C32-C31-C30	2.06	103.95	114.37	3	1
4	A	427	PX4	O8-C23-C24	2.06	115.72	123.78	13	1
4	A	348	PX4	C14-C13-C12	2.06	103.96	114.37	8	1
4	A	354	PX4	C5-N1-C2	2.06	101.73	109.91	5	1
4	A	366	PX4	C1-C2-N1	2.06	122.43	115.82	9	1
4	A	383	PX4	C8-O5-C9	2.06	124.64	117.12	13	1
4	A	396	PX4	C28-C27-C26	2.06	103.97	114.37	6	1
4	A	396	PX4	C34-C33-C32	2.06	103.96	114.37	14	1
4	A	401	PX4	C22-C21-C20	2.06	99.47	113.36	12	1
4	A	401	PX4	C33-C32-C31	2.06	103.96	114.37	12	1
4	A	403	PX4	O6-C9-C10	2.06	115.73	123.78	8	1
4	A	415	PX4	C3-N1-C2	2.06	118.09	109.91	11	1
4	A	378	PX4	C5-N1-C3	2.06	114.38	108.98	7	1
4	A	370	PX4	C13-C12-C11	2.06	103.97	114.37	6	1
4	A	399	PX4	C14-C13-C12	2.06	103.97	114.37	7	2
4	A	418	PX4	C16-C15-C14	2.06	103.97	114.37	13	2
4	A	311	PX4	C11-C10-C9	2.06	106.16	113.69	13	1
4	A	339	PX4	C3-N1-C2	2.06	101.74	109.91	5	1
4	A	350	PX4	C11-C10-C9	2.06	106.16	113.69	9	1
4	A	367	PX4	C13-C12-C11	2.06	103.98	114.37	9	1
4	A	400	PX4	C30-C29-C28	2.06	103.98	114.37	9	1
4	A	419	PX4	C34-C33-C32	2.05	103.98	114.37	12	1
4	A	422	PX4	C29-C28-C27	2.05	103.98	114.37	11	1
4	A	425	PX4	O6-C9-C10	2.06	115.74	123.78	9	1
4	A	429	PX4	C13-C12-C11	2.06	103.98	114.37	1	1
4	A	322	PX4	C16-C15-C14	2.05	103.99	114.37	6	1
4	A	335	PX4	C17-C16-C15	2.05	103.99	114.37	13	1
4	A	401	PX4	C5-N1-C2	2.05	118.08	109.91	3	1
4	A	429	PX4	C8-O5-C9	2.05	124.63	117.12	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	352	PX4	O3-C1-C2	2.05	119.53	109.65	14	1
4	A	374	PX4	C14-C13-C12	2.05	103.99	114.37	7	1
4	A	326	PX4	C30-C29-C28	2.05	104.00	114.37	3	1
4	A	364	PX4	C14-C13-C12	2.05	104.00	114.37	3	1
4	A	384	PX4	C26-C25-C24	2.05	105.59	113.13	4	1
4	A	391	PX4	C19-C18-C17	2.05	104.00	114.37	3	1
4	A	393	PX4	C27-C26-C25	2.05	103.99	114.37	2	1
4	A	409	PX4	O8-C23-C24	2.05	115.75	123.78	1	1
4	A	338	PX4	O3-C1-C2	2.05	119.51	109.65	8	1
4	A	366	PX4	C11-C10-C9	2.05	106.18	113.69	13	1
4	A	419	PX4	C17-C16-C15	2.05	104.00	114.37	4	1
4	A	425	PX4	C16-C15-C14	2.05	104.00	114.37	7	1
4	A	322	PX4	C13-C12-C11	2.05	104.01	114.37	3	1
4	A	333	PX4	C32-C31-C30	2.05	104.01	114.37	10	1
4	A	371	PX4	C4-N1-C2	2.05	118.06	109.91	11	1
4	A	321	PX4	C25-C24-C23	2.05	106.19	113.69	13	1
4	A	323	PX4	C16-C15-C14	2.05	104.02	114.37	6	1
4	A	353	PX4	C3-N1-C2	2.05	118.05	109.91	4	2
4	A	353	PX4	C8-O5-C9	2.05	109.63	117.12	7	1
4	A	347	PX4	C16-C15-C14	2.05	104.02	114.37	10	1
4	A	363	PX4	C19-C18-C17	2.05	104.02	114.37	4	1
4	A	368	PX4	C34-C33-C32	2.05	104.01	114.37	1	1
4	A	381	PX4	C11-C10-C9	2.05	106.18	113.69	5	1
4	A	406	PX4	C20-C19-C18	2.05	104.01	114.37	6	1
4	A	410	PX4	C5-N1-C2	2.05	118.06	109.91	5	2
4	A	333	PX4	O1-P1-O3	2.05	116.84	107.57	1	1
4	A	364	PX4	C18-C17-C16	2.05	104.02	114.37	7	1
4	A	372	PX4	C25-C24-C23	2.05	106.19	113.69	2	1
4	A	306	PX4	C33-C32-C31	2.05	104.03	114.37	4	1
4	A	347	PX4	C28-C27-C26	2.05	104.03	114.37	10	1
4	A	330	PX4	O1-P1-O3	2.04	116.83	107.57	2	1
4	A	337	PX4	O7-C7-C8	2.04	115.68	108.34	14	1
4	A	375	PX4	C13-C12-C11	2.04	104.04	114.37	9	1
4	A	428	PX4	C29-C28-C27	2.04	104.03	114.37	7	1
4	A	321	PX4	C33-C32-C31	2.04	104.04	114.37	4	1
4	A	328	PX4	C34-C33-C32	2.04	104.04	114.37	8	1
4	A	343	PX4	C8-O5-C9	2.04	109.65	117.12	2	1
4	A	344	PX4	C20-C19-C18	2.04	104.04	114.37	3	1
4	A	380	PX4	C12-C11-C10	2.04	105.63	113.13	8	1
4	A	426	PX4	C32-C31-C30	2.04	104.05	114.37	1	1
4	A	330	PX4	C13-C12-C11	2.04	104.05	114.37	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	306	PX4	C30-C29-C28	2.04	104.06	114.37	9	1
4	A	331	PX4	C33-C32-C31	2.04	104.06	114.37	13	1
4	A	378	PX4	C34-C33-C32	2.04	104.05	114.37	9	1
4	A	341	PX4	C3-N1-C2	2.04	118.02	109.91	12	1
4	A	357	PX4	C34-C33-C32	2.04	104.06	114.37	2	1
4	A	331	PX4	O1-P1-O4	2.04	116.80	107.57	9	1
4	A	332	PX4	C33-C32-C31	2.04	104.07	114.37	11	1
4	A	366	PX4	C17-C16-C15	2.04	104.06	114.37	9	1
4	A	368	PX4	C17-C16-C15	2.04	104.06	114.37	7	1
4	A	337	PX4	C15-C14-C13	2.04	104.07	114.37	10	1
4	A	350	PX4	C32-C31-C30	2.04	104.07	114.37	6	1
4	A	374	PX4	C32-C31-C30	2.04	104.07	114.37	4	1
4	A	377	PX4	C34-C33-C32	2.04	104.07	114.37	2	1
4	A	378	PX4	C13-C12-C11	2.04	104.07	114.37	7	1
4	A	401	PX4	C14-C13-C12	2.04	104.07	114.37	13	1
4	A	404	PX4	C13-C12-C11	2.04	104.06	114.37	3	1
4	A	413	PX4	O8-C23-C24	2.04	115.81	123.78	13	1
4	A	306	PX4	C19-C18-C17	2.04	104.08	114.37	7	1
4	A	345	PX4	C27-C26-C25	2.04	104.08	114.37	6	1
4	A	377	PX4	C3-N1-C2	2.04	118.00	109.91	1	1
4	A	405	PX4	C17-C16-C15	2.04	104.07	114.37	2	1
4	A	408	PX4	C3-N1-C2	2.04	101.82	109.91	11	1
4	A	418	PX4	C25-C24-C23	2.04	106.24	113.69	4	1
4	A	428	PX4	C27-C26-C25	2.04	104.08	114.37	3	1
4	A	314	PX4	C26-C25-C24	2.04	105.65	113.13	4	1
4	A	328	PX4	O3-C1-C2	2.04	119.44	109.65	5	1
4	A	342	PX4	C32-C31-C30	2.03	104.08	114.37	2	1
4	A	372	PX4	O1-P1-O4	2.03	116.78	107.57	3	1
4	A	321	PX4	C30-C29-C28	2.03	104.10	114.37	8	1
4	A	334	PX4	C12-C11-C10	2.03	120.59	113.13	9	1
4	A	382	PX4	C25-C24-C23	2.03	121.14	113.69	8	1
4	A	391	PX4	C5-N1-C2	2.03	117.98	109.91	6	1
4	A	420	PX4	C27-C26-C25	2.03	104.10	114.37	12	1
4	A	337	PX4	O1-P1-O3	2.03	98.37	107.57	3	1
4	A	349	PX4	C25-C24-C23	2.03	106.25	113.69	14	1
4	A	402	PX4	C33-C32-C31	2.03	104.11	114.37	5	1
4	A	352	PX4	O6-C9-C10	2.03	115.85	123.78	6	1
4	A	357	PX4	O4-P1-O2	2.03	100.89	108.94	8	1
4	A	392	PX4	C36-C35-C34	2.03	99.66	113.36	9	1
4	A	365	PX4	C32-C31-C30	2.03	104.12	114.37	10	1
4	A	370	PX4	C27-C26-C25	2.03	104.12	114.37	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	406	PX4	C8-O5-C9	2.03	109.70	117.12	6	1
4	A	321	PX4	C27-C26-C25	2.03	104.12	114.37	13	1
4	A	327	PX4	C25-C24-C23	2.03	121.12	113.69	13	1
4	A	369	PX4	O3-P1-O2	2.03	116.97	108.94	3	2
4	A	402	PX4	O8-C23-C24	2.03	115.86	123.78	7	1
4	A	409	PX4	C11-C10-C9	2.03	121.12	113.69	7	1
4	A	338	PX4	C5-N1-C2	2.02	101.87	109.91	5	1
4	A	353	PX4	C7-O7-C23	2.02	112.95	117.80	2	1
4	A	371	PX4	C31-C30-C29	2.02	104.14	114.37	7	1
4	A	375	PX4	C3-N1-C2	2.02	101.86	109.91	4	1
4	A	385	PX4	C32-C31-C30	2.02	104.14	114.37	2	1
4	A	418	PX4	O4-P1-O2	2.02	100.91	108.94	5	1
4	A	323	PX4	C30-C29-C28	2.02	104.14	114.37	12	1
4	A	369	PX4	O5-C9-C10	2.02	118.00	111.83	13	1
4	A	420	PX4	C18-C17-C16	2.02	104.14	114.37	14	1
4	A	381	PX4	C20-C19-C18	2.02	104.15	114.37	4	1
4	A	392	PX4	C4-N1-C2	2.02	117.95	109.91	2	1
4	A	398	PX4	C31-C30-C29	2.02	104.15	114.37	11	1
4	A	309	PX4	C19-C18-C17	2.02	104.15	114.37	4	1
4	A	408	PX4	C20-C19-C18	2.02	104.15	114.37	9	1
4	A	369	PX4	C22-C21-C20	2.02	99.73	113.36	9	1
4	A	375	PX4	C15-C14-C13	2.02	104.16	114.37	11	1
4	A	411	PX4	C29-C28-C27	2.02	104.15	114.37	2	1
4	A	361	PX4	C21-C20-C19	2.02	97.53	115.25	5	1
4	A	383	PX4	C27-C26-C25	2.02	104.16	114.37	9	1
4	A	415	PX4	C20-C19-C18	2.02	104.16	114.37	9	1
4	A	318	PX4	C30-C29-C28	2.02	104.17	114.37	11	1
4	A	358	PX4	C28-C27-C26	2.02	104.16	114.37	1	1
4	A	405	PX4	C15-C14-C13	2.02	104.16	114.37	11	1
4	A	421	PX4	O6-C9-C10	2.02	115.89	123.78	1	1
4	A	364	PX4	C20-C19-C18	2.02	104.17	114.37	9	1
4	A	306	PX4	C13-C12-C11	2.02	104.17	114.37	7	1
4	A	384	PX4	C15-C14-C13	2.02	104.17	114.37	14	1
4	A	392	PX4	C29-C28-C27	2.02	104.17	114.37	9	1
4	A	307	PX4	O7-C7-C6	2.02	115.58	108.34	12	1
4	A	418	PX4	C5-N1-C4	2.02	114.27	108.98	1	1
4	A	308	PX4	C13-C12-C11	2.01	104.18	114.37	8	1
4	A	309	PX4	C29-C28-C27	2.01	104.18	114.37	13	1
4	A	312	PX4	C14-C13-C12	2.02	104.18	114.37	14	1
4	A	333	PX4	C11-C10-C9	2.02	106.31	113.69	3	1
4	A	333	PX4	C28-C27-C26	2.02	104.18	114.37	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	336	PX4	O1-P1-O4	2.01	116.70	107.57	5	1
4	A	362	PX4	C34-C33-C32	2.02	104.18	114.37	10	1
4	A	403	PX4	C28-C27-C26	2.01	104.18	114.37	13	1
4	A	405	PX4	C30-C29-C28	2.01	104.19	114.37	14	1
4	A	408	PX4	O6-C9-C10	2.01	115.91	123.78	5	1
4	A	427	PX4	C15-C14-C13	2.01	104.18	114.37	14	1
4	A	325	PX4	C20-C19-C18	2.01	104.19	114.37	2	1
4	A	354	PX4	C3-N1-C2	2.01	117.92	109.91	1	1
4	A	368	PX4	C30-C29-C28	2.01	104.19	114.37	10	1
4	A	369	PX4	C4-N1-C2	2.01	117.91	109.91	13	1
4	A	417	PX4	C18-C17-C16	2.01	104.19	114.37	6	1
4	A	421	PX4	C18-C17-C16	2.01	104.19	114.37	14	1
4	A	308	PX4	C28-C27-C26	2.01	104.20	114.37	11	1
4	A	379	PX4	C16-C15-C14	2.01	104.20	114.37	2	1
4	A	379	PX4	O1-P1-O3	2.01	98.45	107.57	11	1
4	A	387	PX4	C3-N1-C2	2.01	117.91	109.91	11	1
4	A	306	PX4	C17-C16-C15	2.01	104.20	114.37	5	1
4	A	365	PX4	O1-P1-O4	2.01	116.68	107.57	7	1
4	A	386	PX4	C12-C11-C10	2.01	105.74	113.13	3	1
4	A	414	PX4	C34-C33-C32	2.01	104.20	114.37	11	1
4	A	323	PX4	C15-C14-C13	2.01	104.21	114.37	1	1
4	A	342	PX4	O8-C23-C24	2.01	115.92	123.78	14	1
4	A	370	PX4	C34-C33-C32	2.01	104.21	114.37	9	1
4	A	384	PX4	O3-P1-O2	2.01	100.97	108.94	12	1
4	A	307	PX4	O8-C23-C24	2.01	131.63	123.78	7	1
4	A	349	PX4	C17-C16-C15	2.01	104.22	114.37	10	1
4	A	363	PX4	O4-P1-O2	2.01	100.98	108.94	11	1
4	A	403	PX4	C19-C18-C17	2.01	104.22	114.37	1	1
4	A	430	PX4	C32-C31-C30	2.01	104.22	114.37	8	1
4	A	336	PX4	C16-C15-C14	2.01	104.23	114.37	10	1
4	A	346	PX4	C28-C27-C26	2.01	104.23	114.37	12	1
4	A	362	PX4	O3-C1-C2	2.01	119.30	109.65	13	1
4	A	388	PX4	C31-C30-C29	2.01	104.23	114.37	6	1
4	A	389	PX4	C8-O5-C9	2.01	124.45	117.12	12	1
4	A	412	PX4	C29-C28-C27	2.01	104.23	114.37	1	1
4	A	426	PX4	C14-C13-C12	2.01	104.23	114.37	2	1
4	A	358	PX4	C27-C26-C25	2.00	104.24	114.37	2	1
4	A	359	PX4	C19-C18-C17	2.00	104.24	114.37	9	1
4	A	403	PX4	C30-C29-C28	2.00	104.24	114.37	7	1
4	A	312	PX4	C20-C19-C18	2.00	104.25	114.37	13	1
4	A	315	PX4	O5-C9-O6	2.00	118.62	123.63	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	317	PX4	C28-C27-C26	2.00	104.25	114.37	14	1
4	A	420	PX4	C35-C34-C33	2.00	97.70	115.25	4	1
4	A	430	PX4	O8-C23-C24	2.00	115.95	123.78	4	1
4	A	316	PX4	C19-C18-C17	2.00	104.26	114.37	9	1
4	A	361	PX4	C15-C14-C13	2.00	104.25	114.37	14	1
4	A	391	PX4	C3-N1-C2	2.00	101.95	109.91	11	1
4	A	351	PX4	C15-C14-C13	2.00	104.26	114.37	14	1
4	A	396	PX4	C32-C31-C30	2.00	104.26	114.37	14	1
4	A	401	PX4	C29-C28-C27	2.00	104.25	114.37	2	1

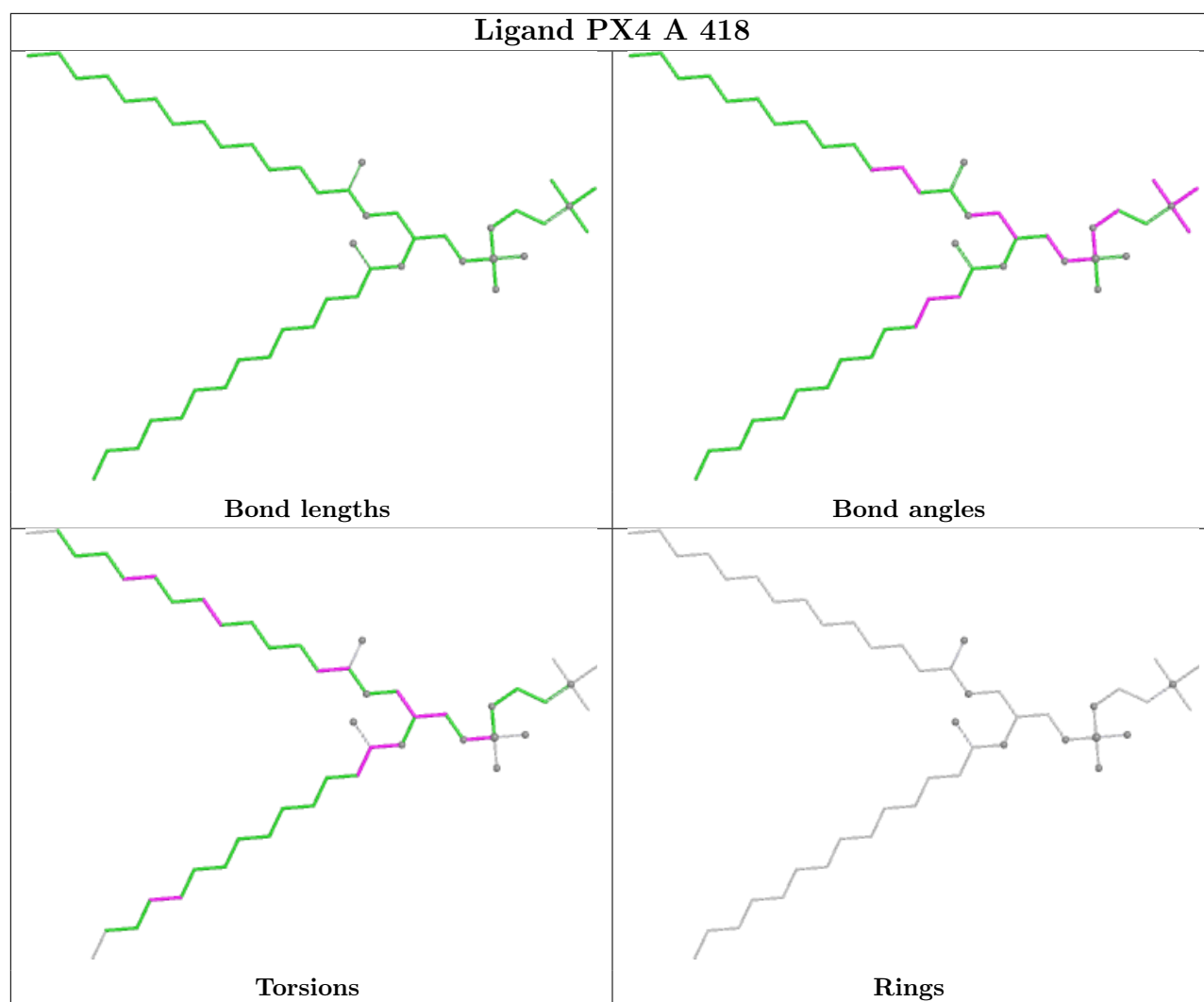
There are no chirality outliers.

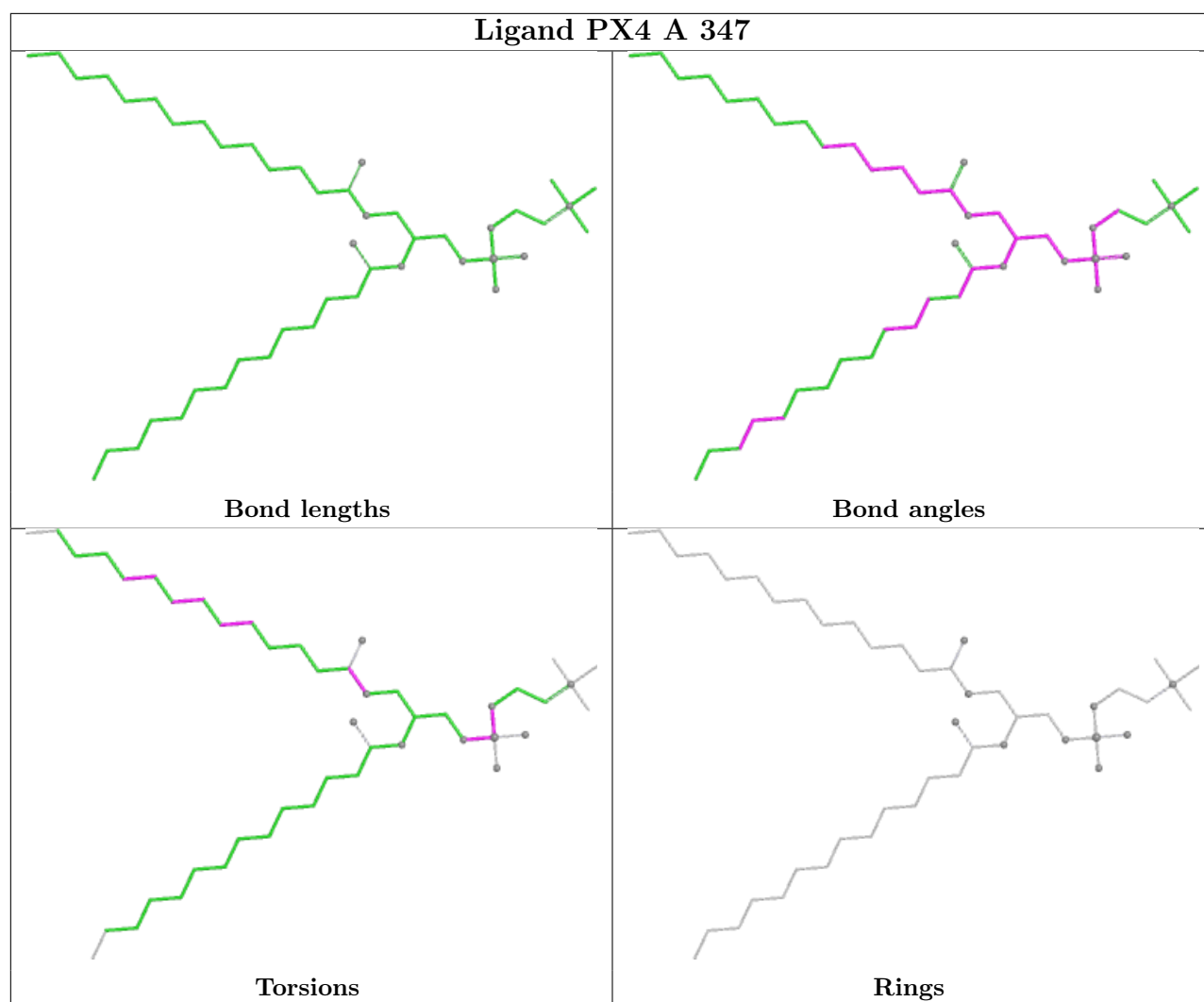
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

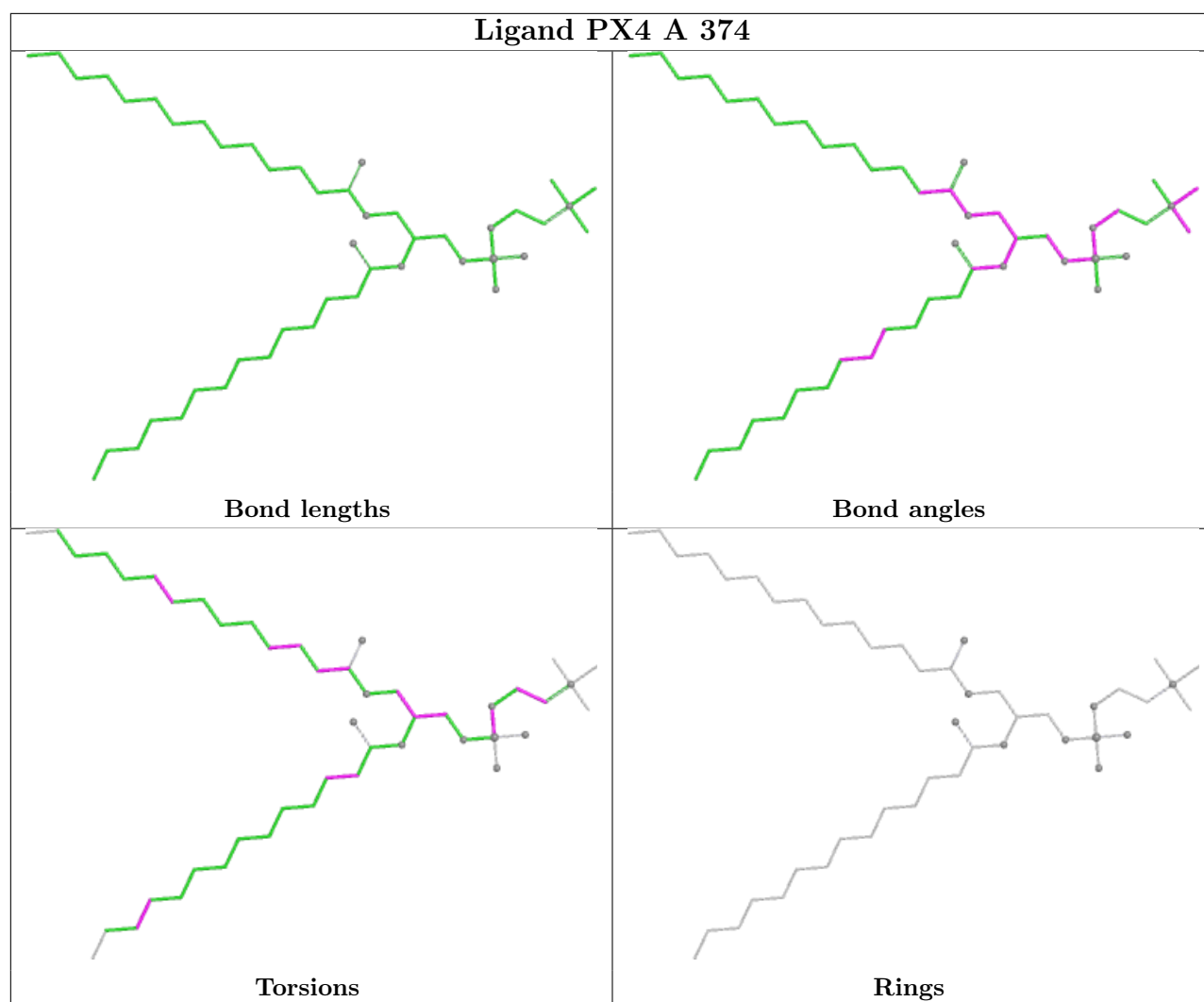
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	371	PX4	O8-C23-O7-C7	13
4	A	307	PX4	O8-C23-O7-C7	7

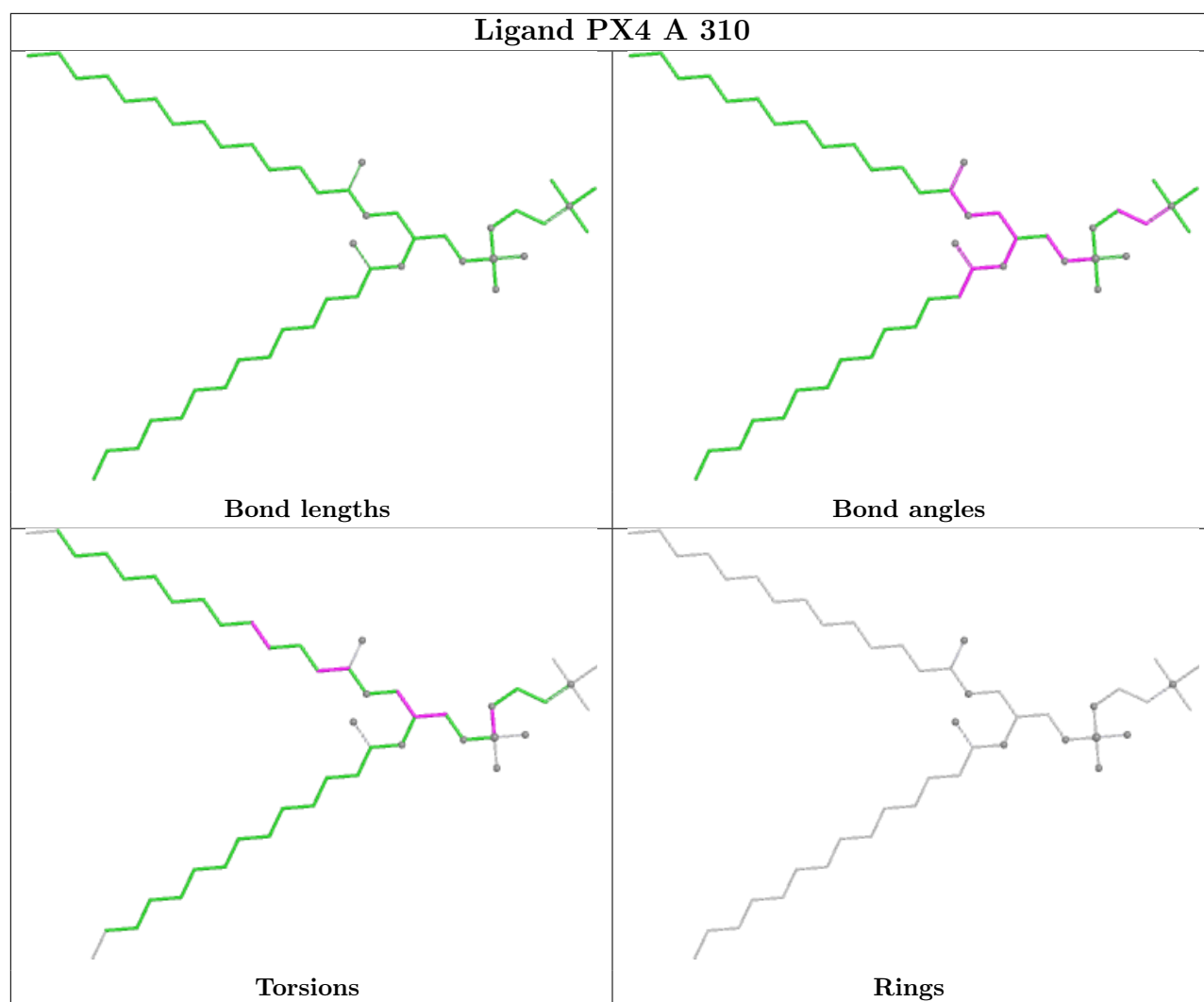
There are no ring outliers.

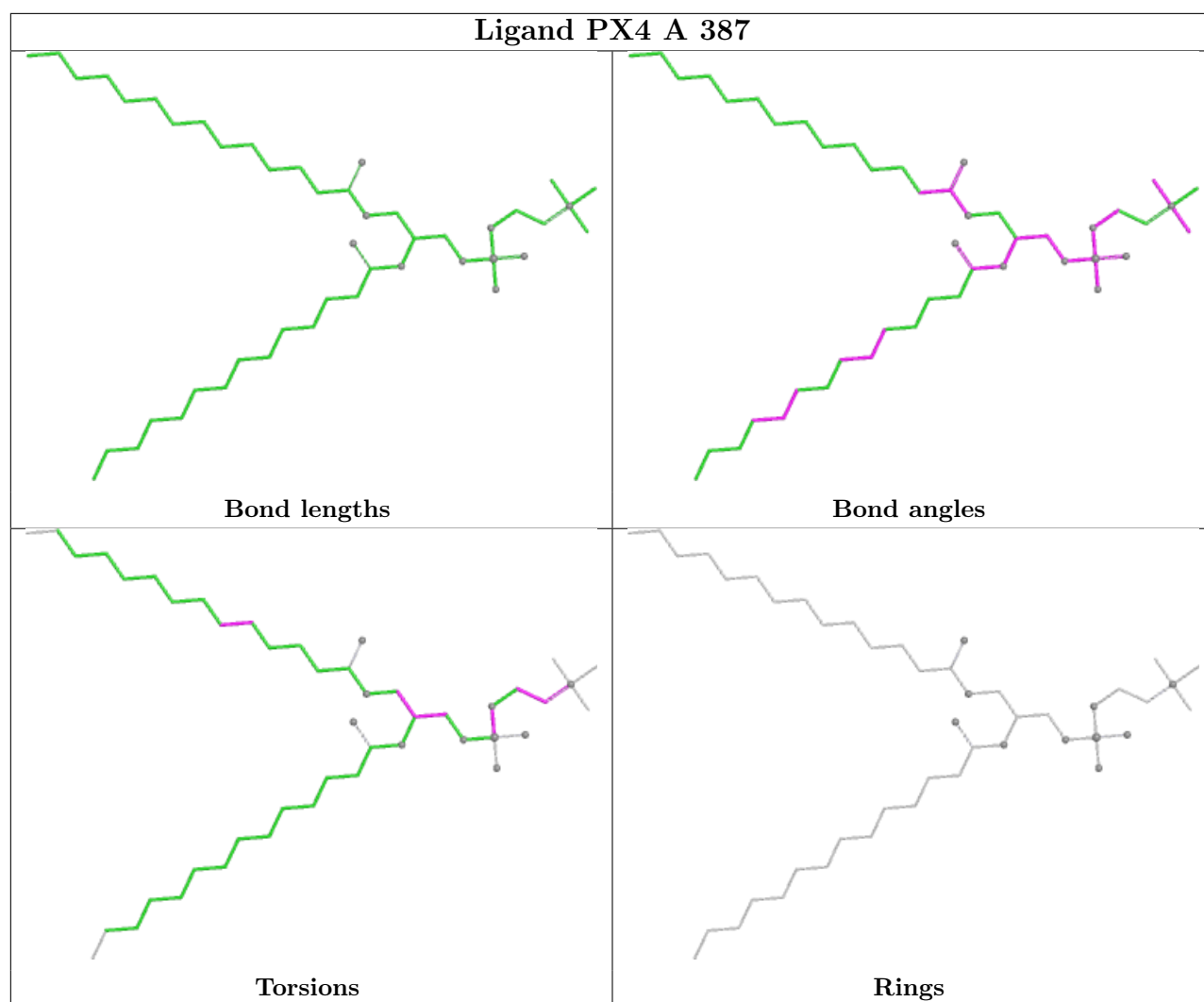
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

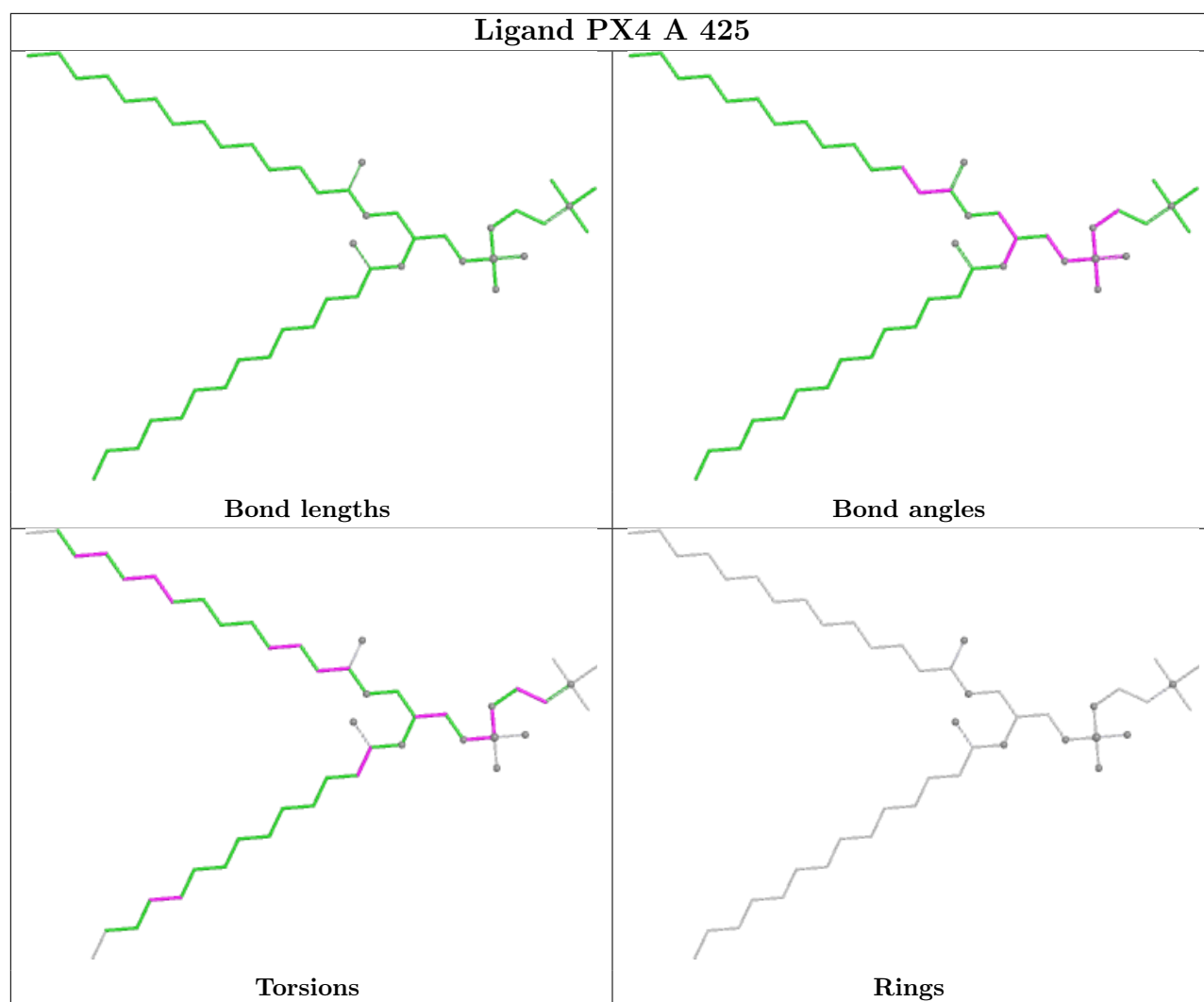


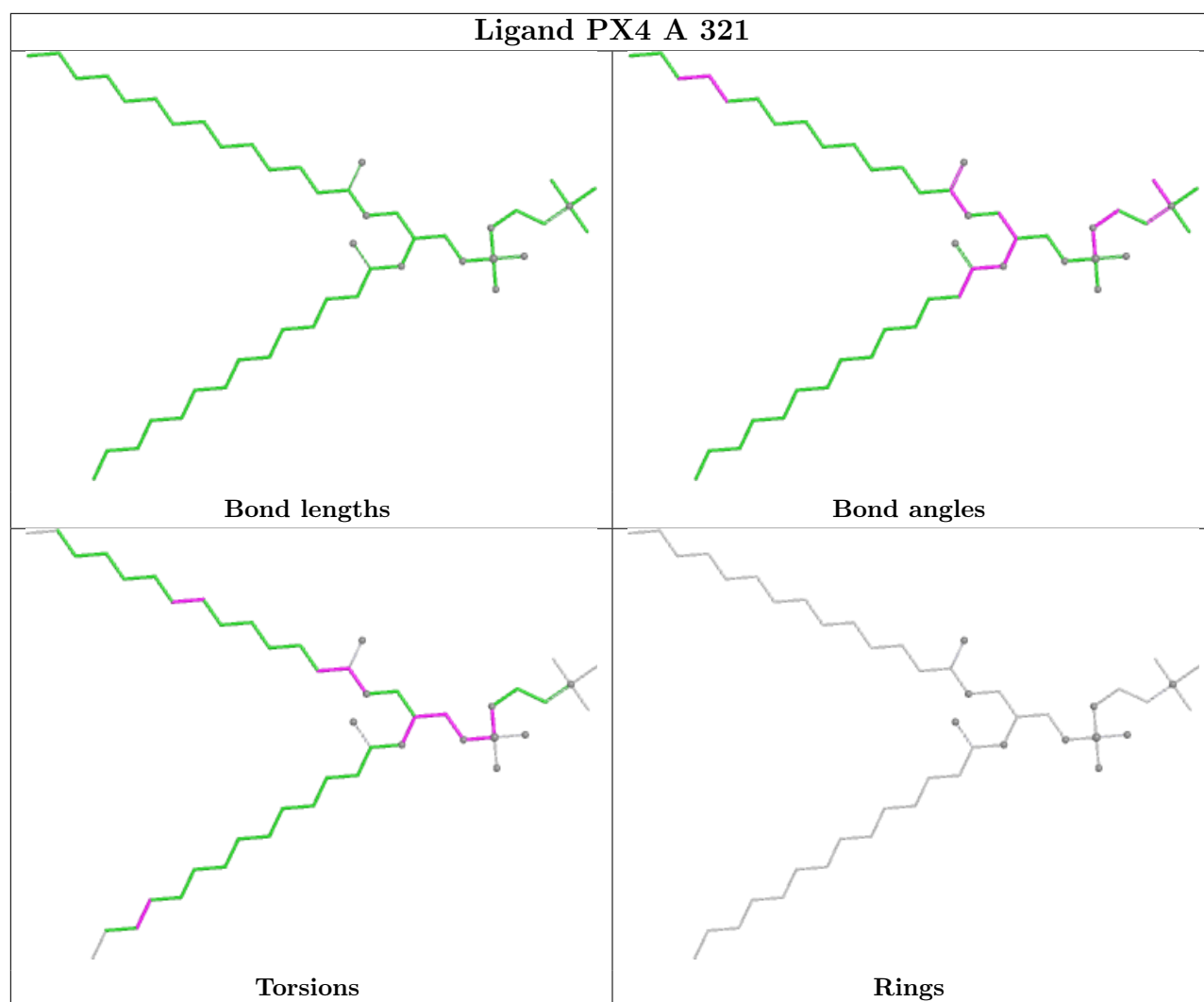


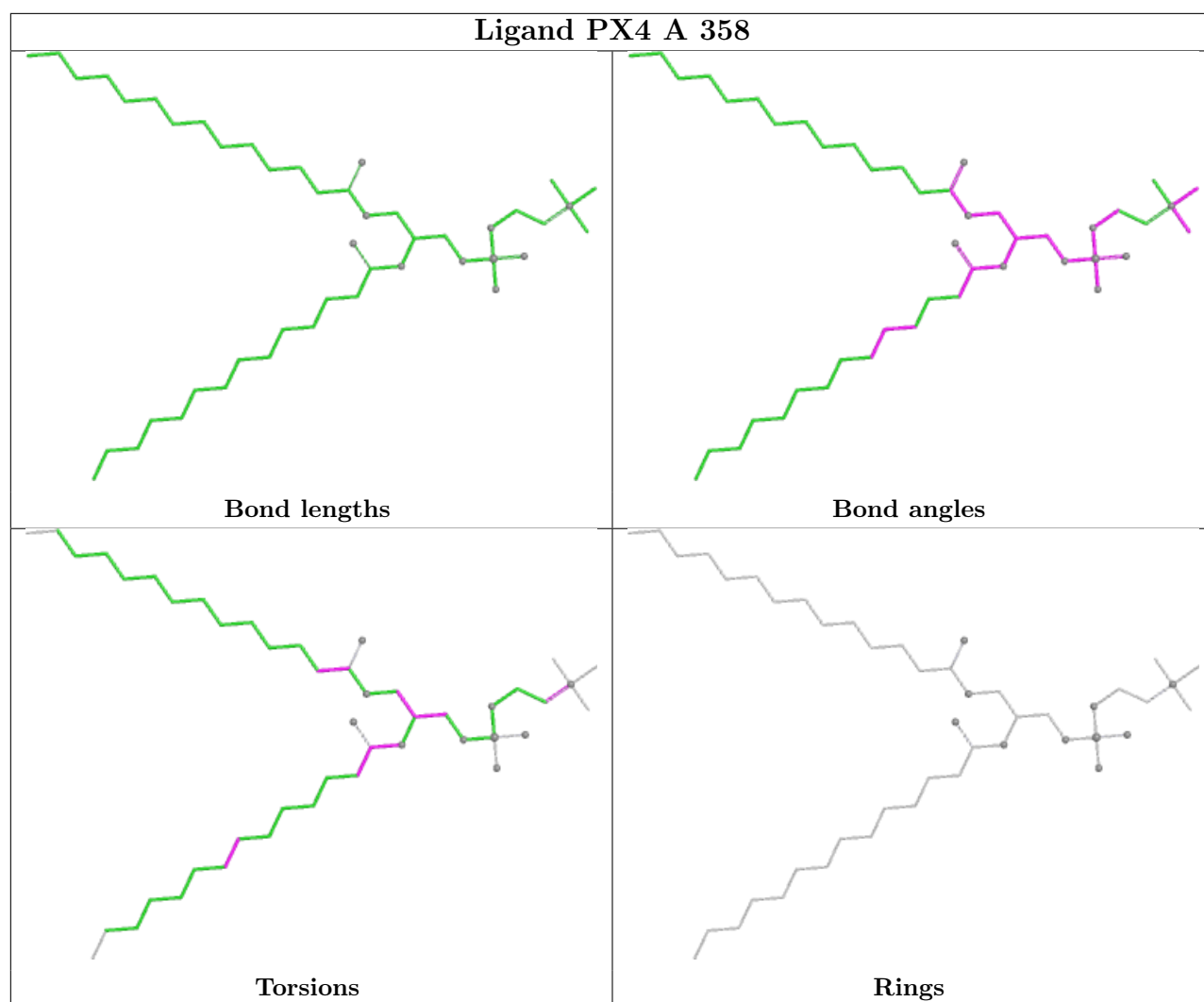


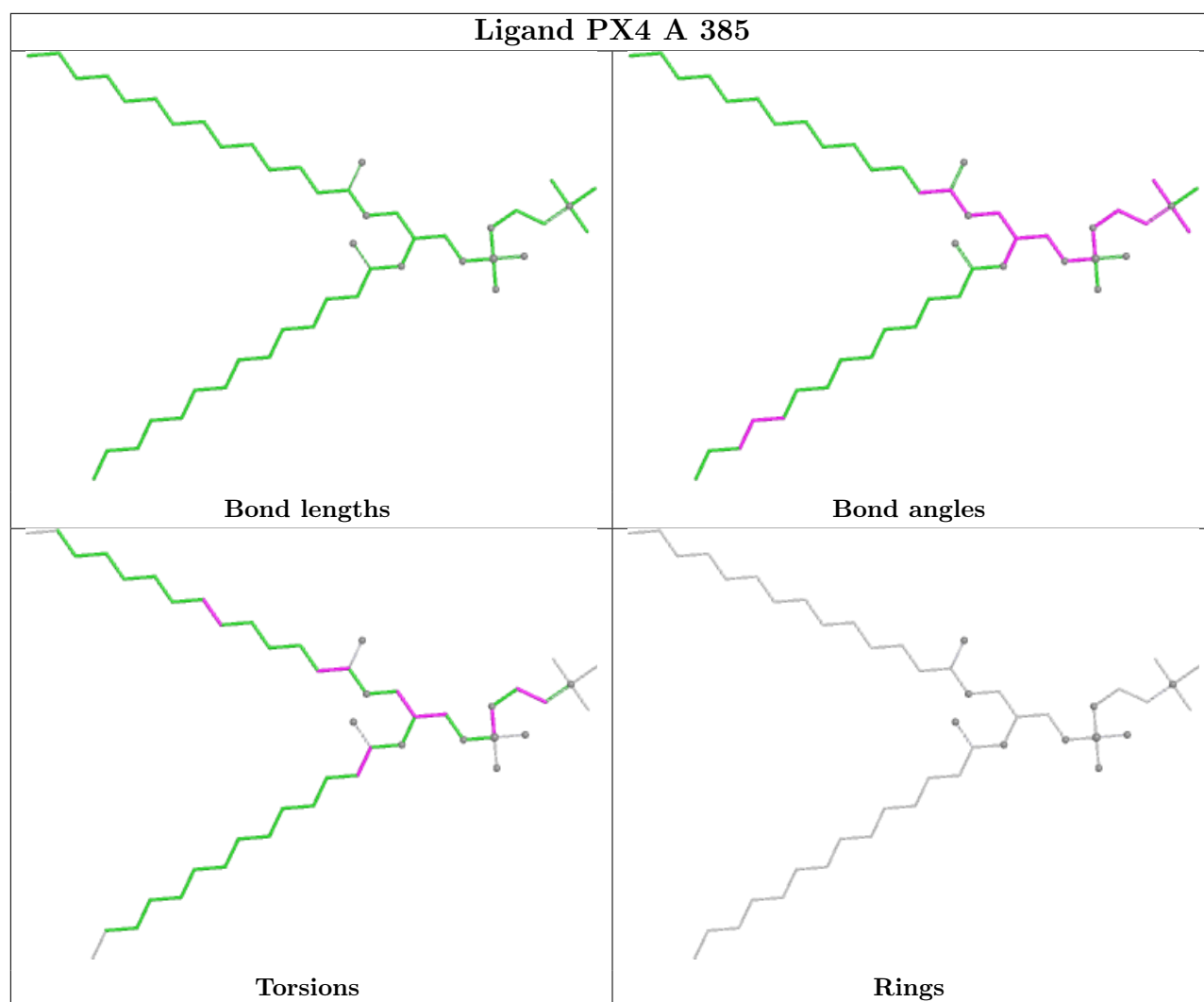


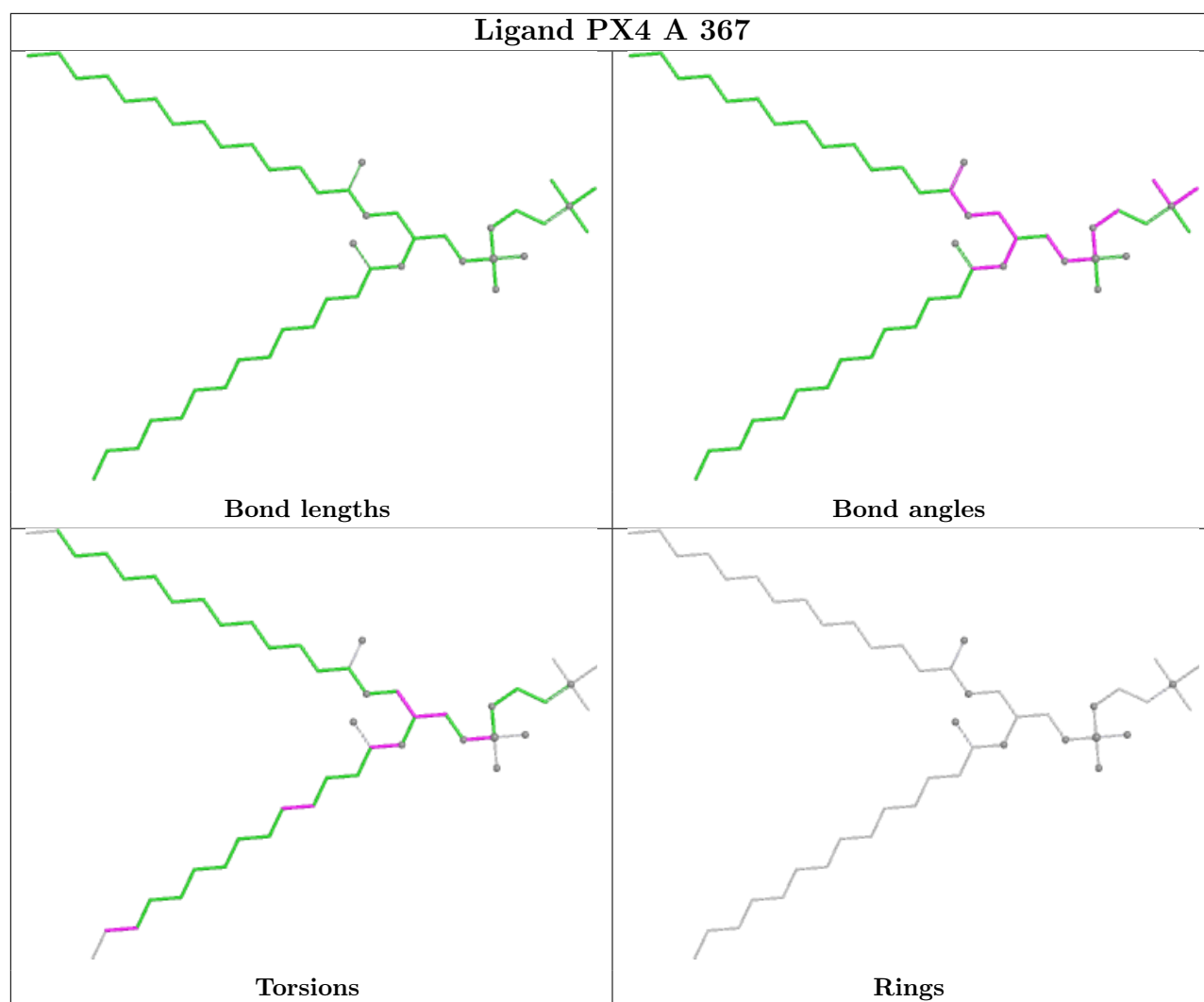


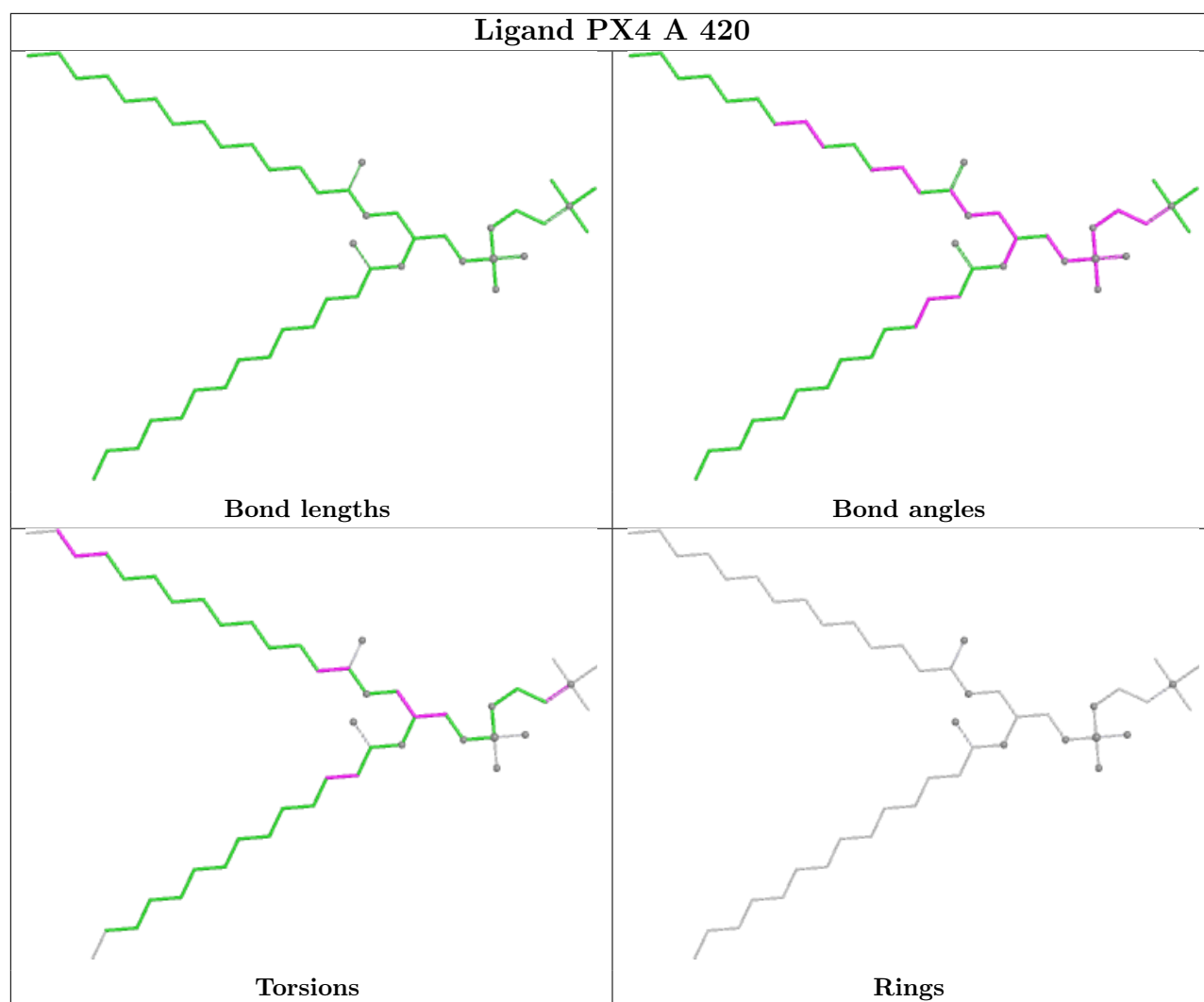


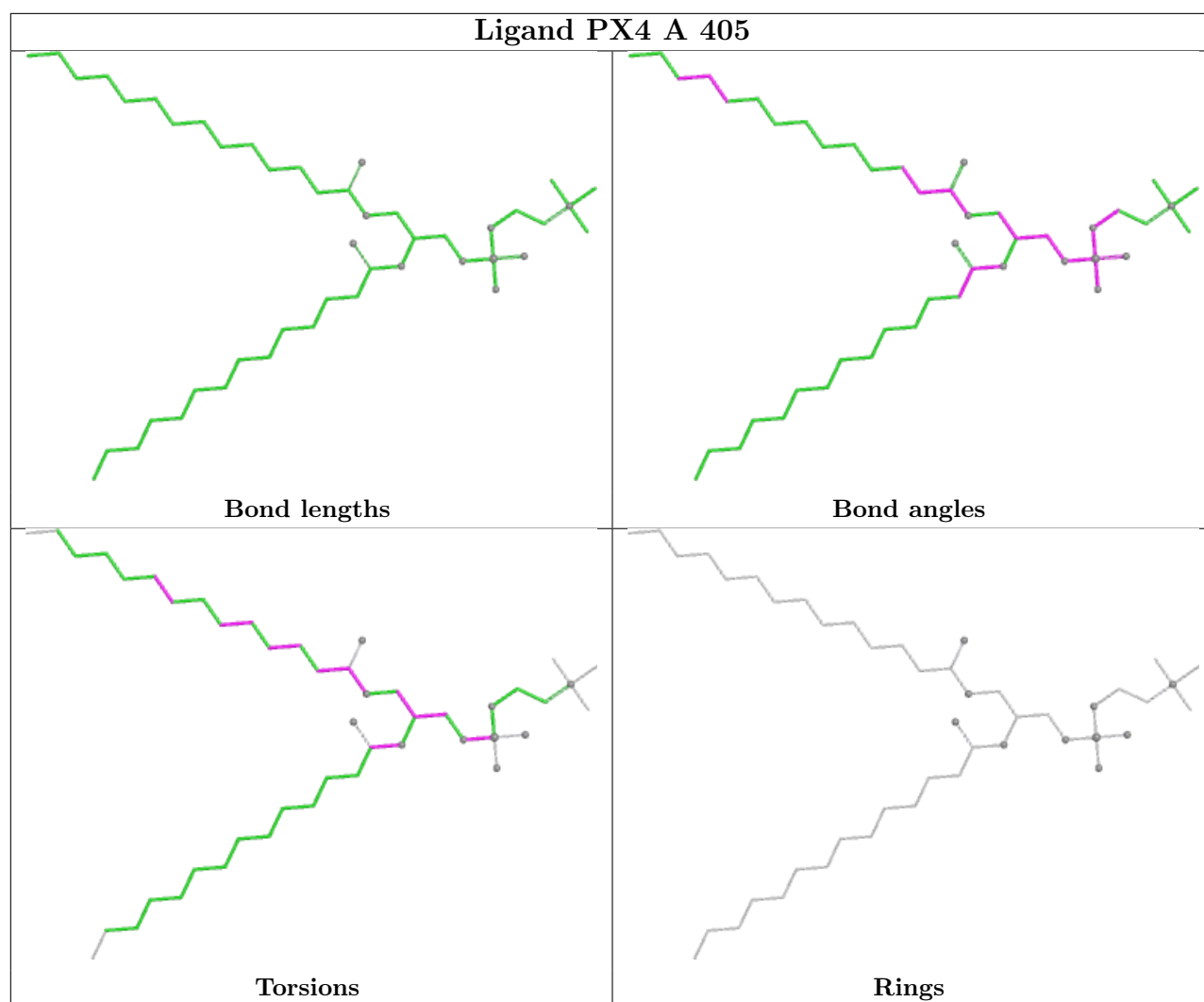


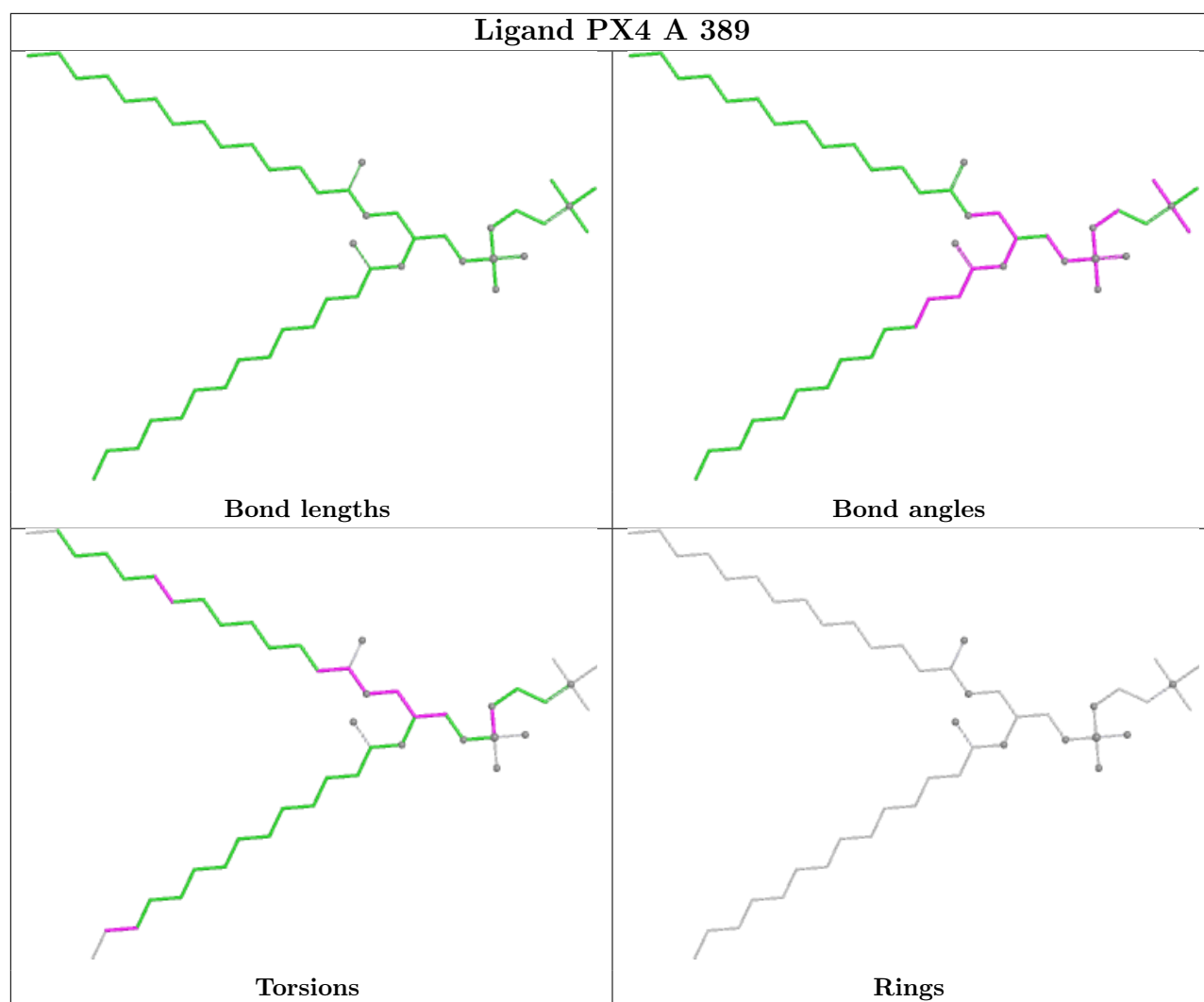


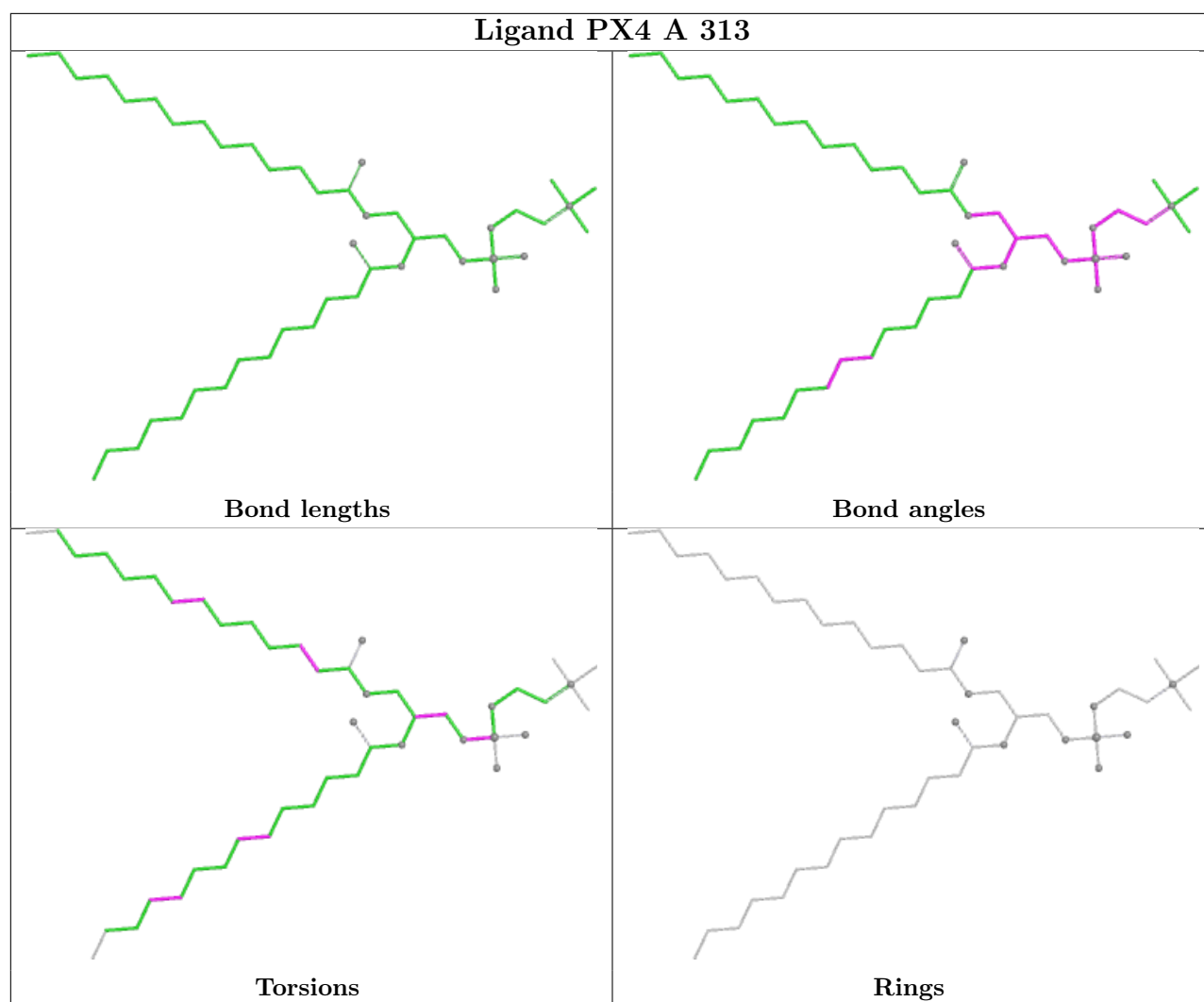


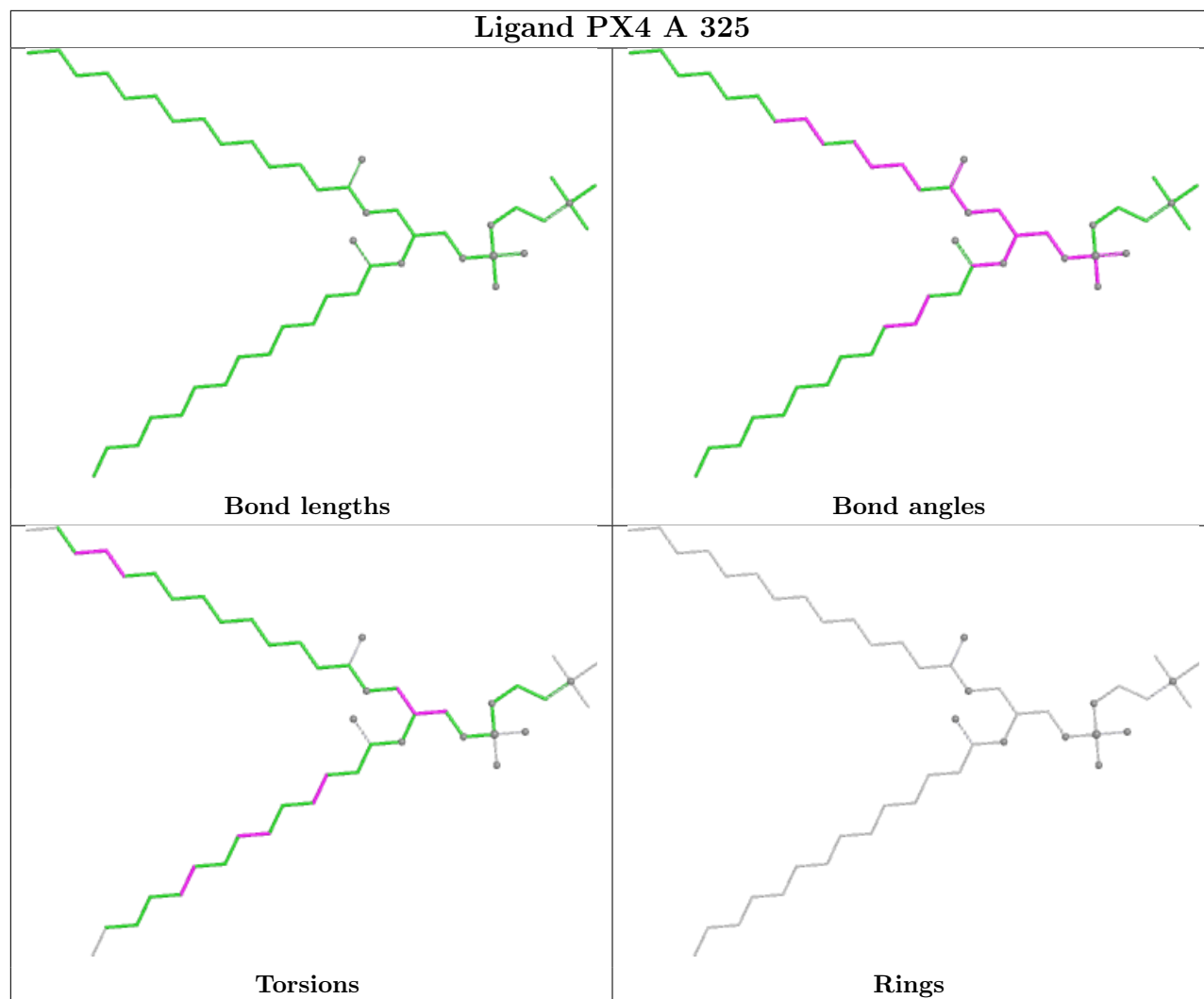


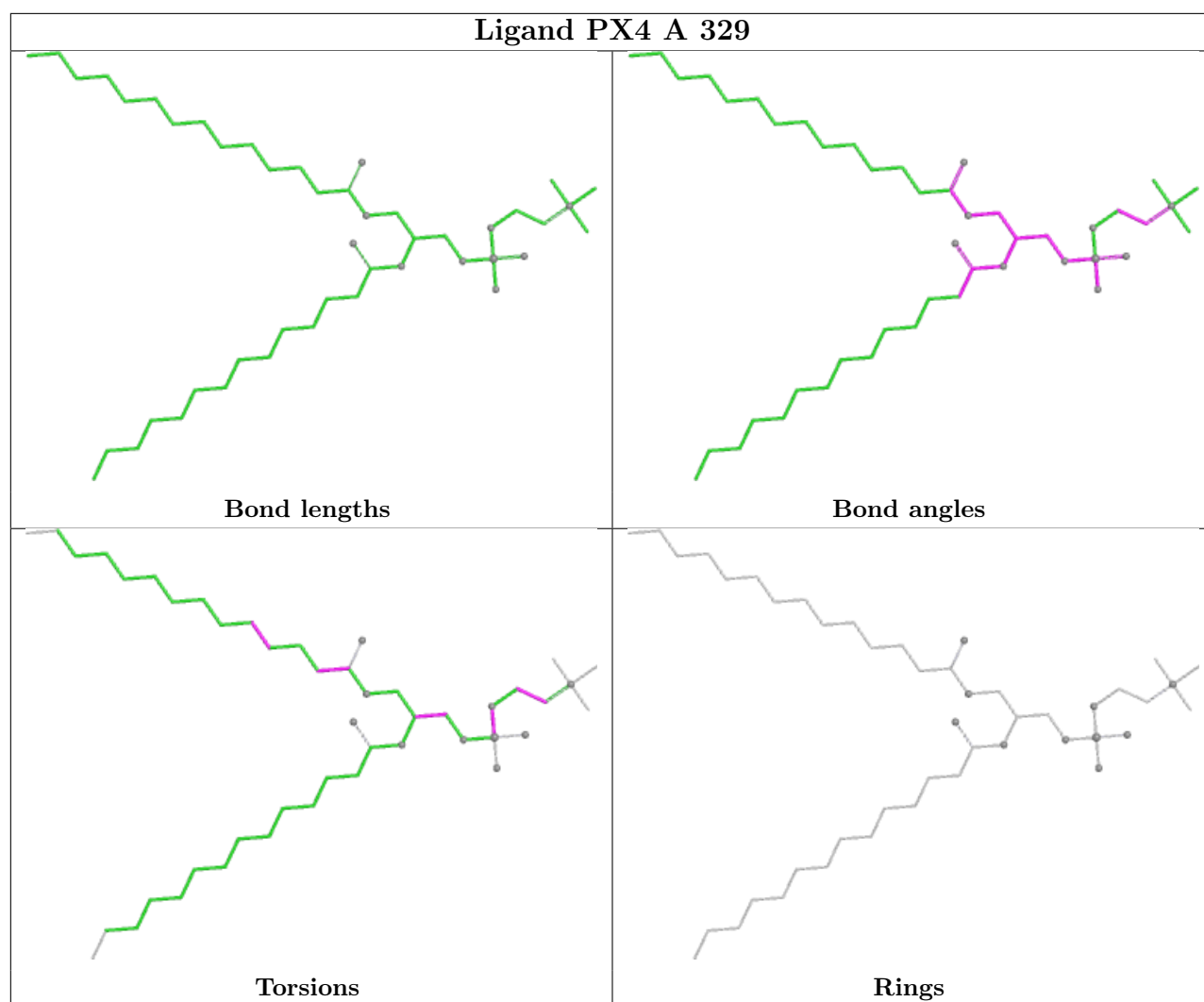


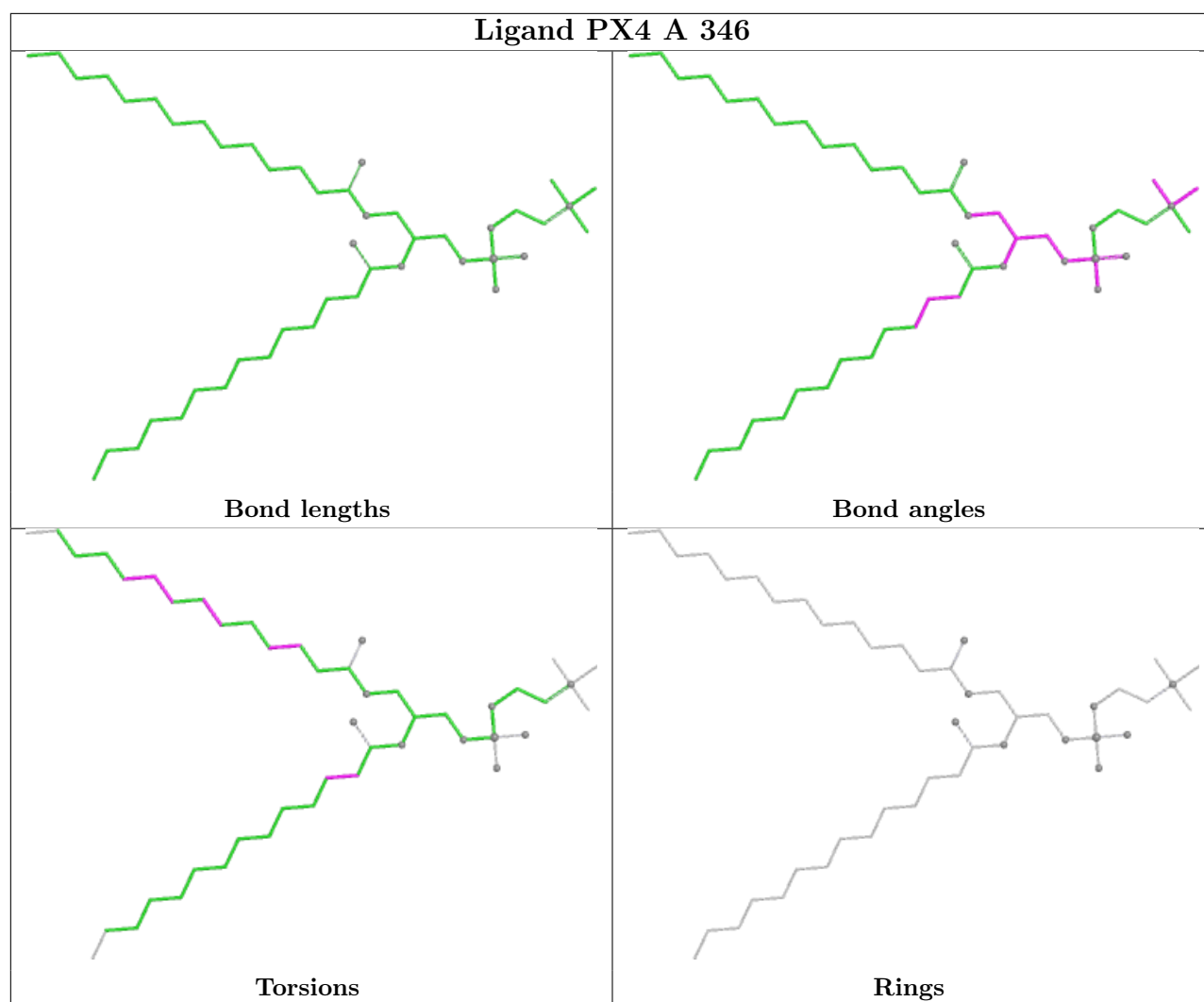


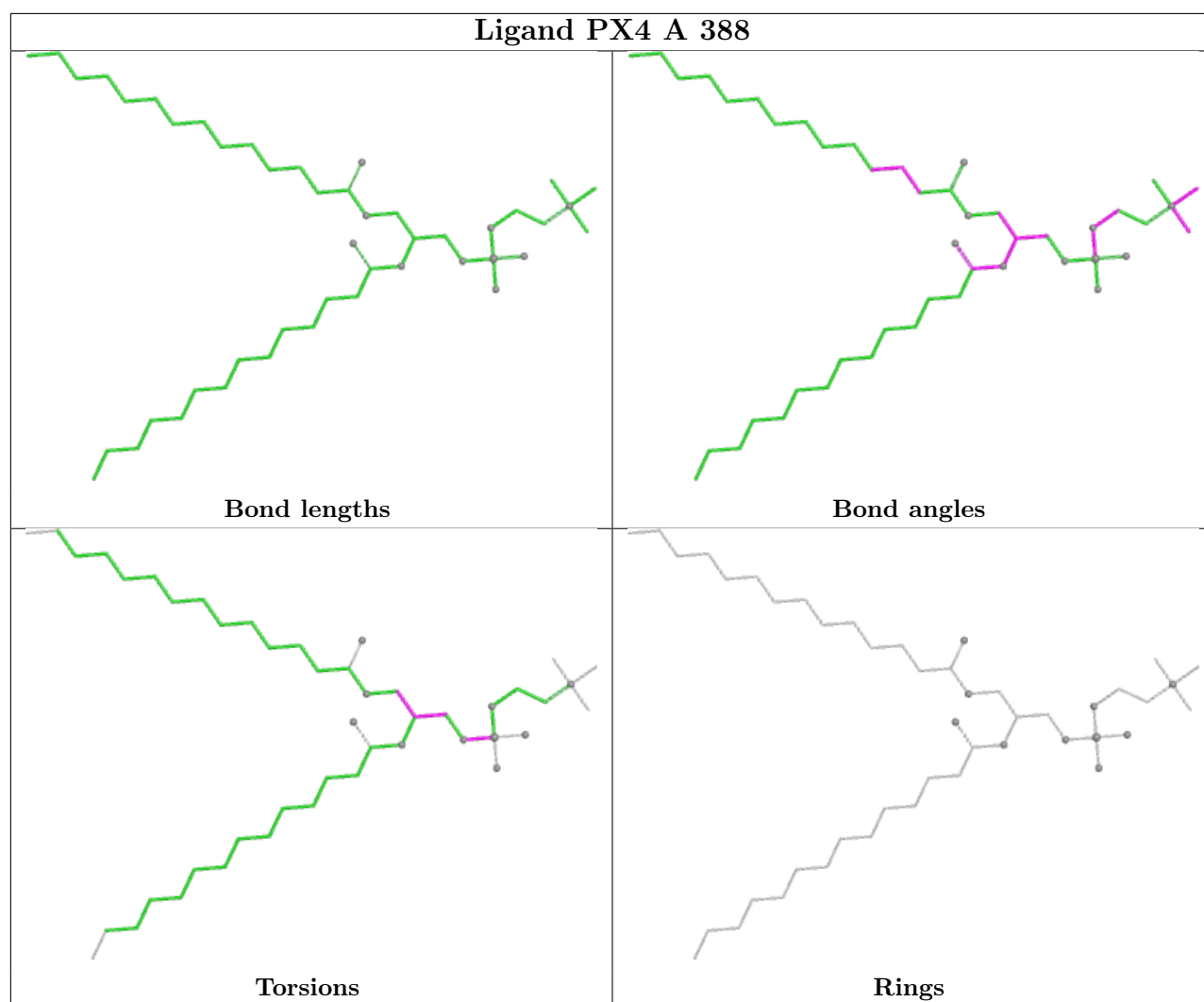


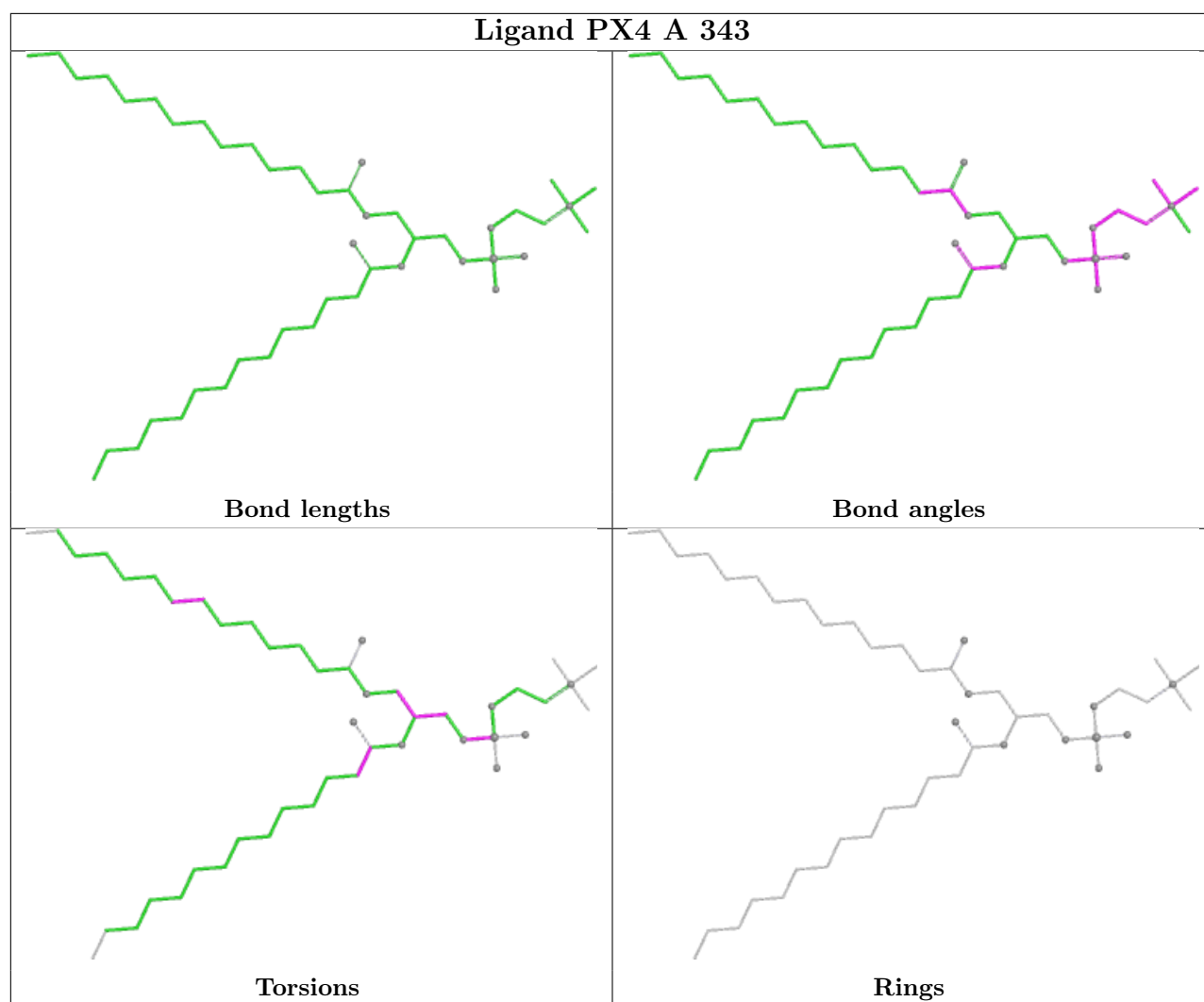


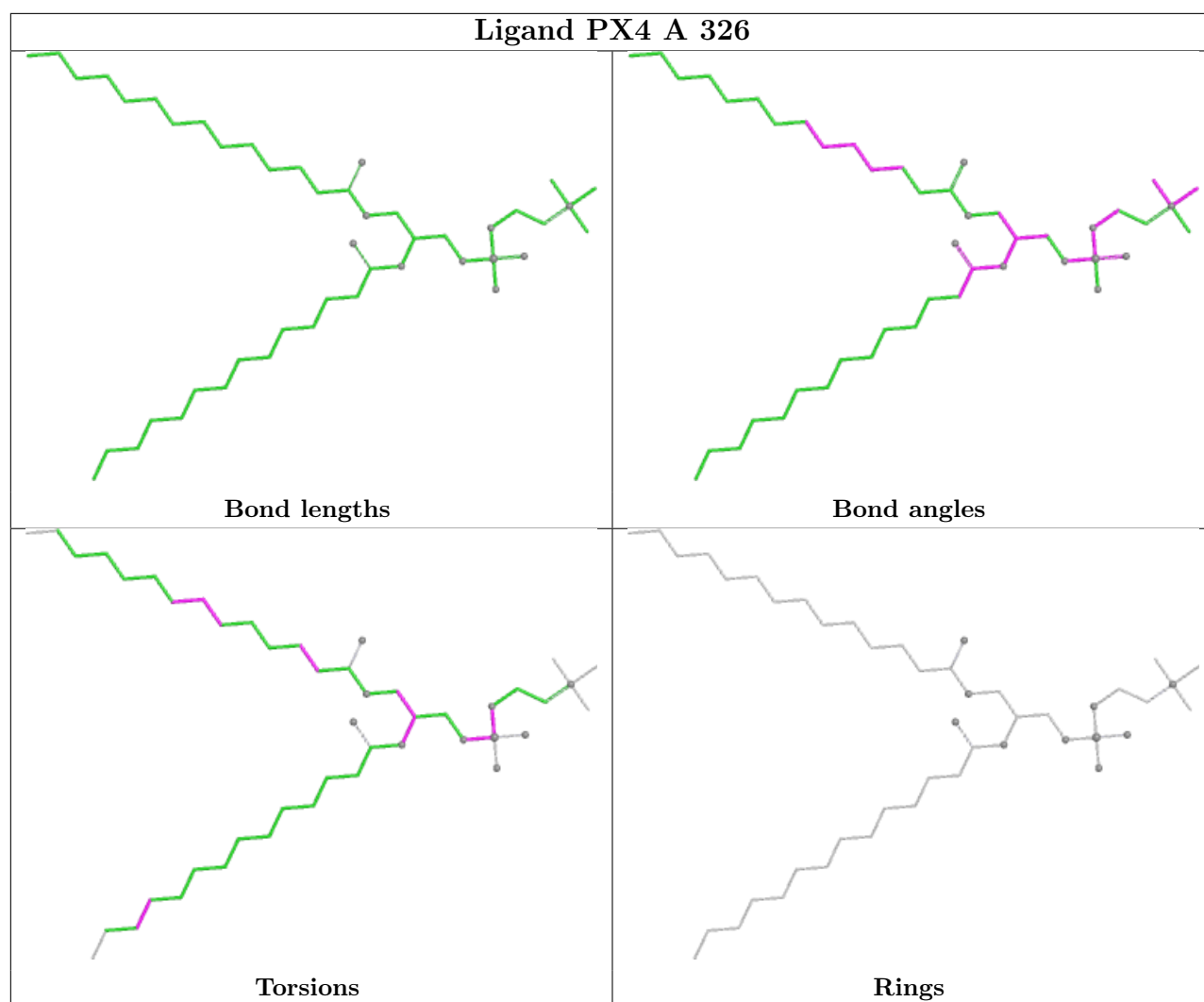


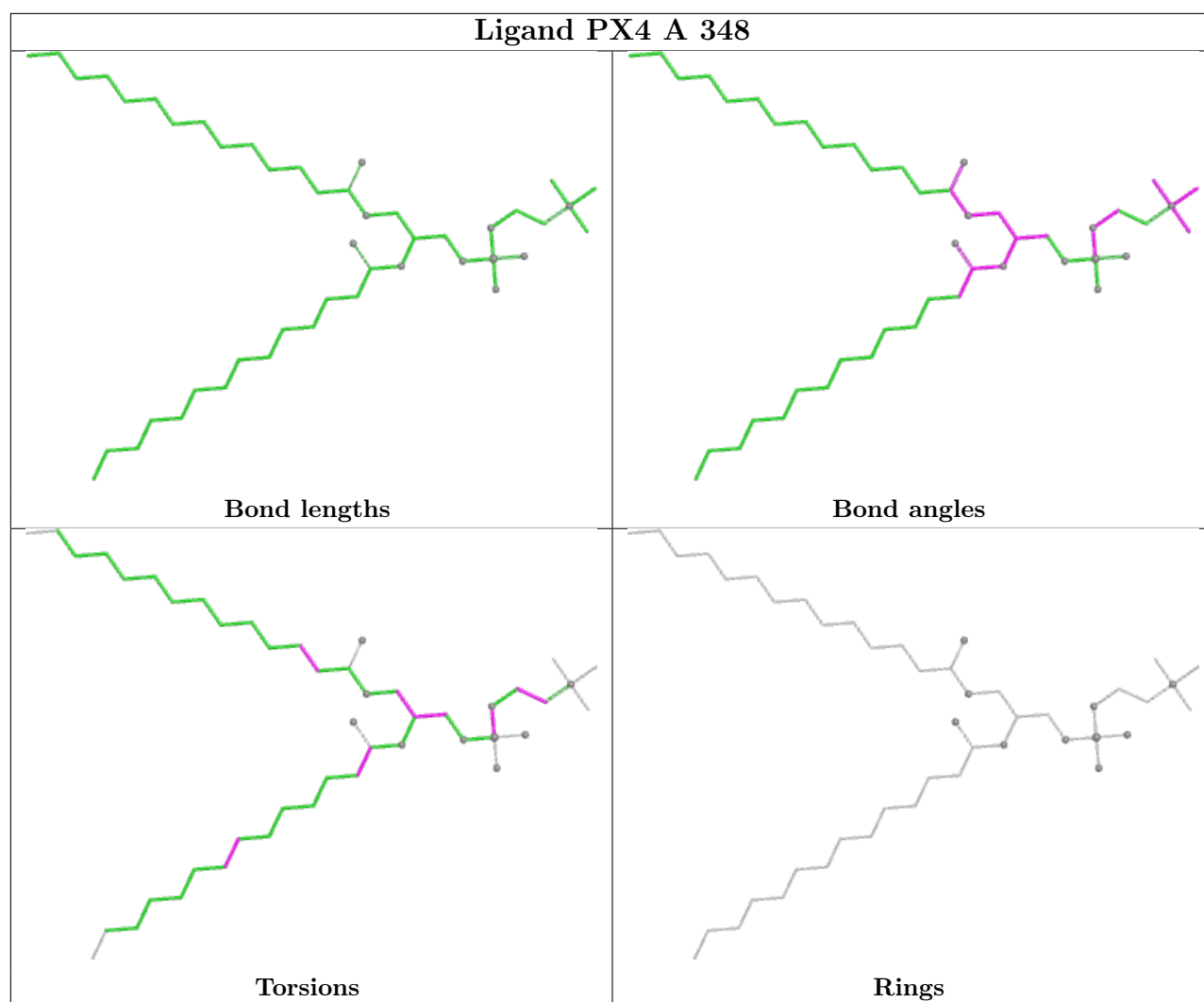


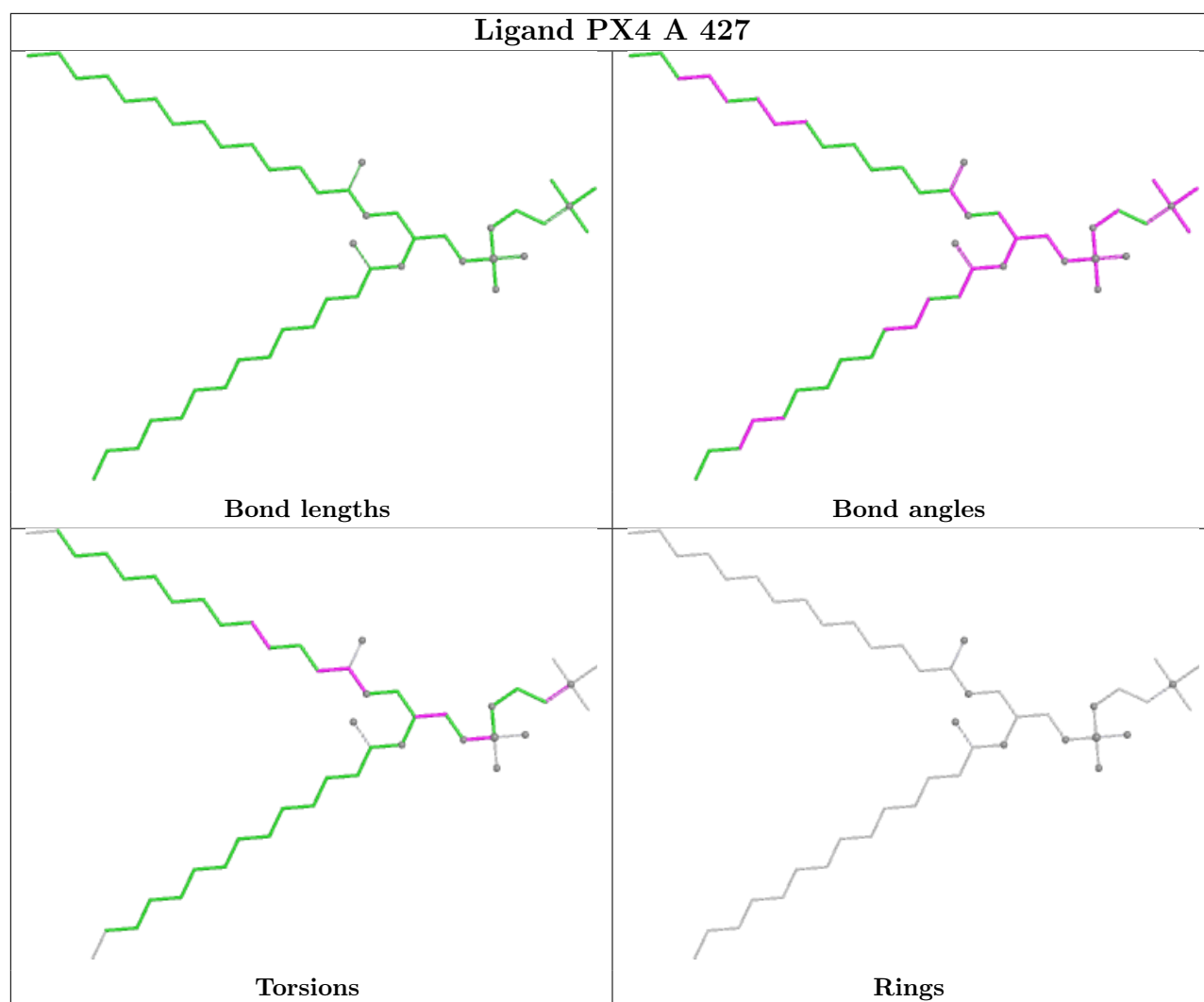


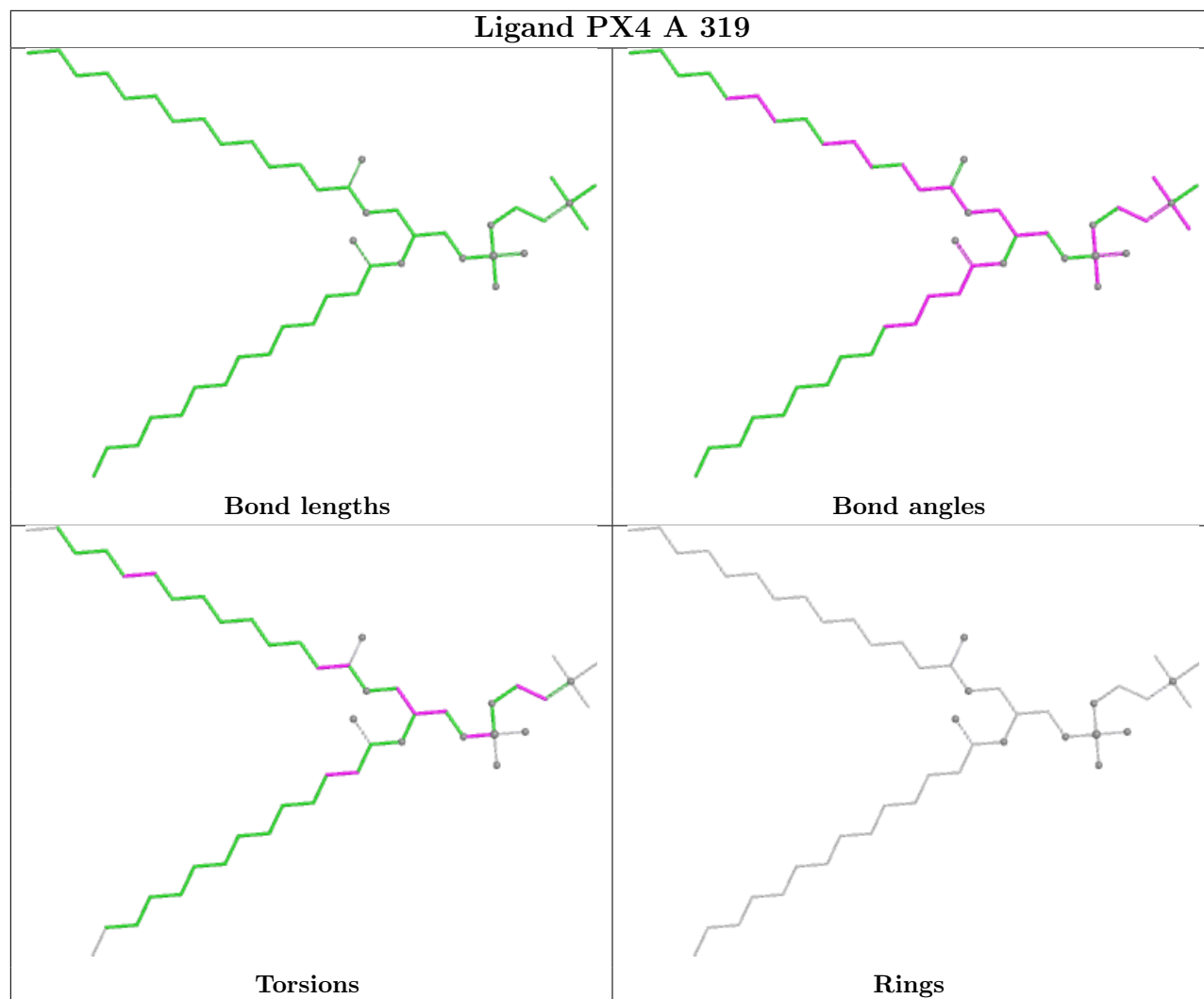


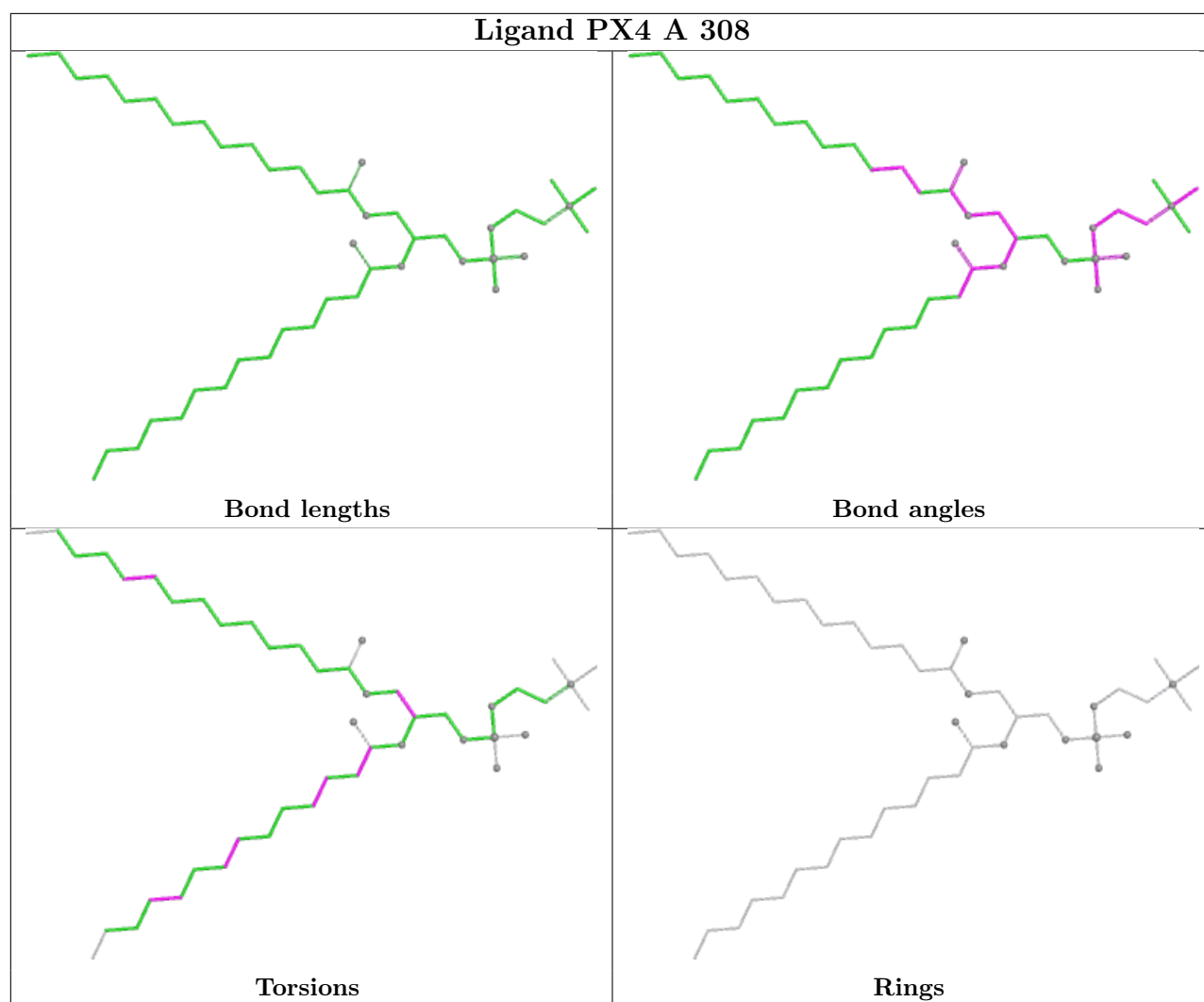


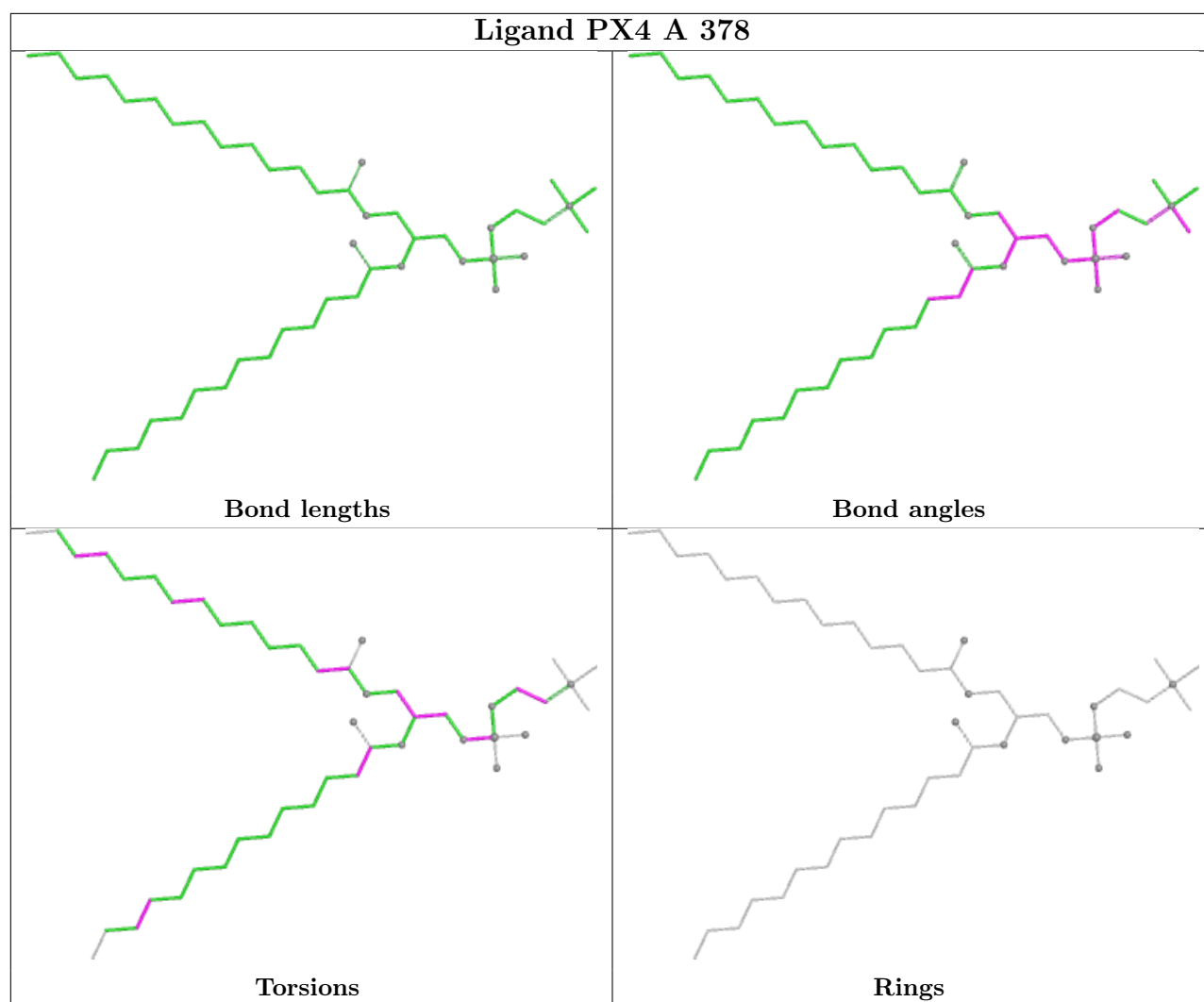


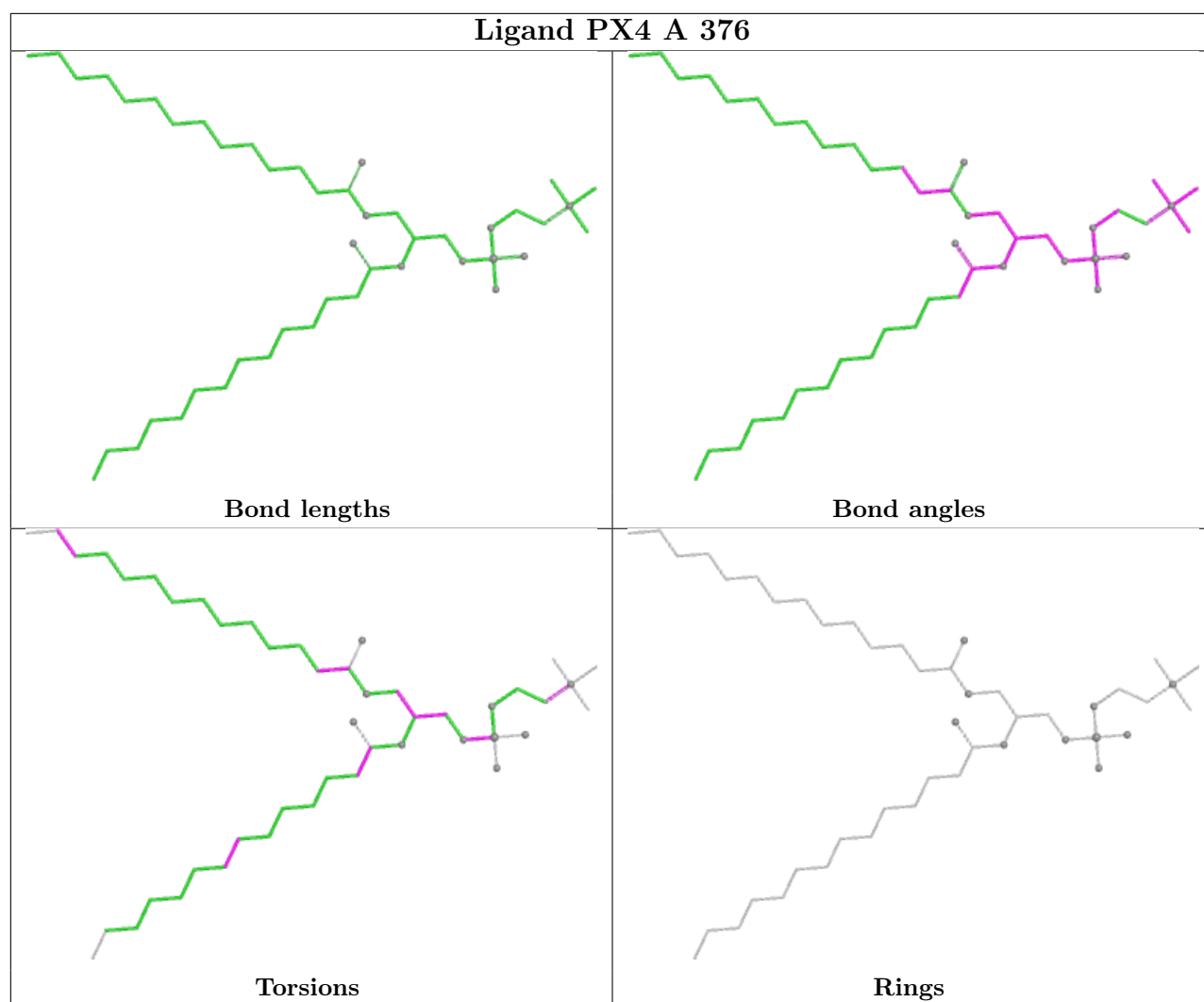


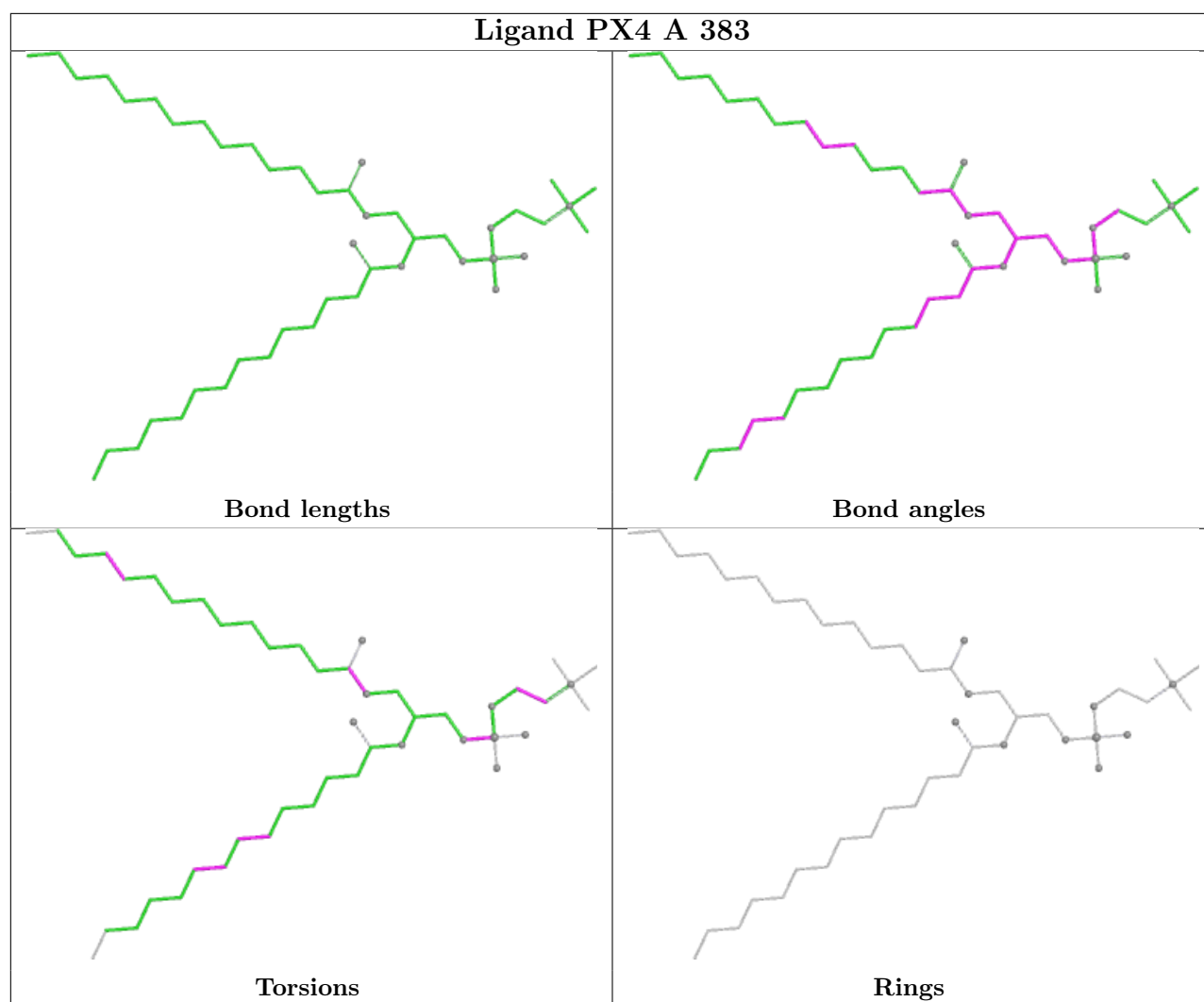


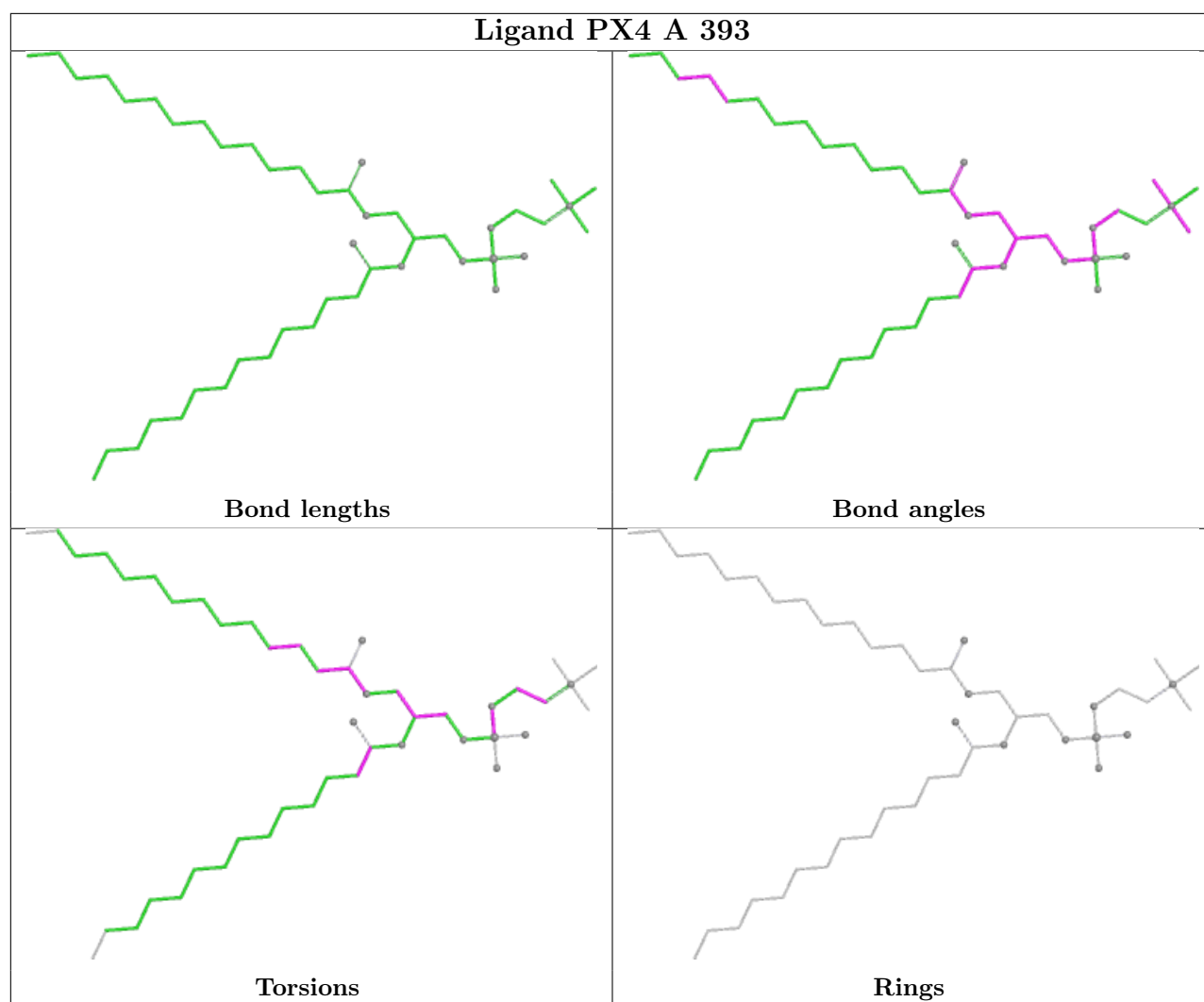


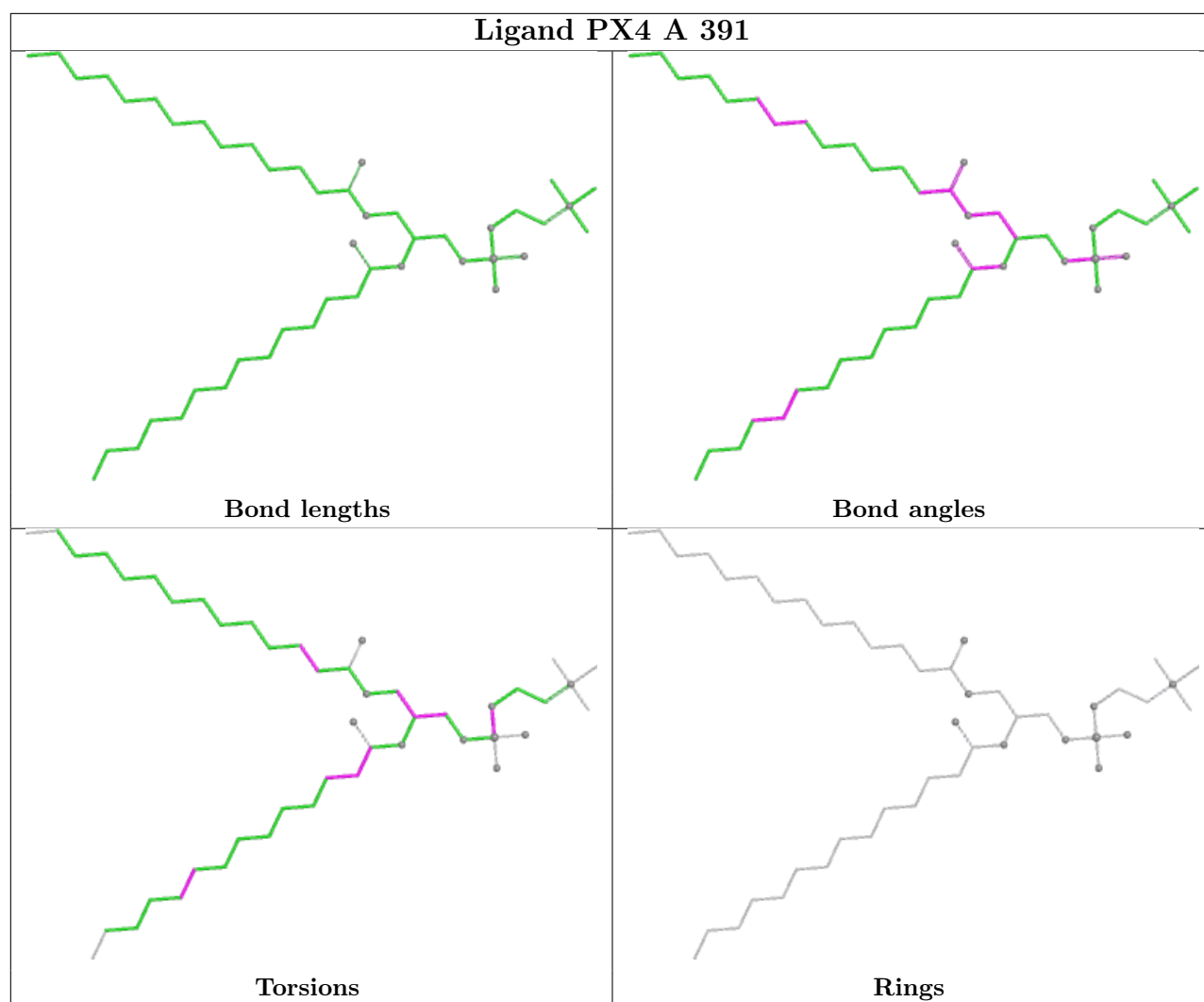


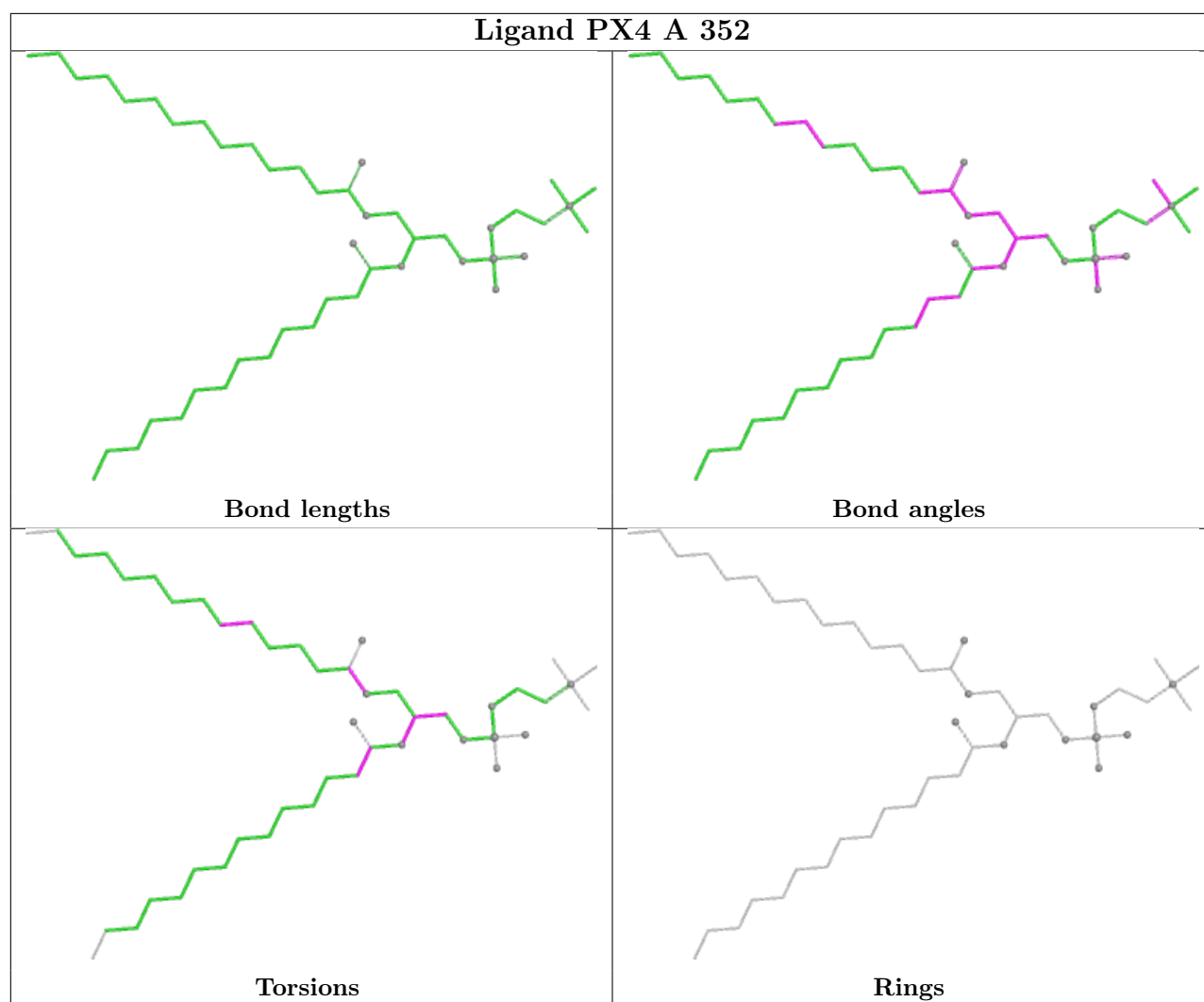


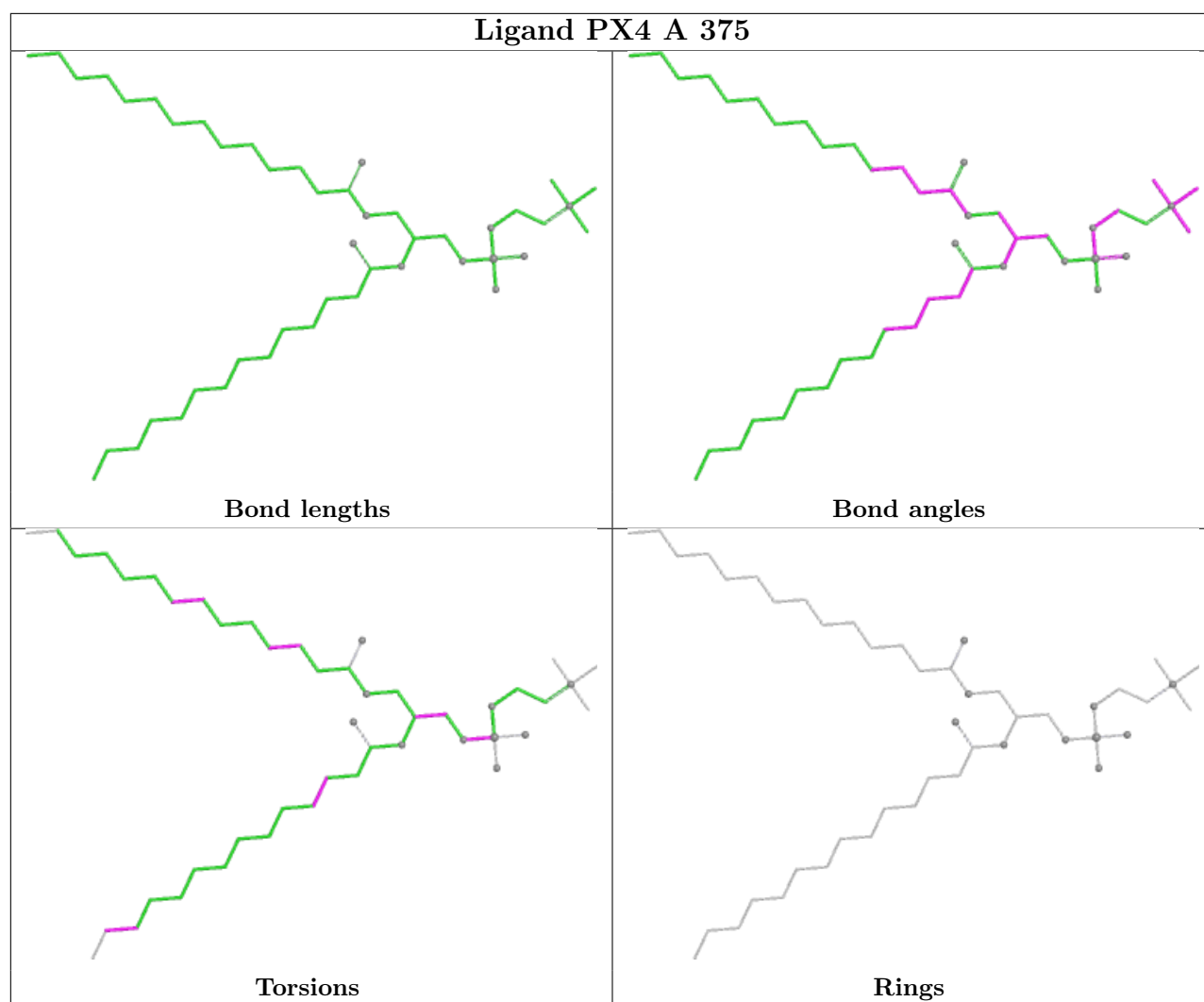


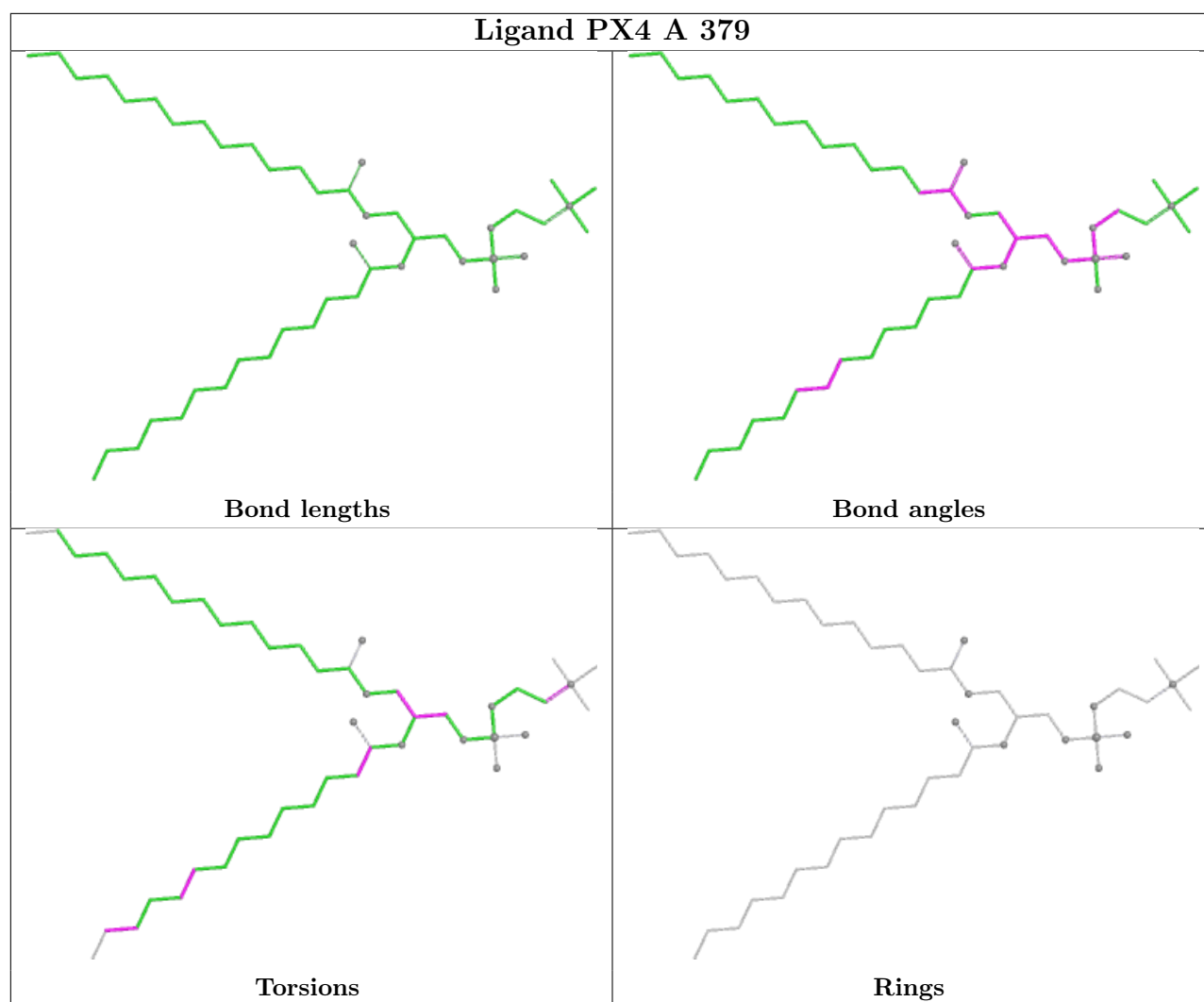


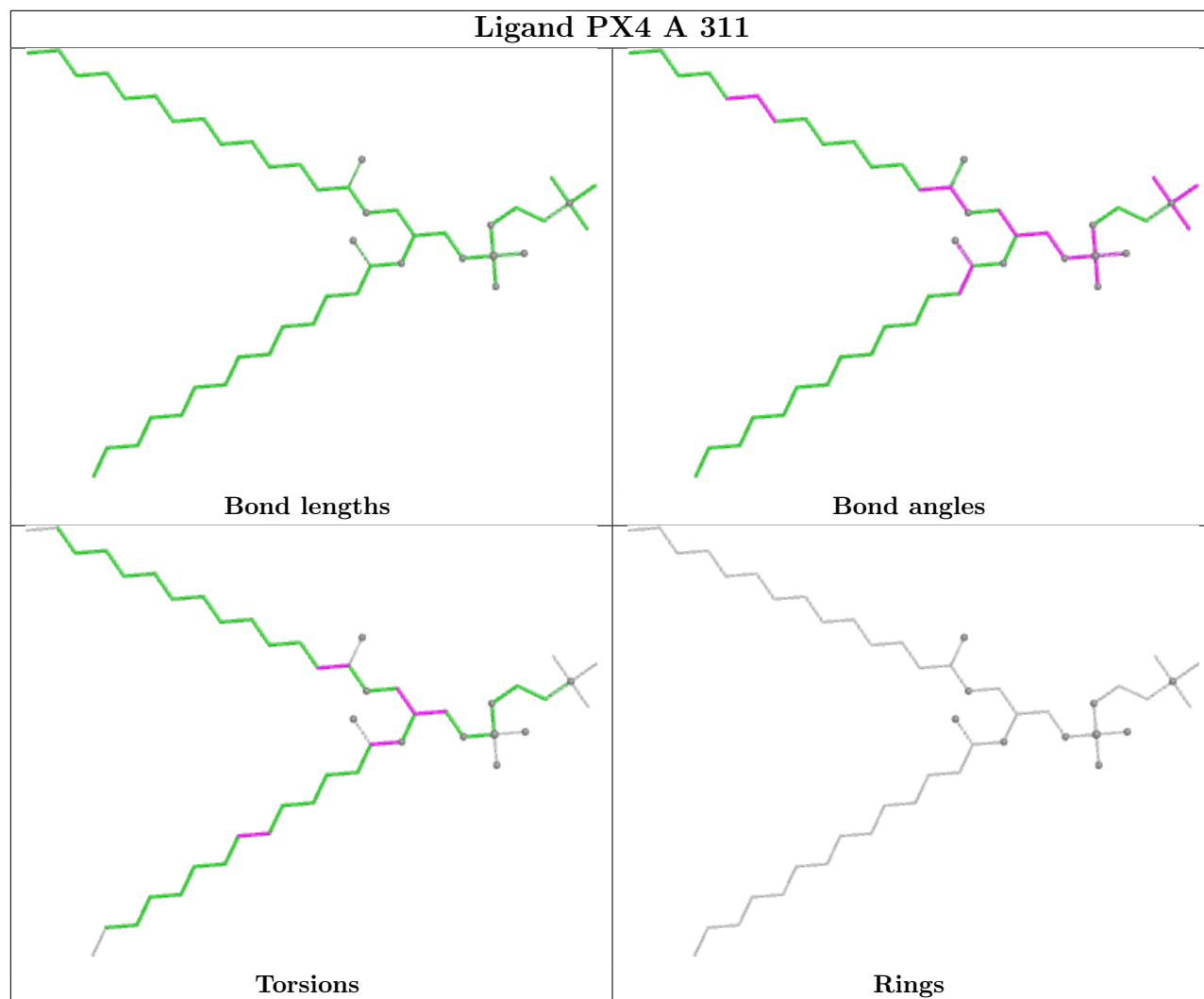


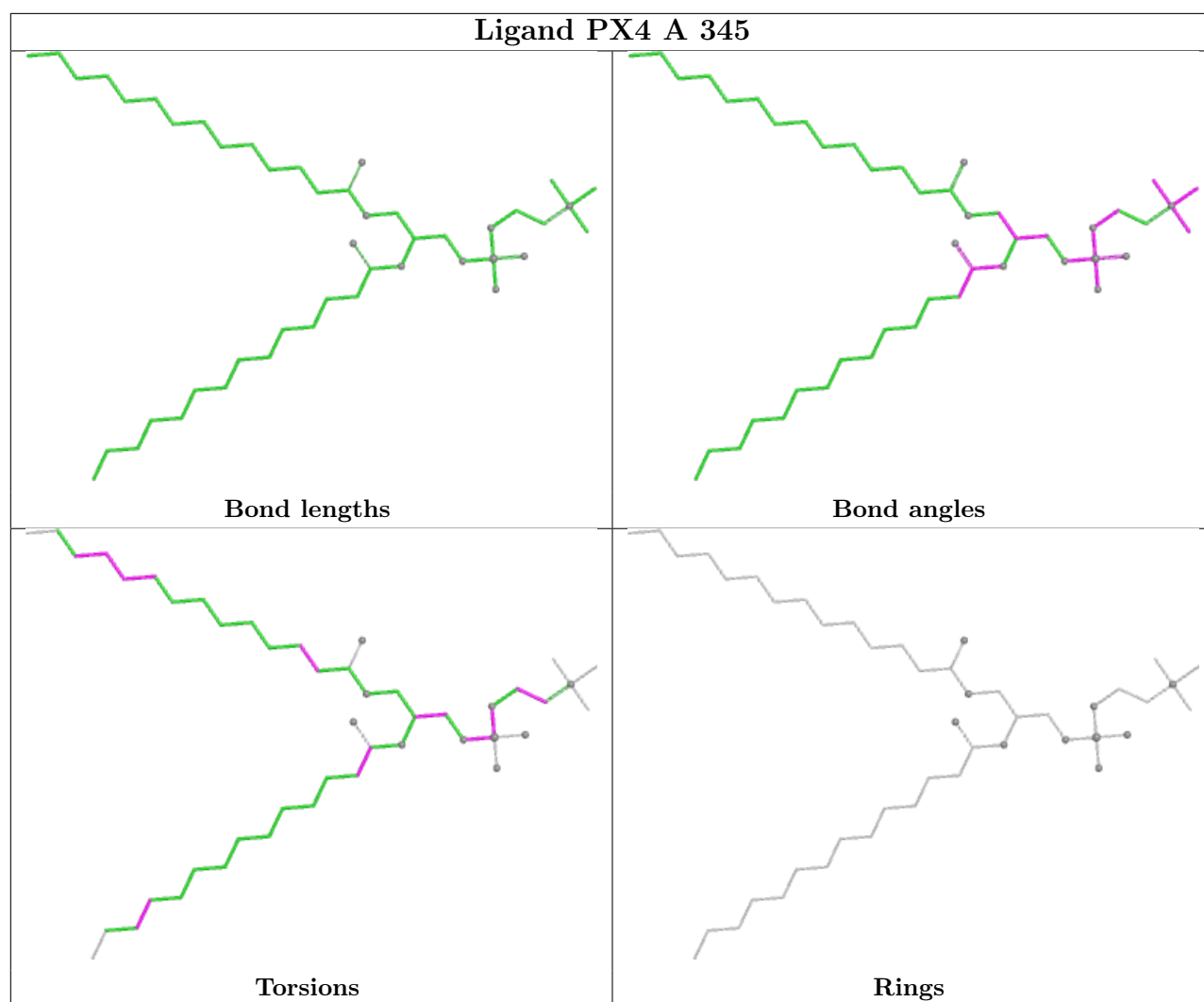


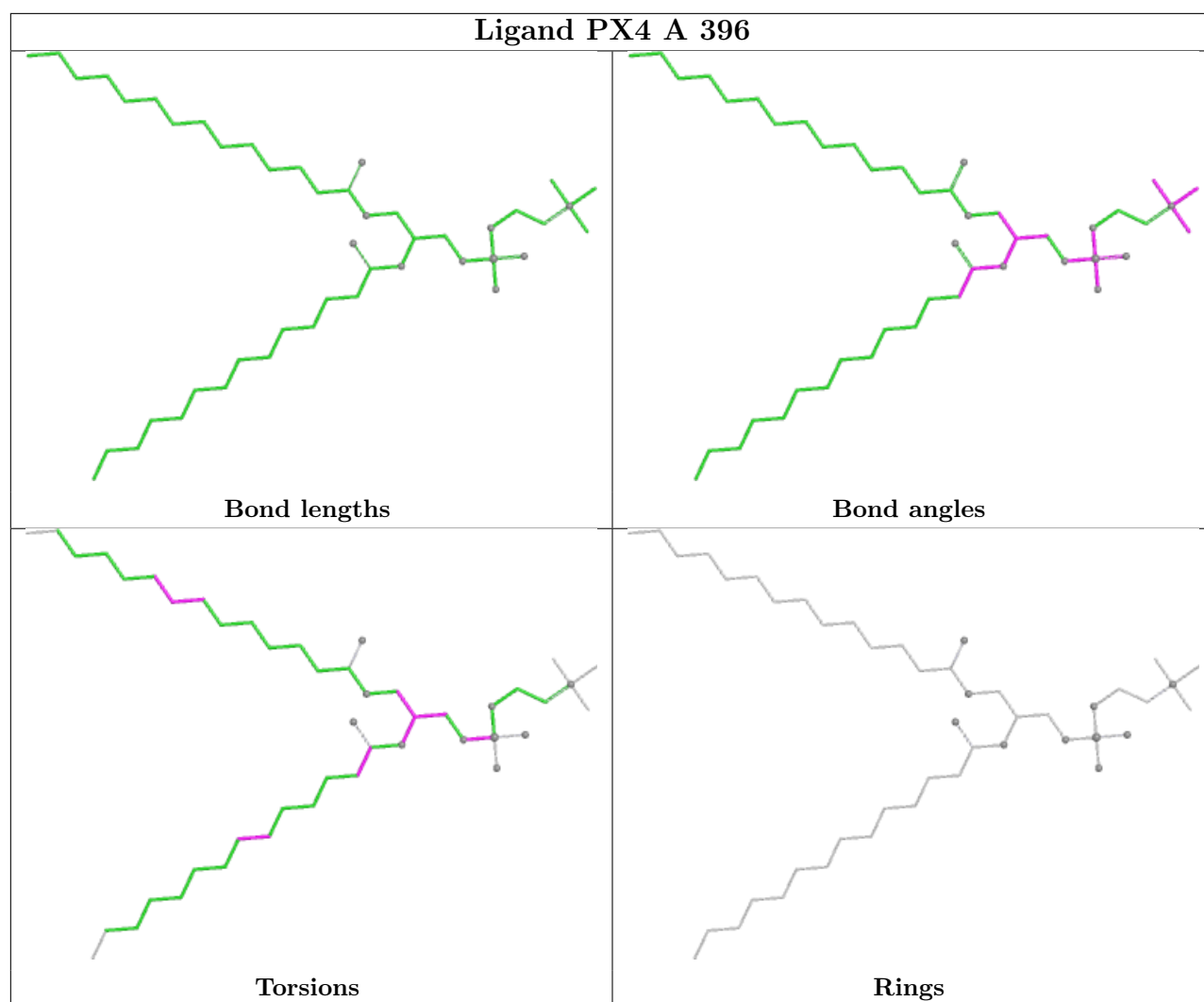


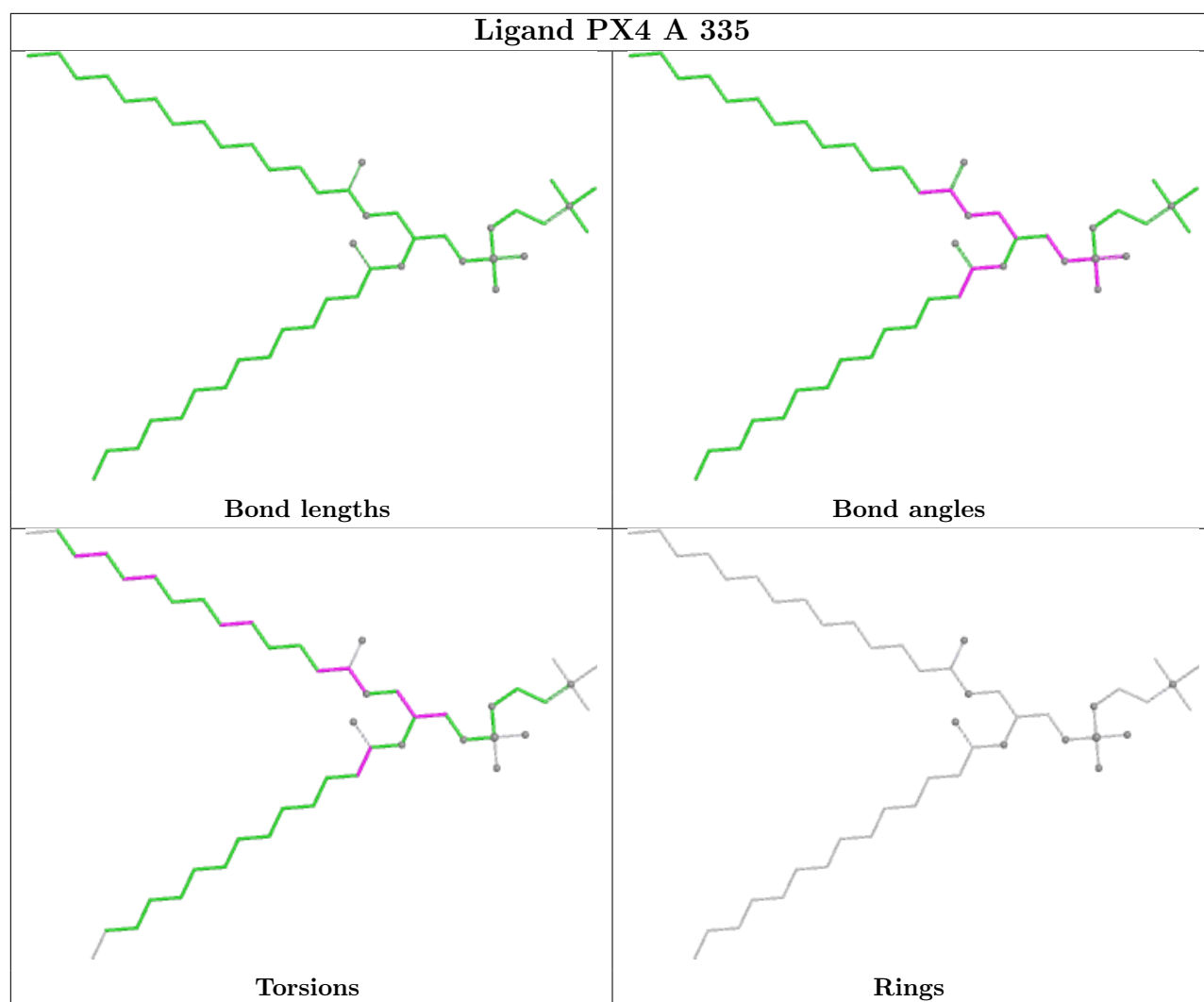


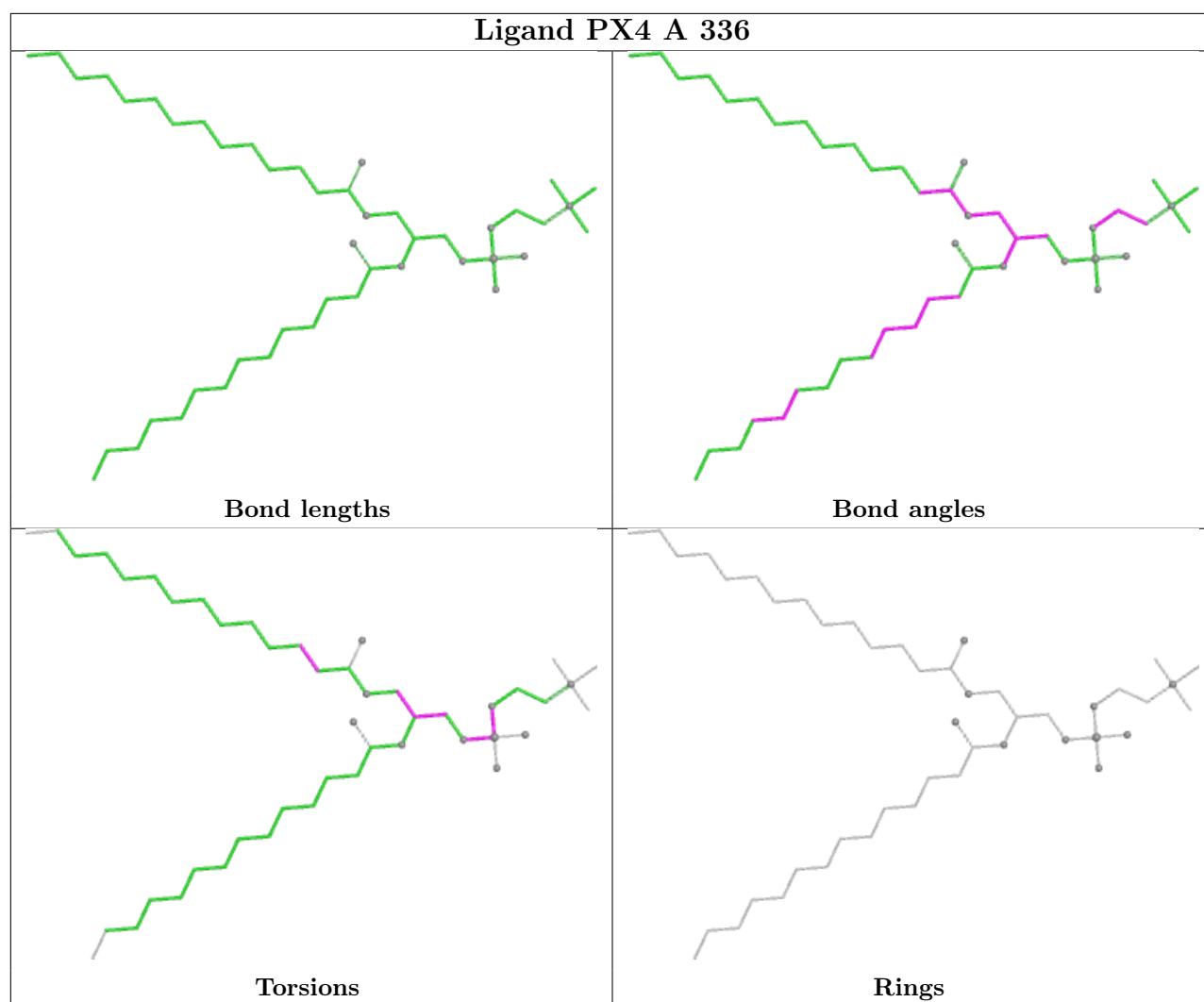


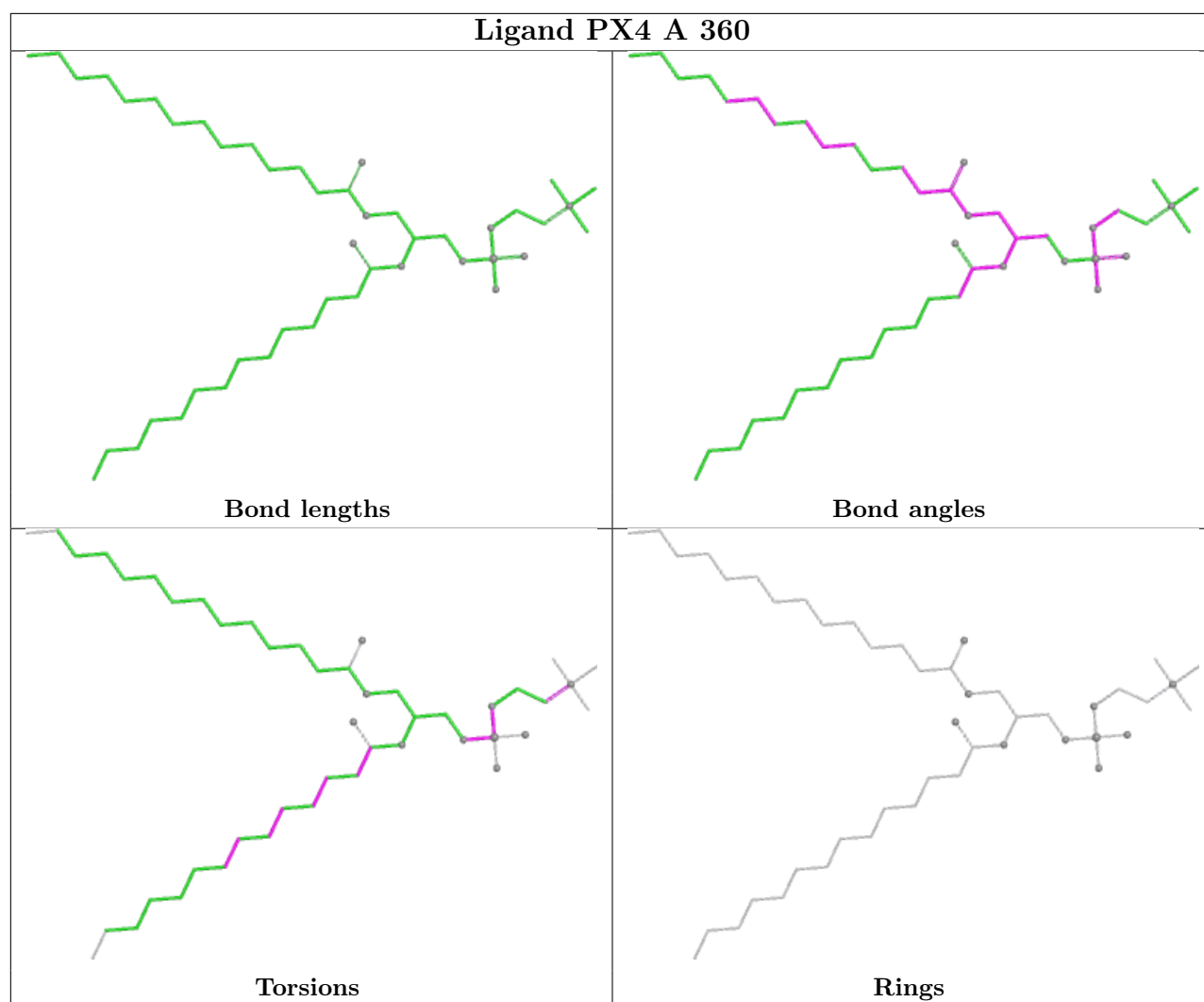


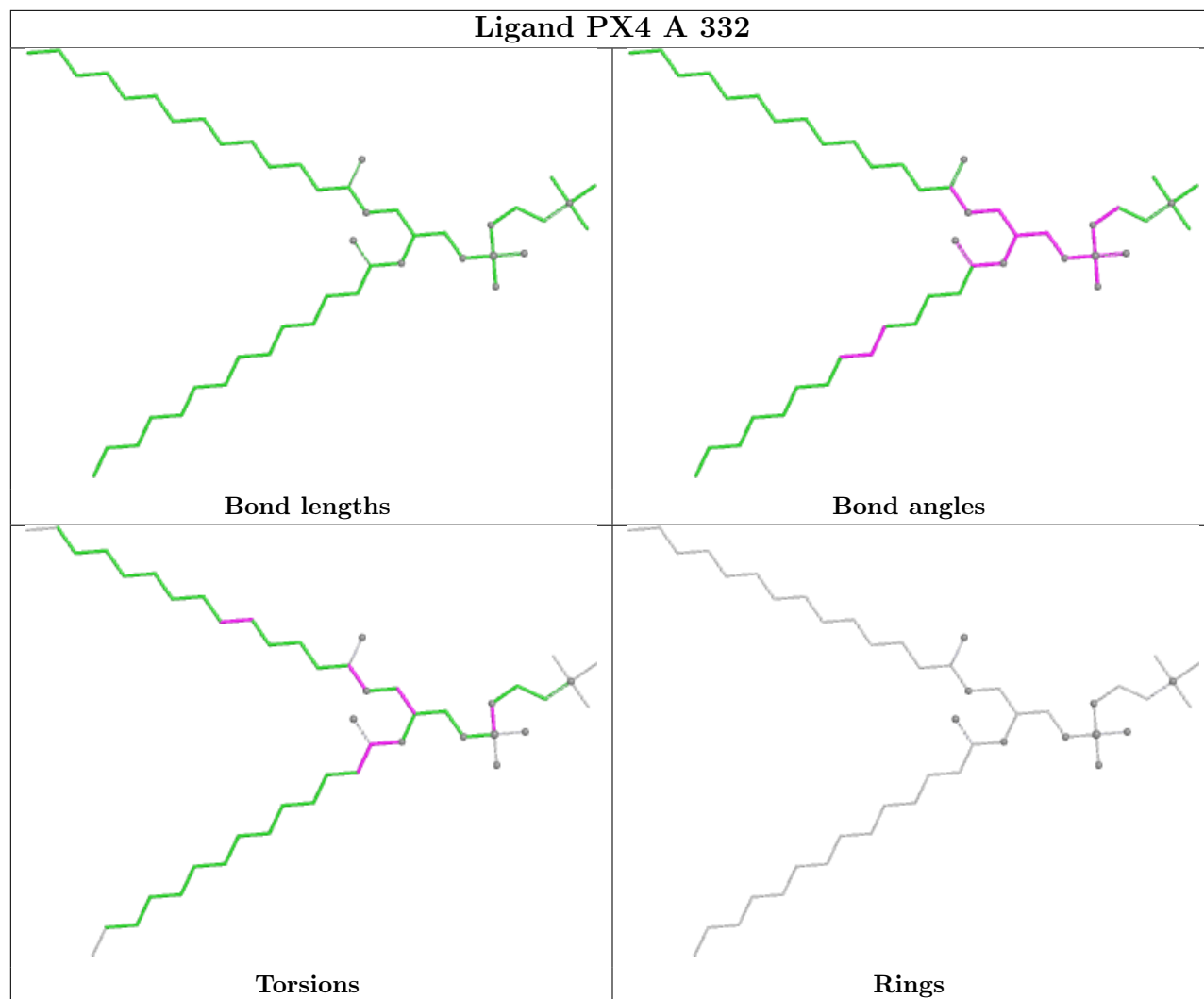


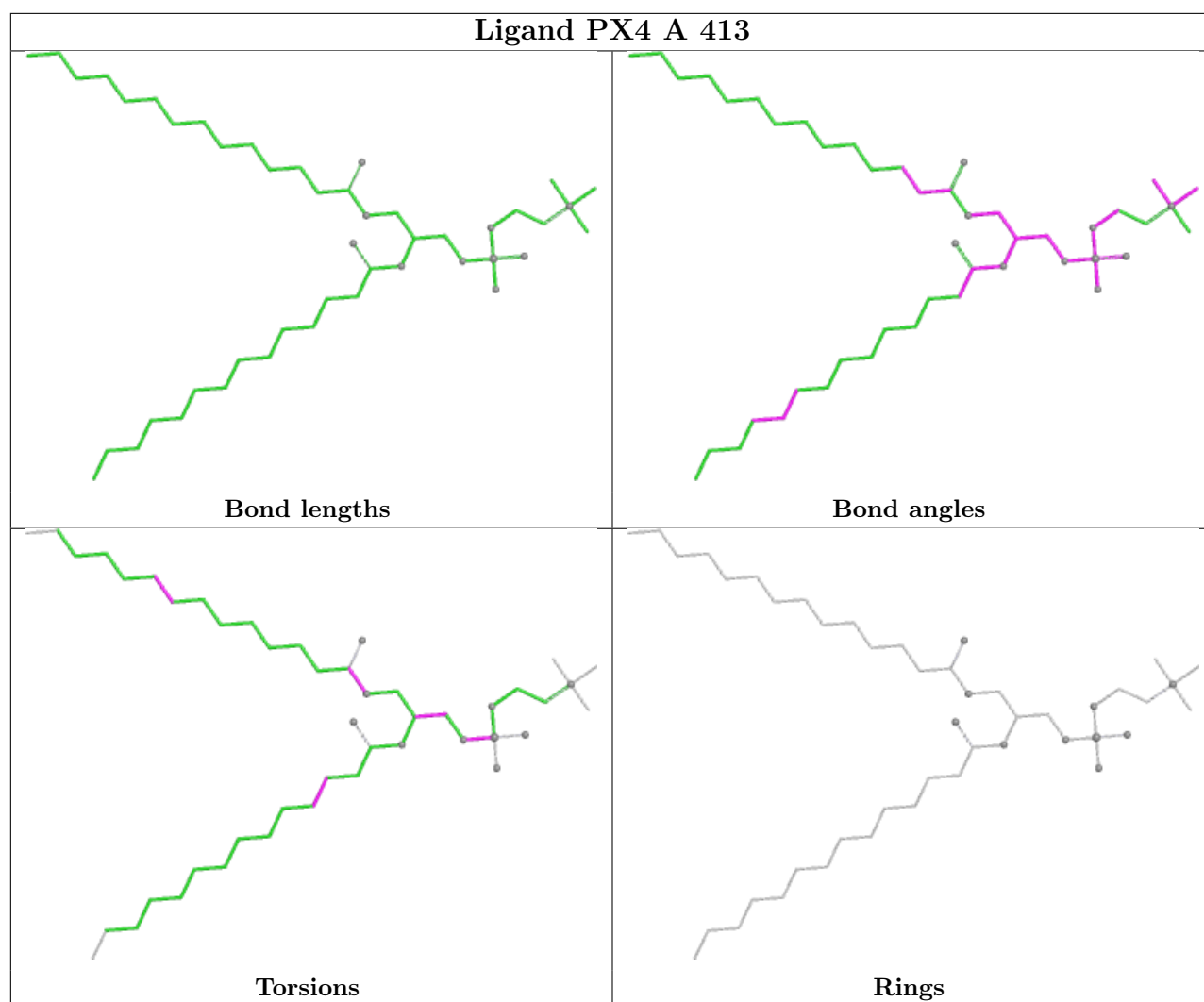


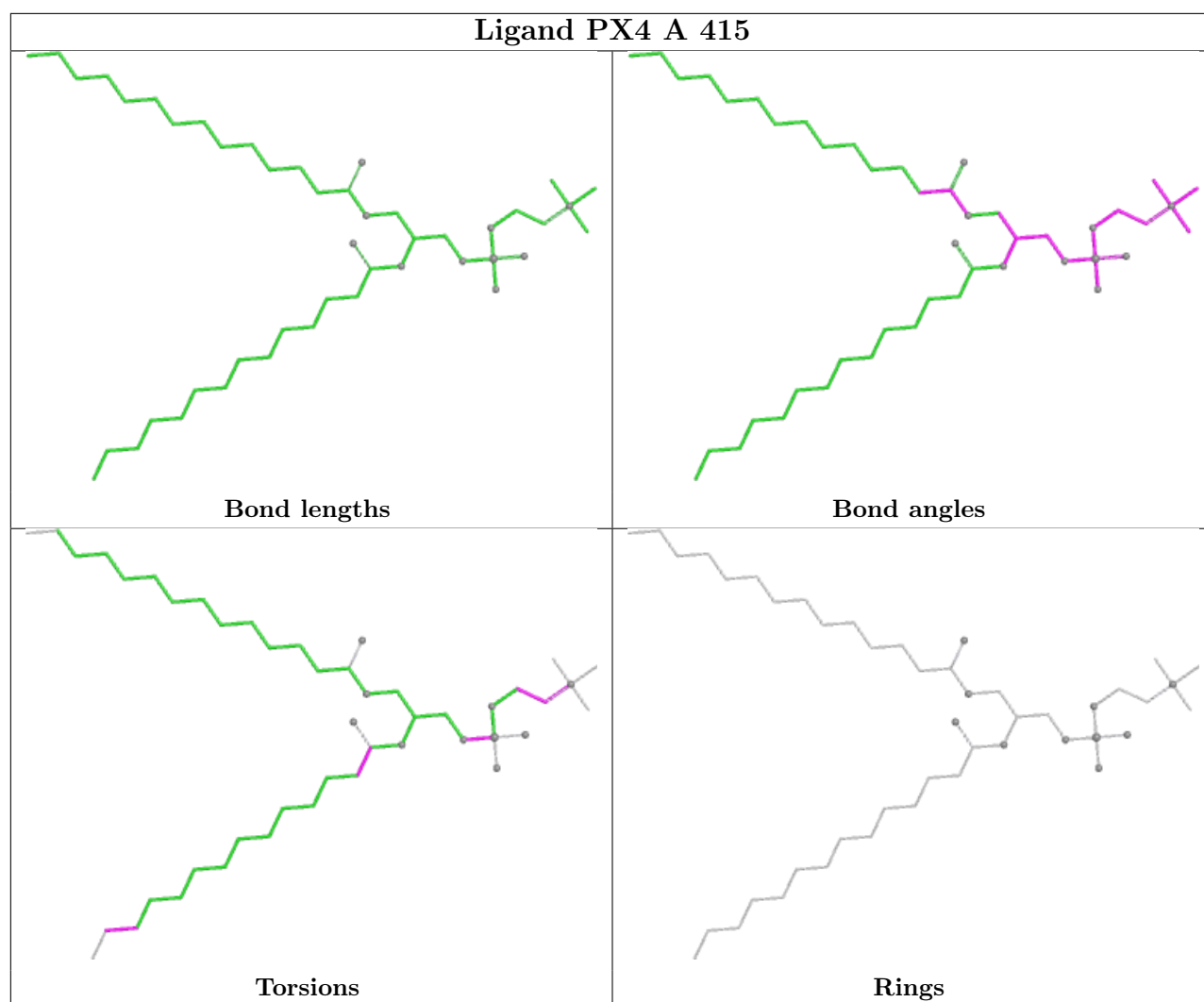


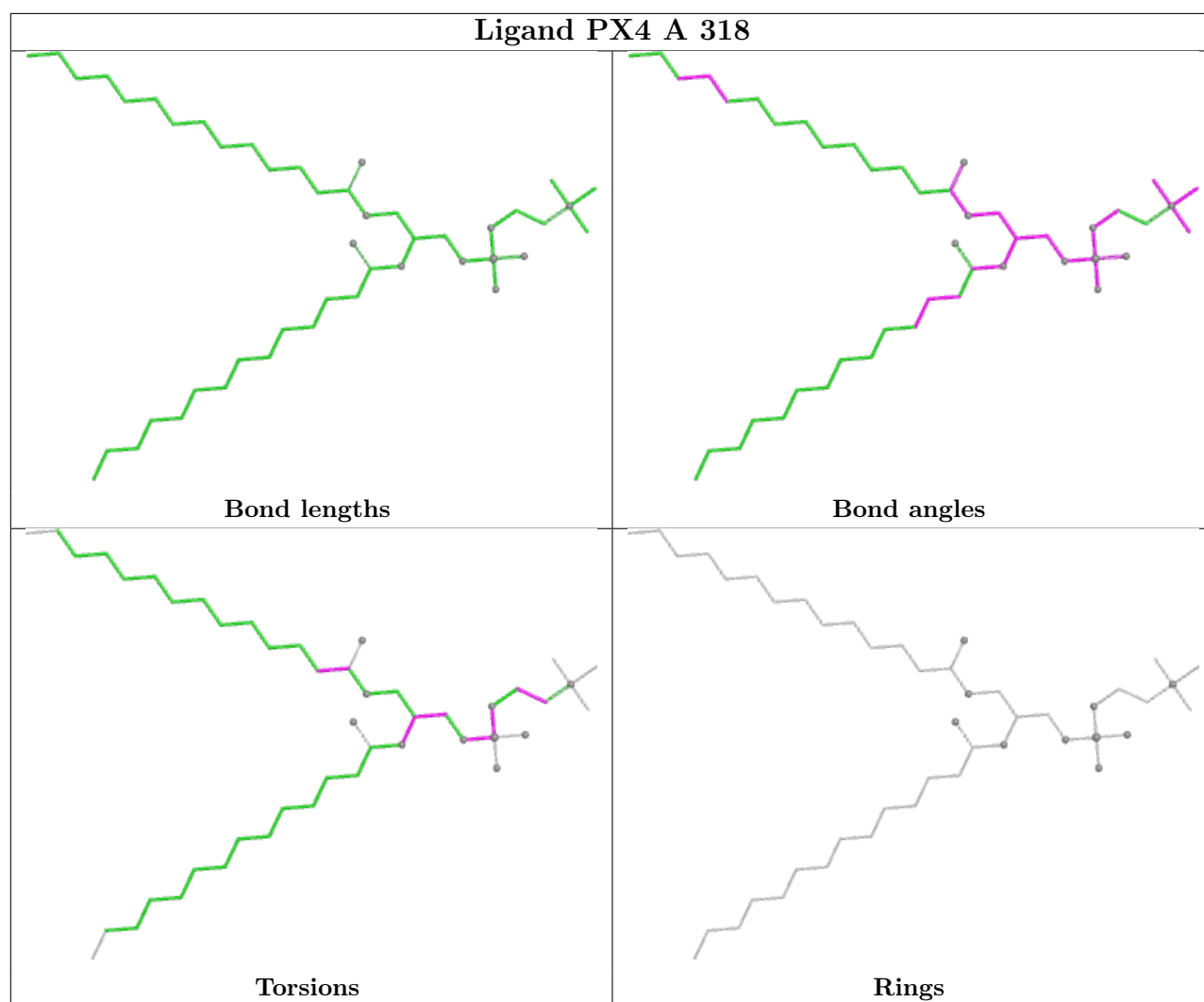


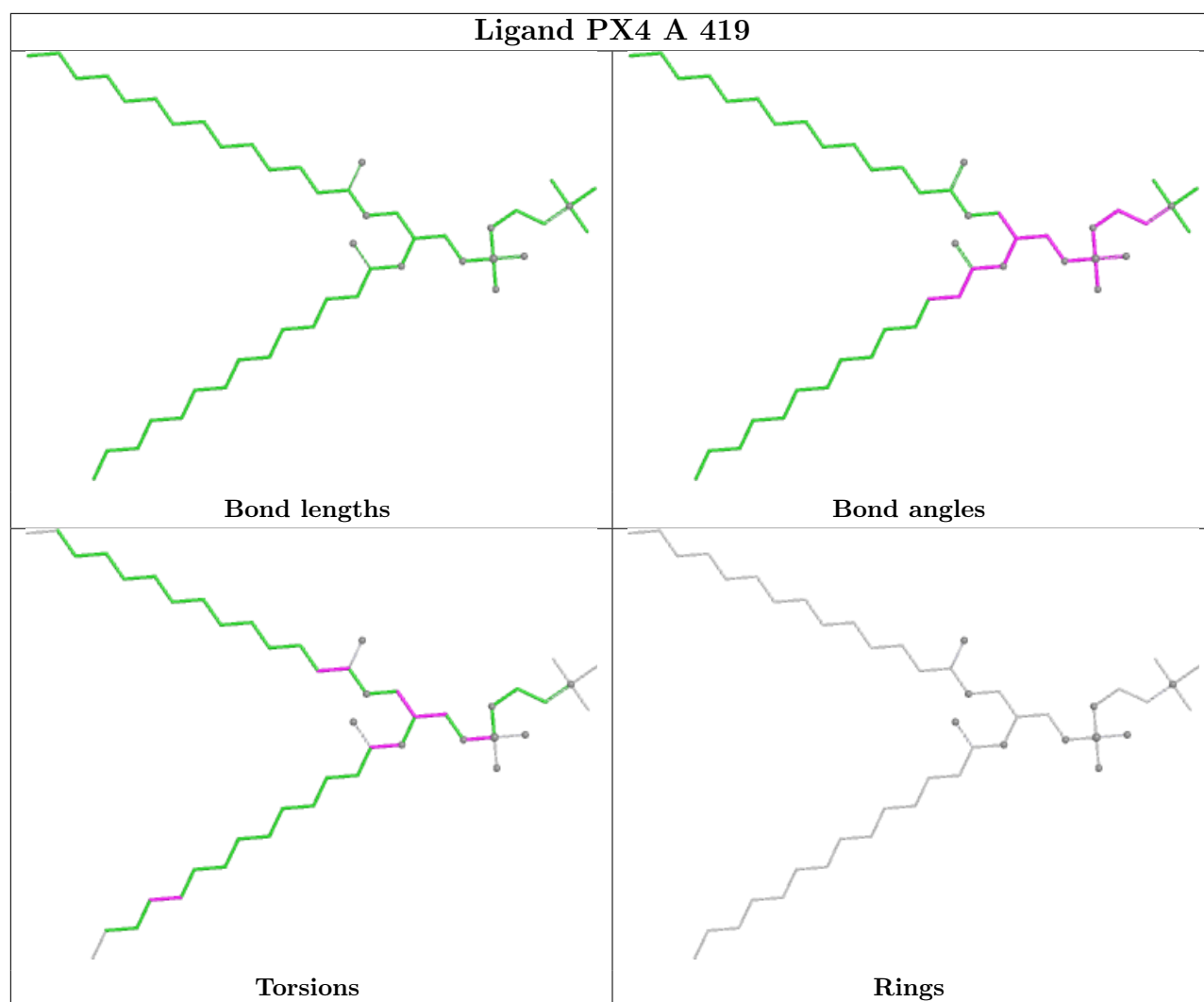


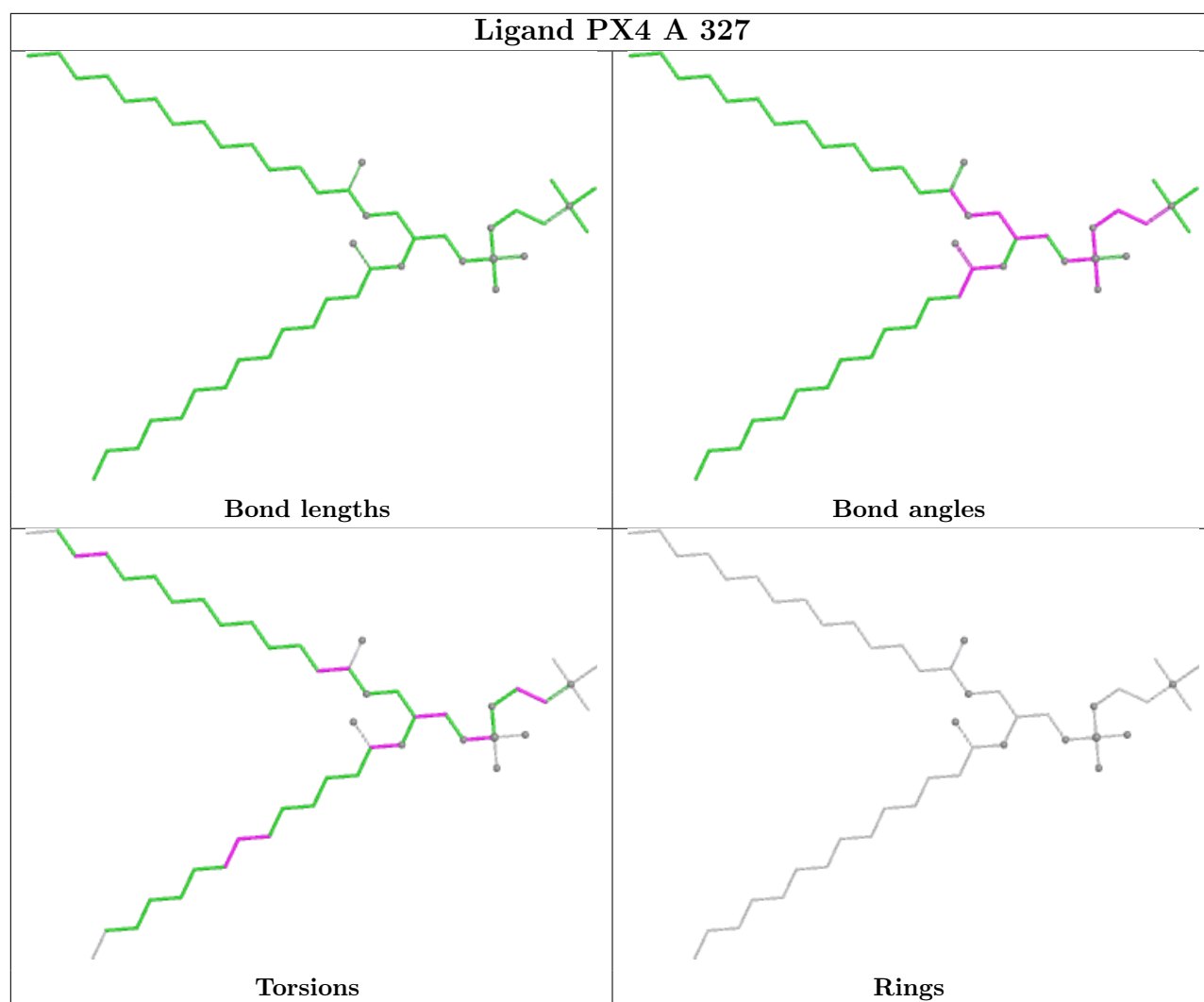


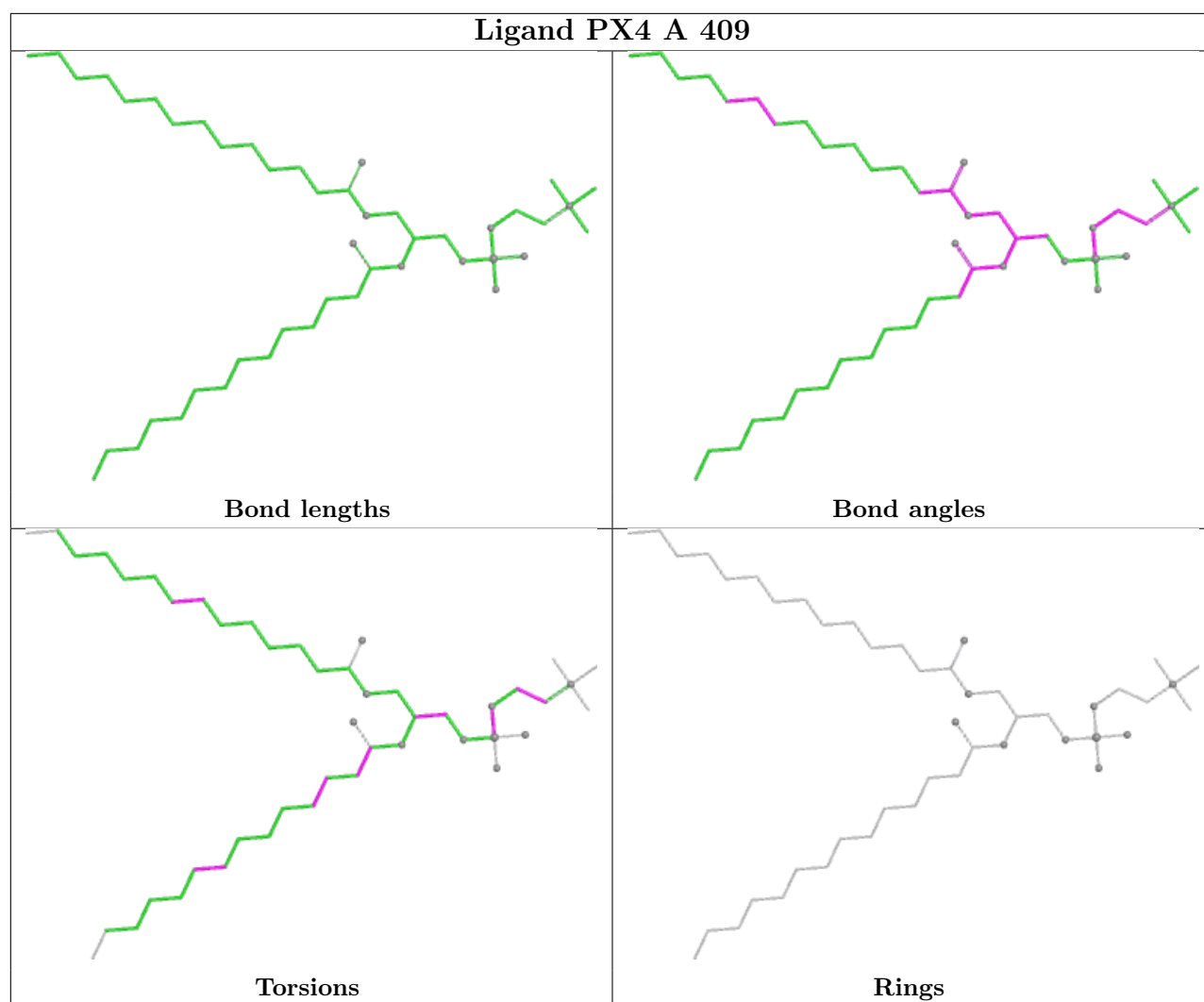


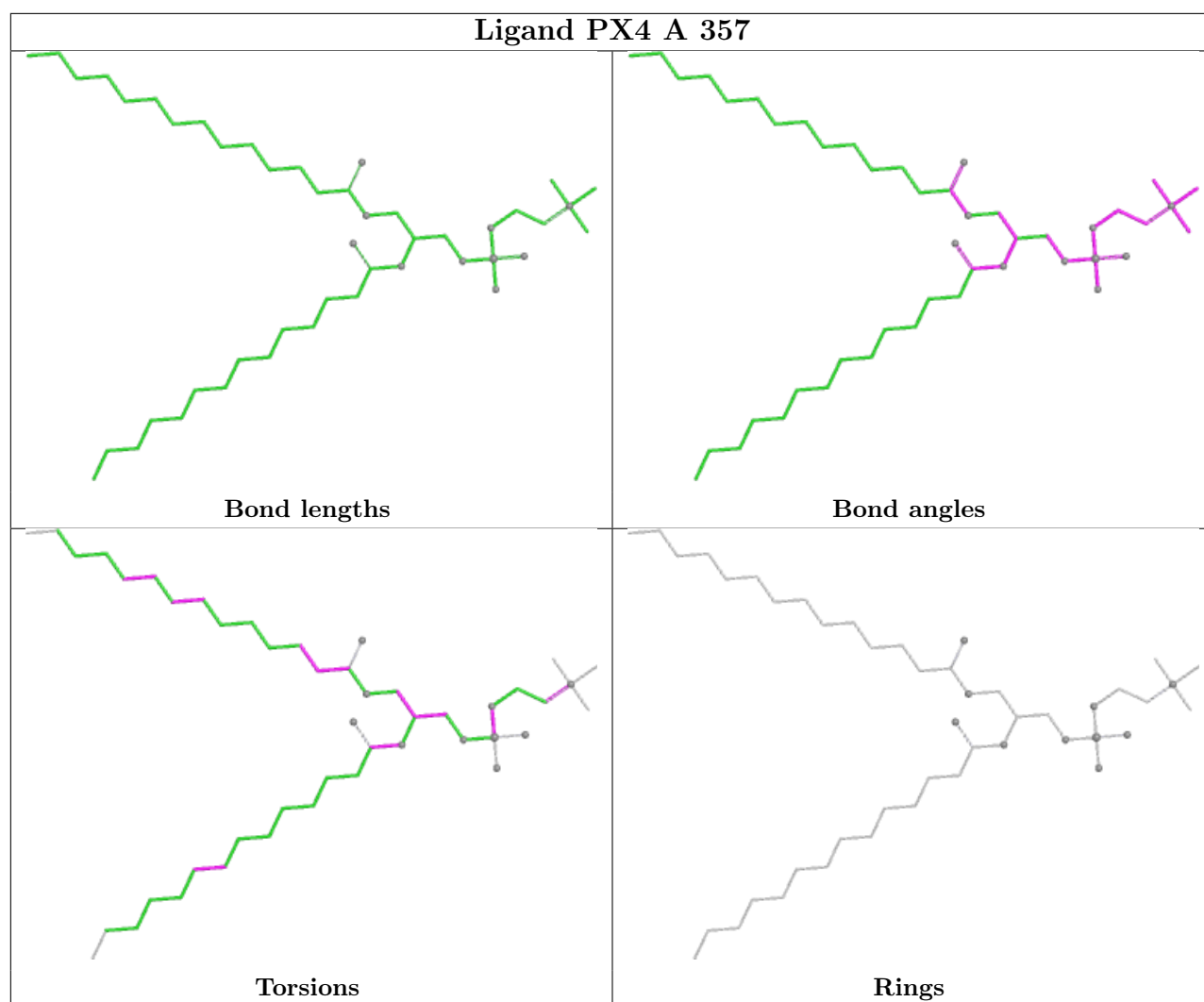


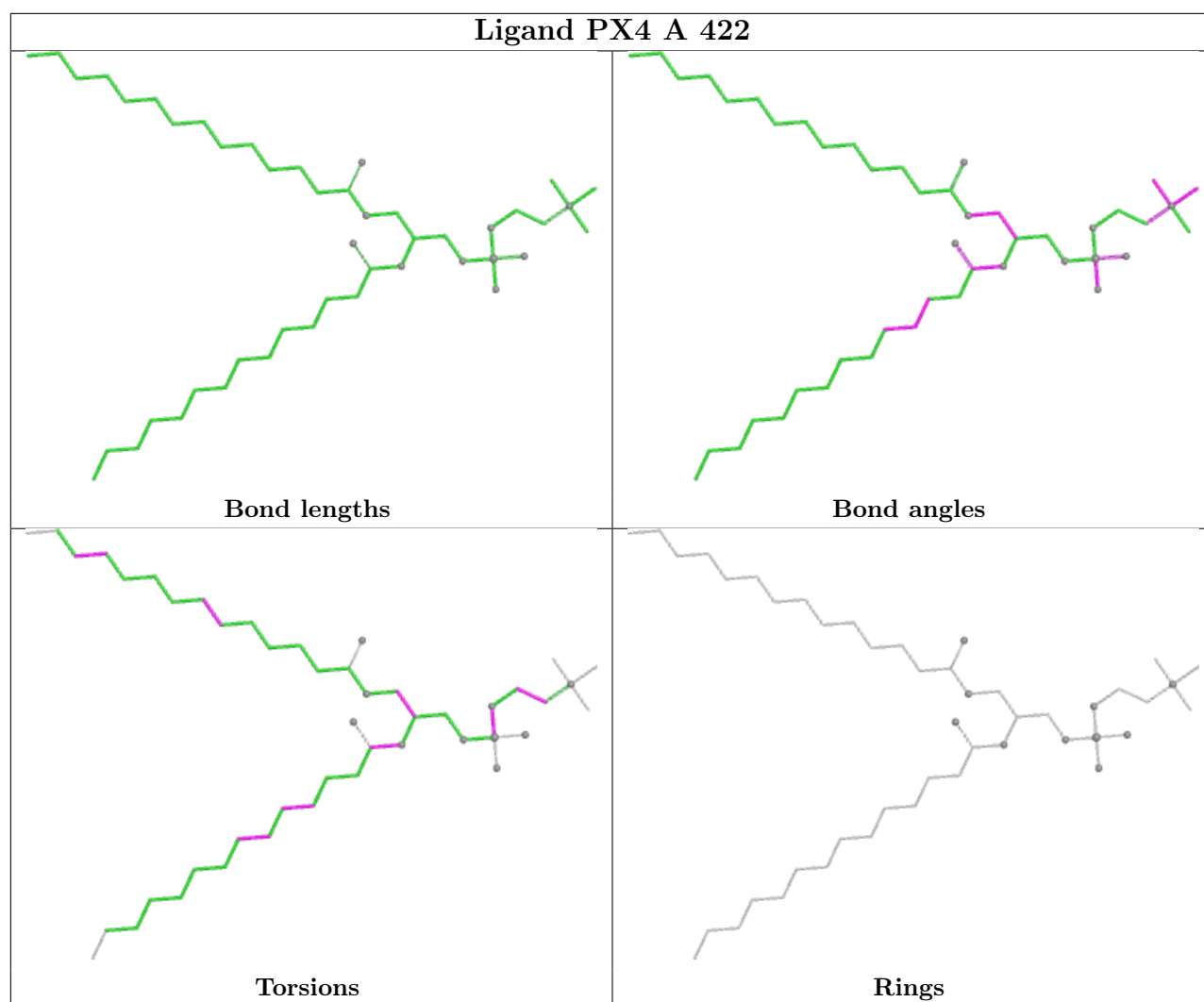


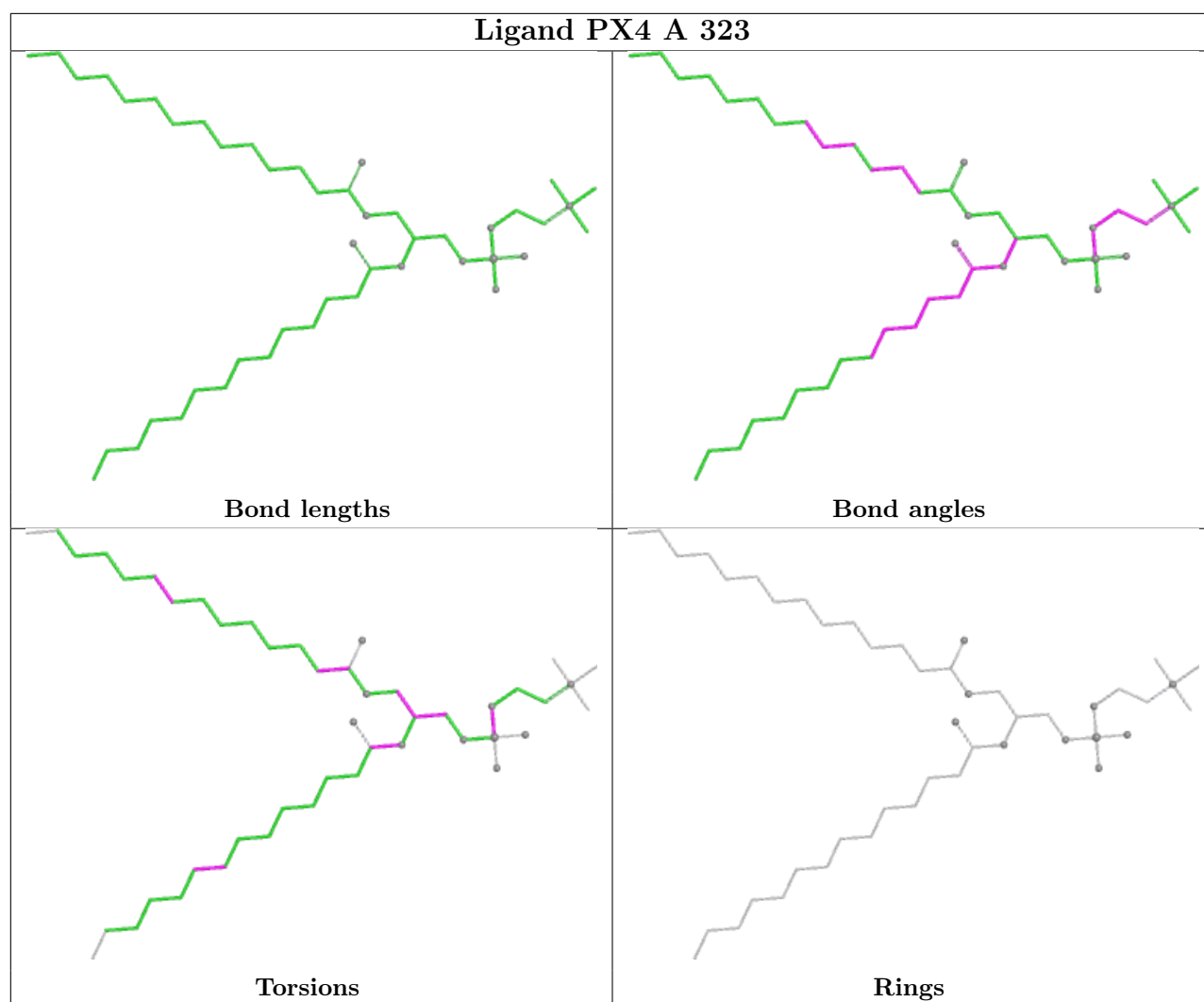


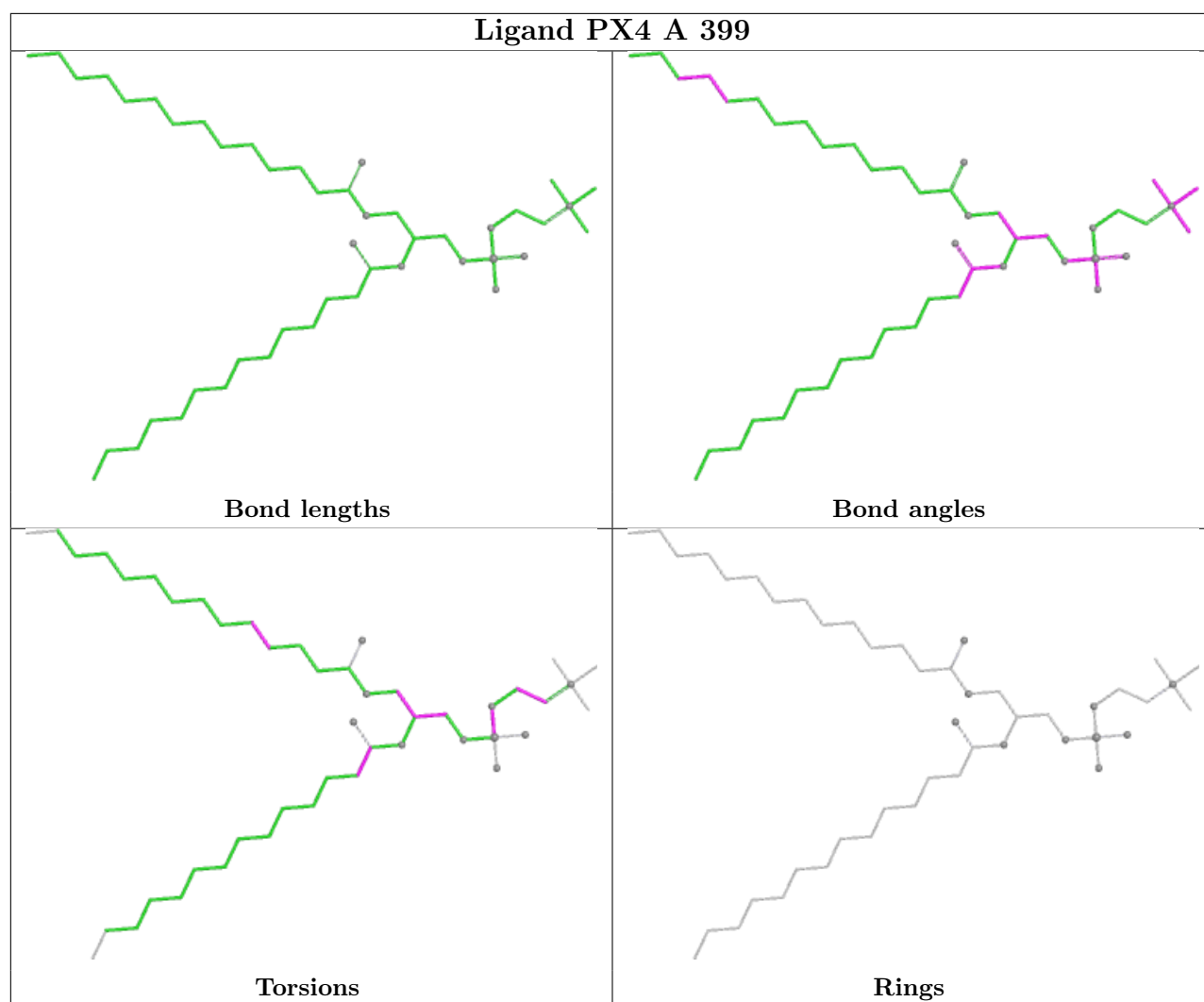


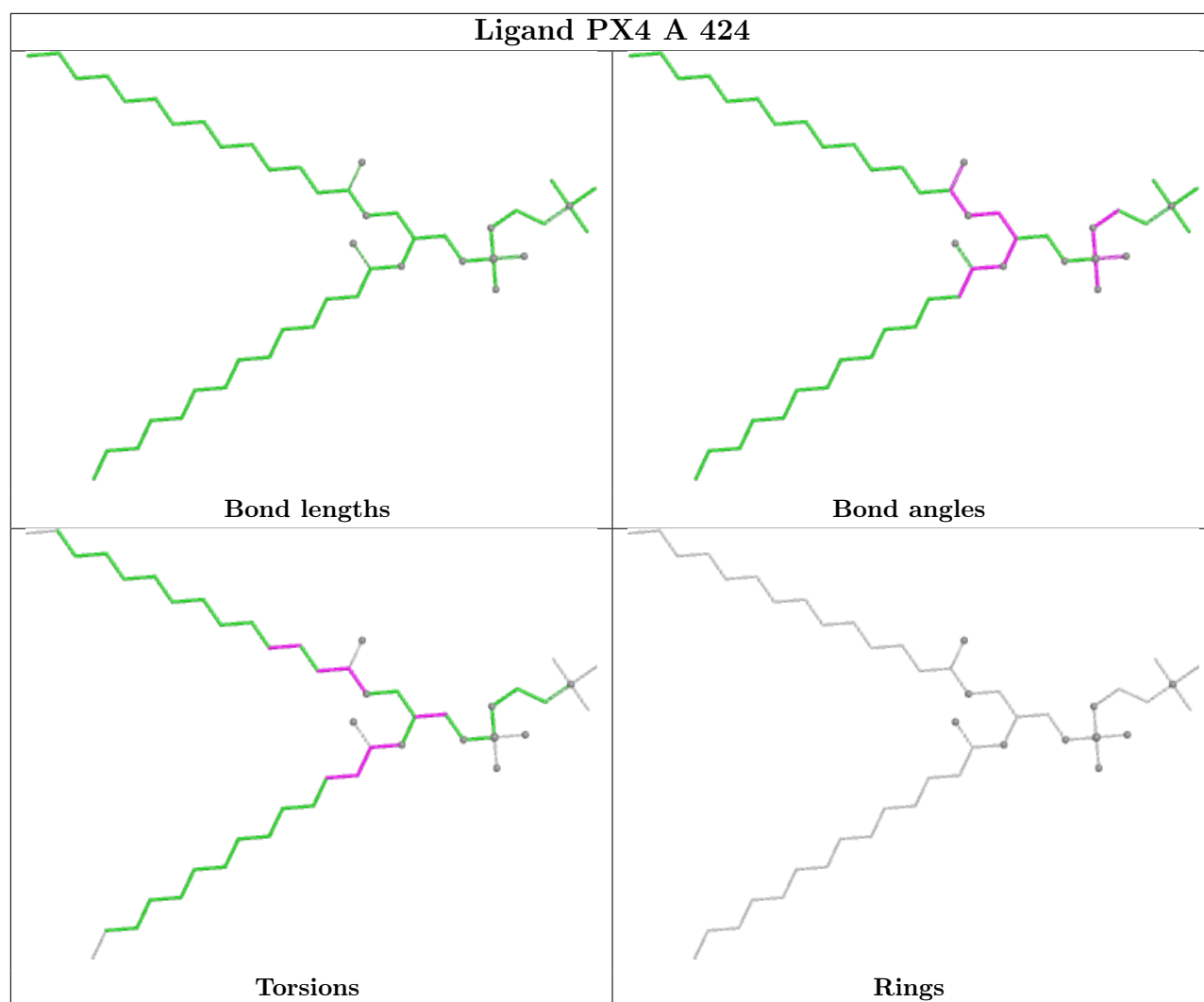


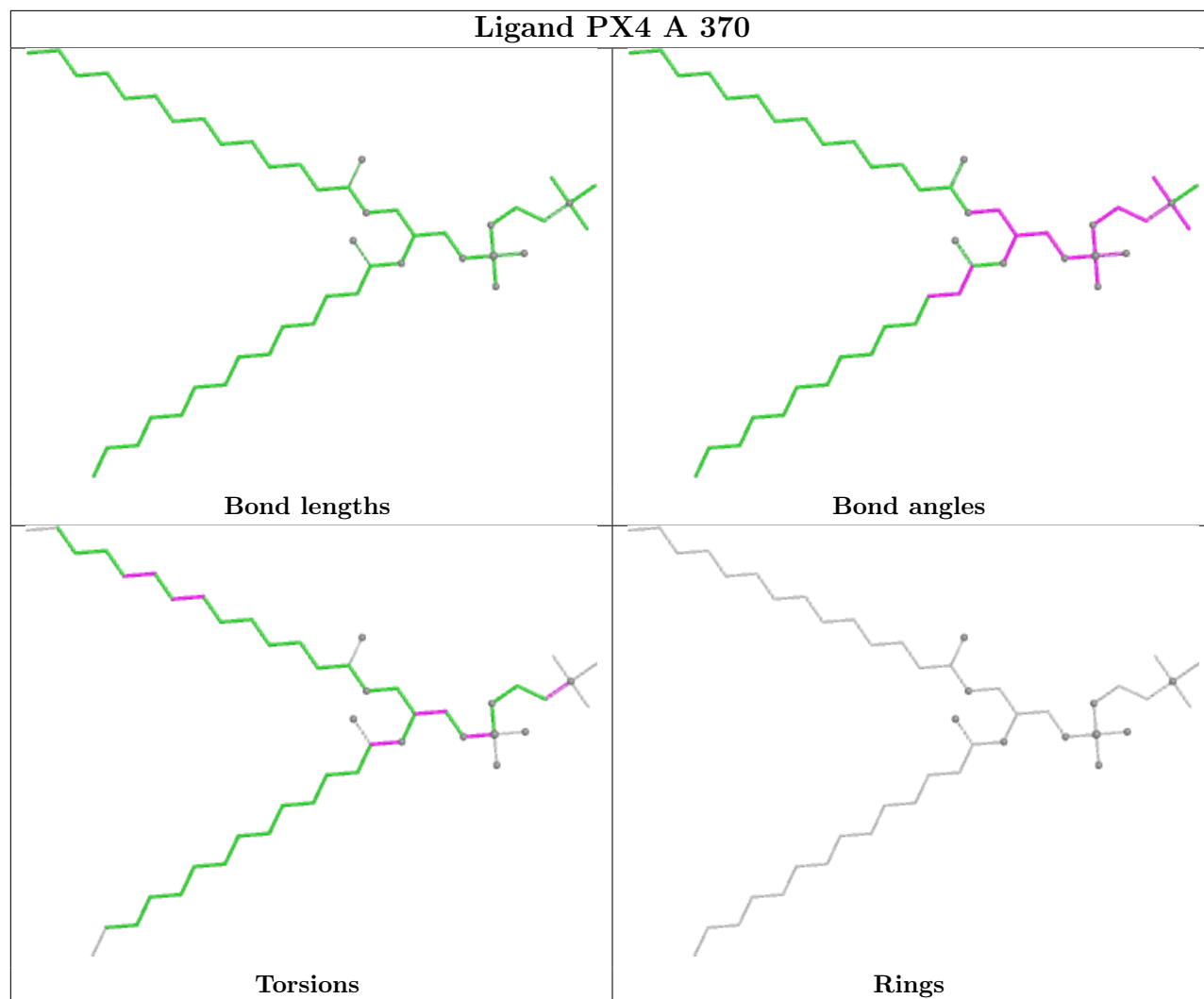


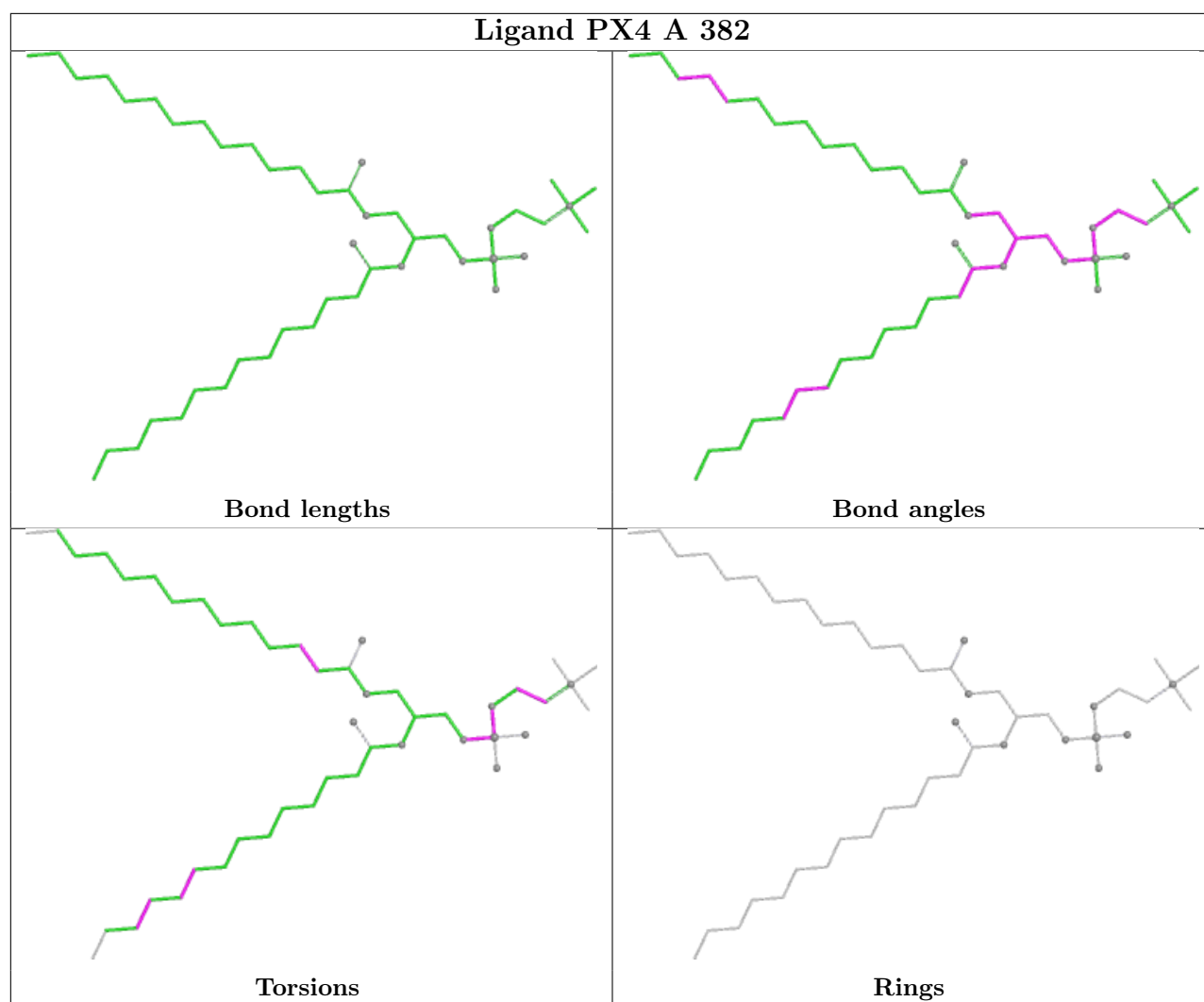


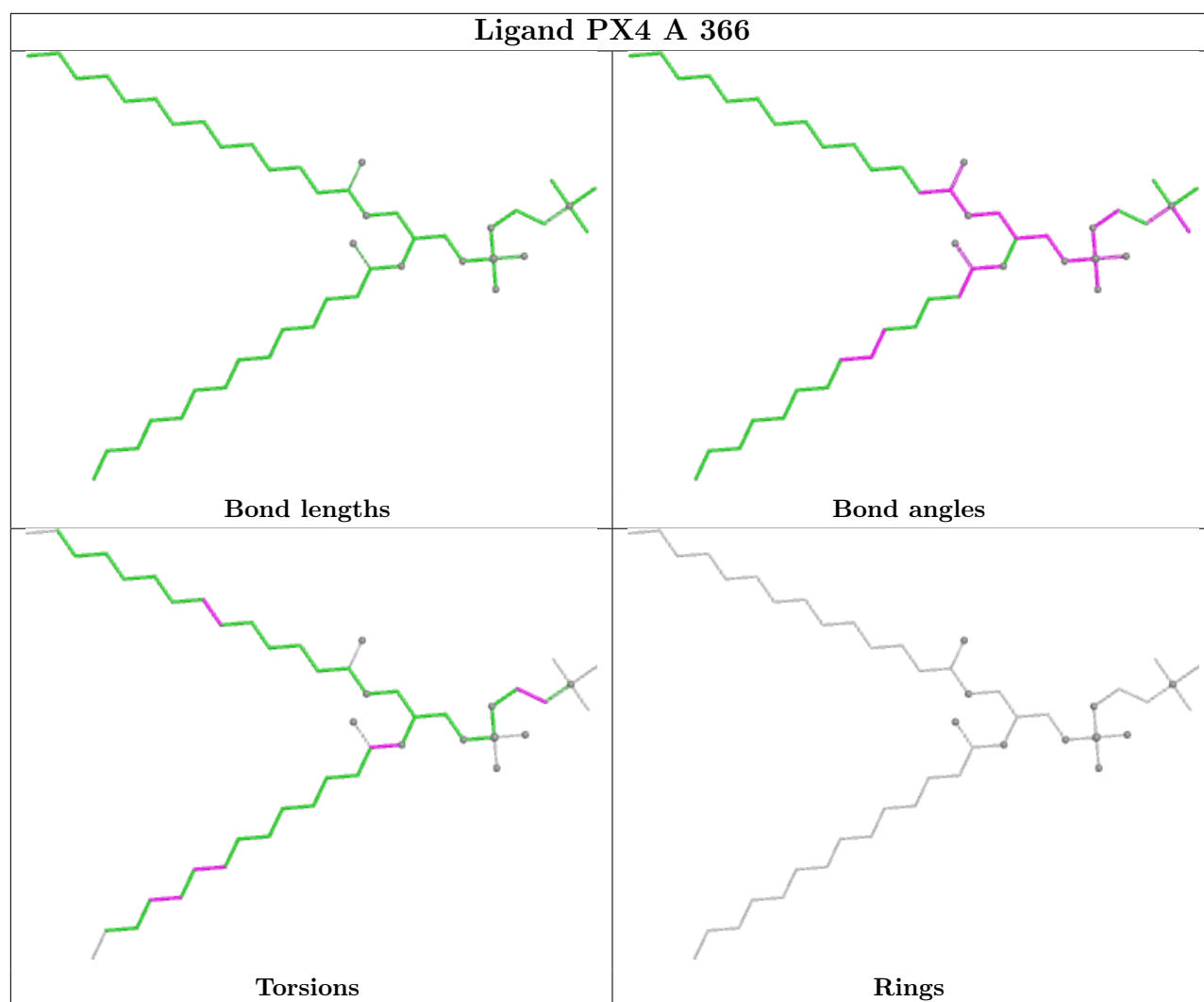


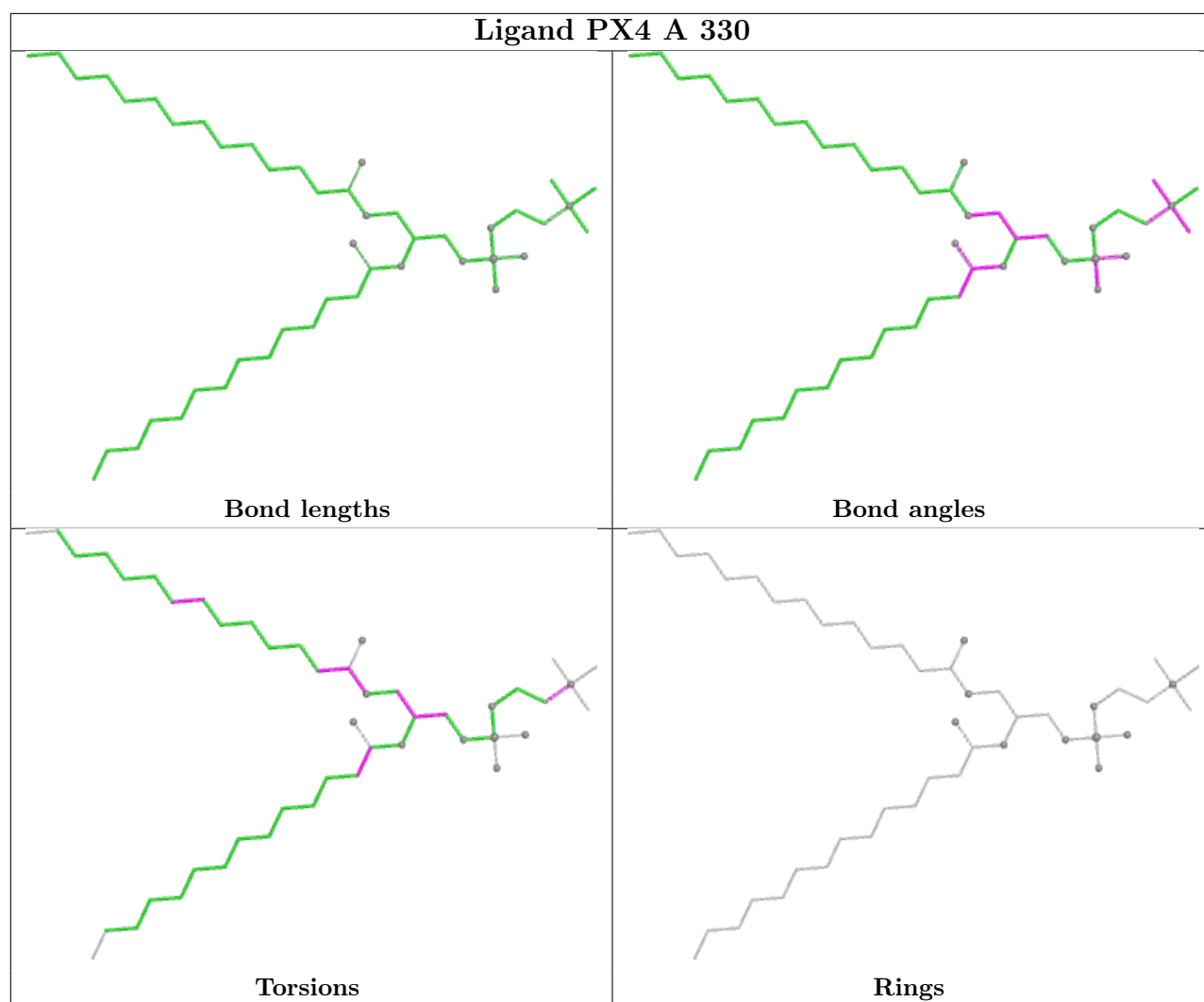


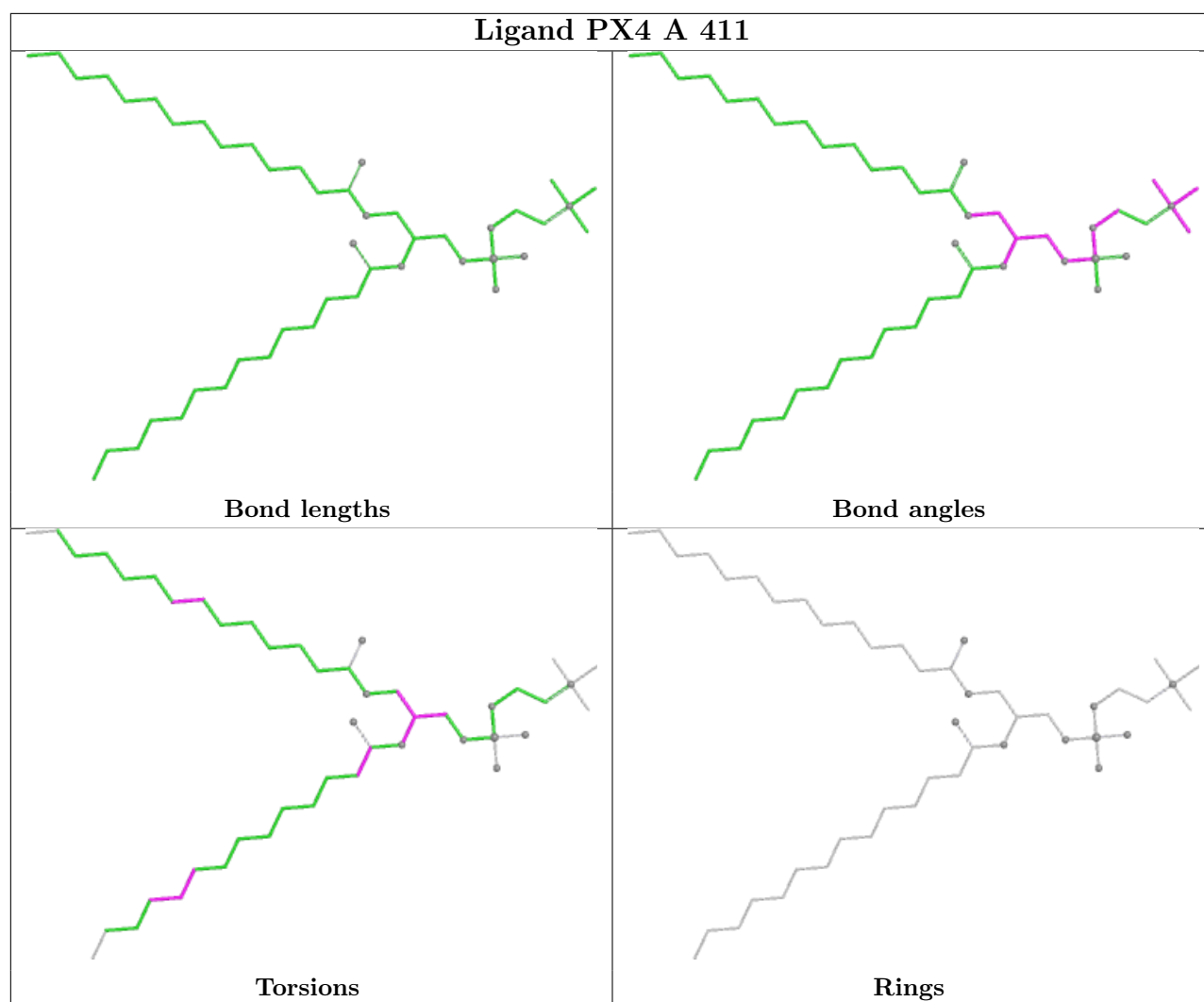


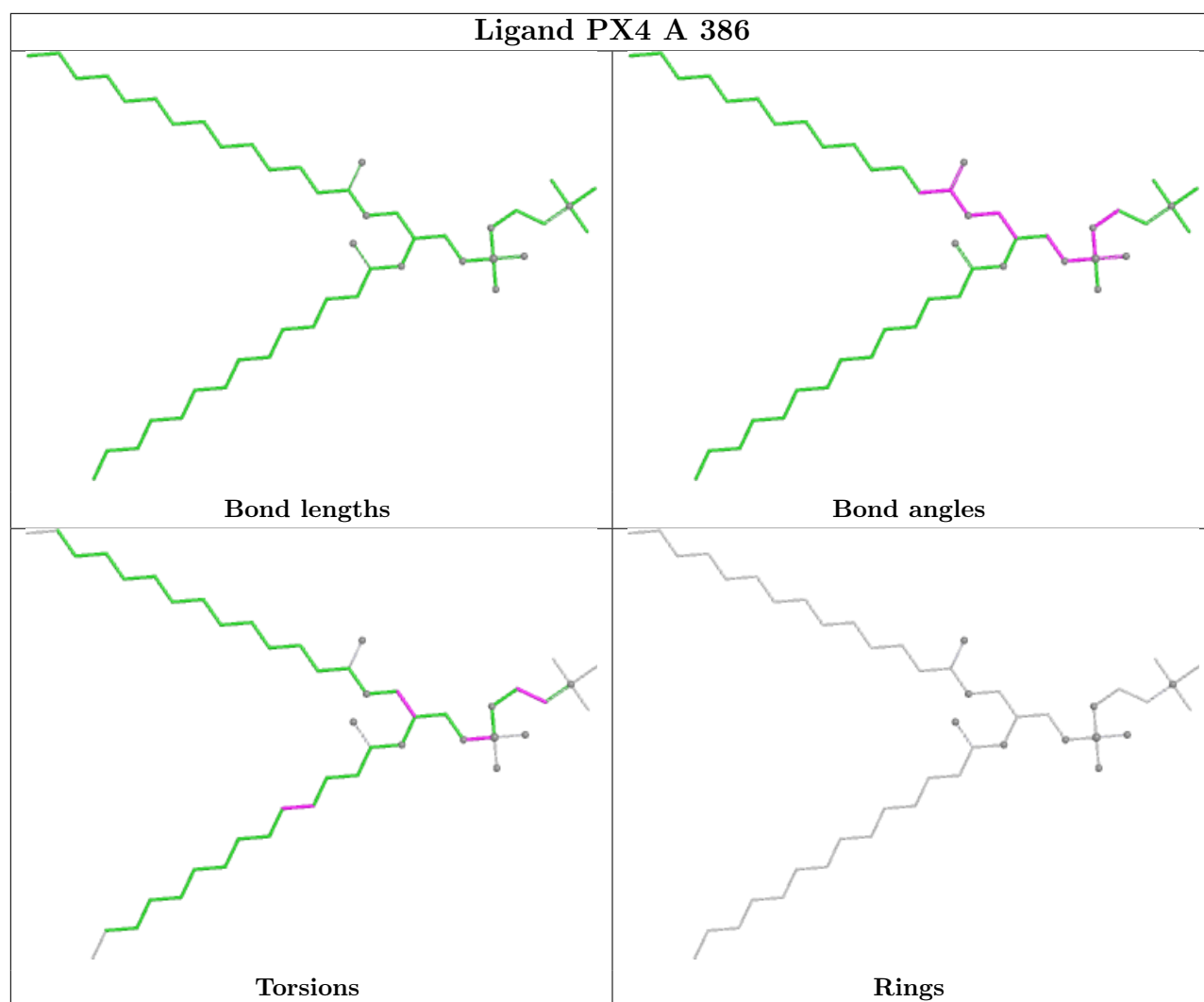


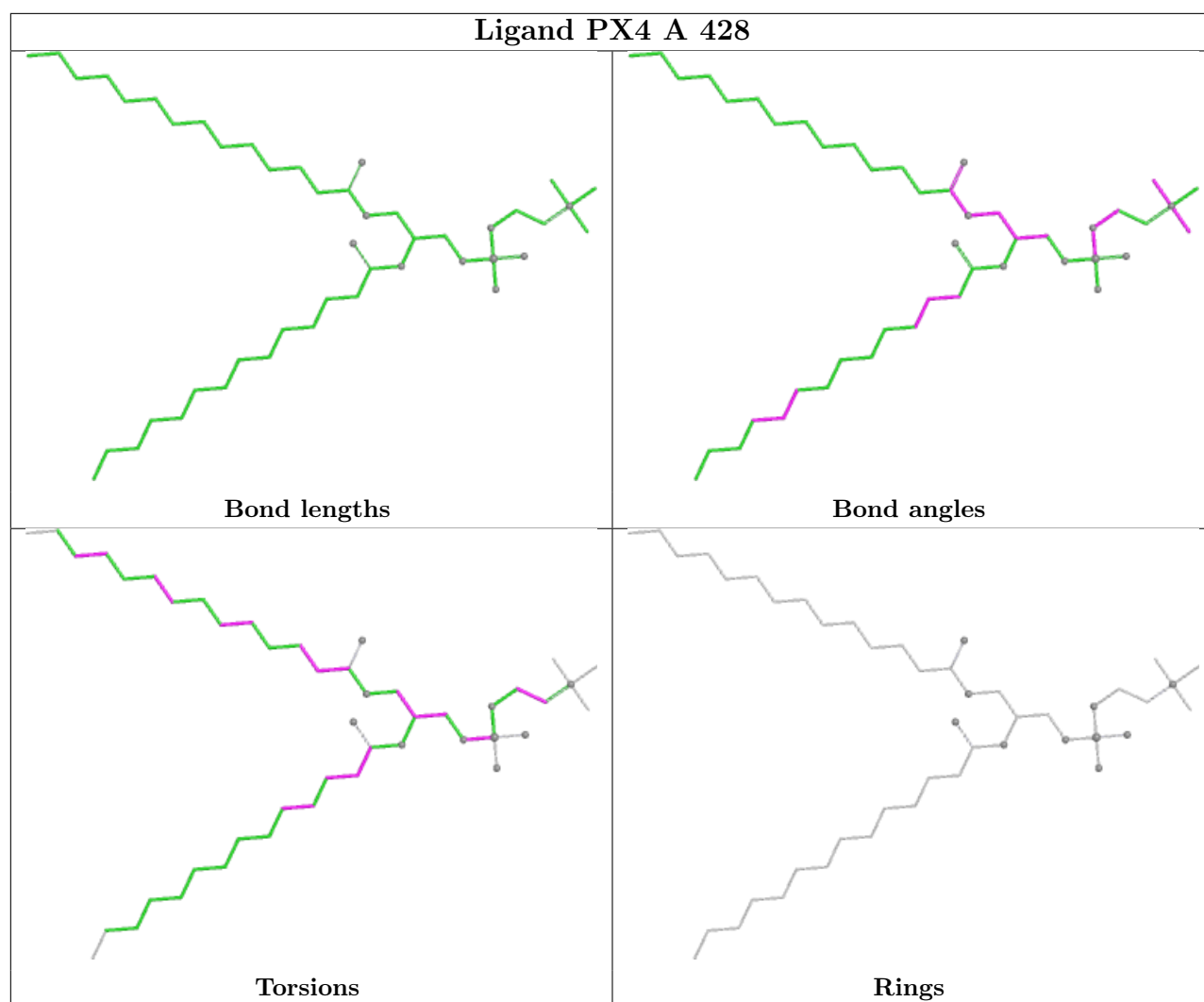


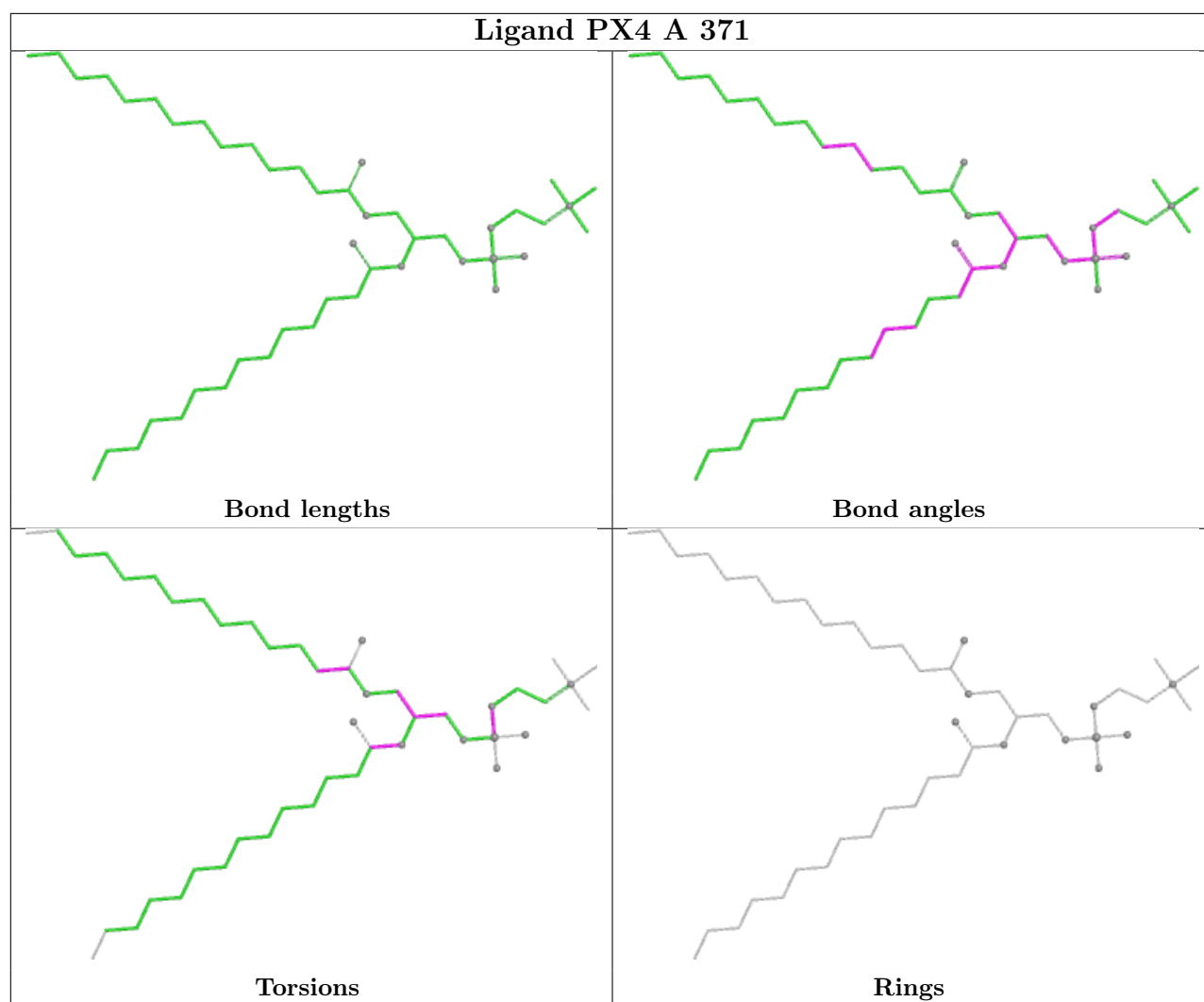


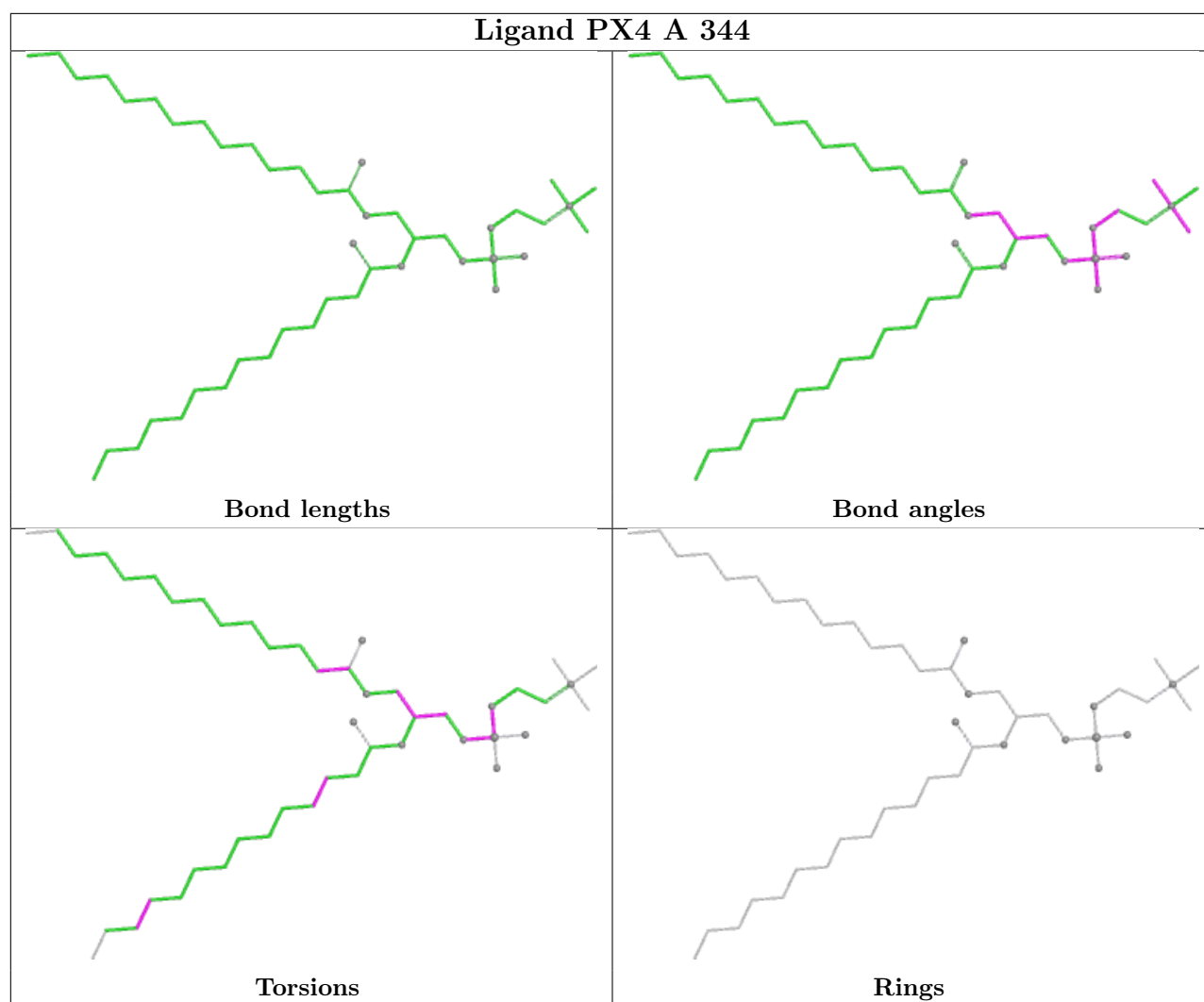


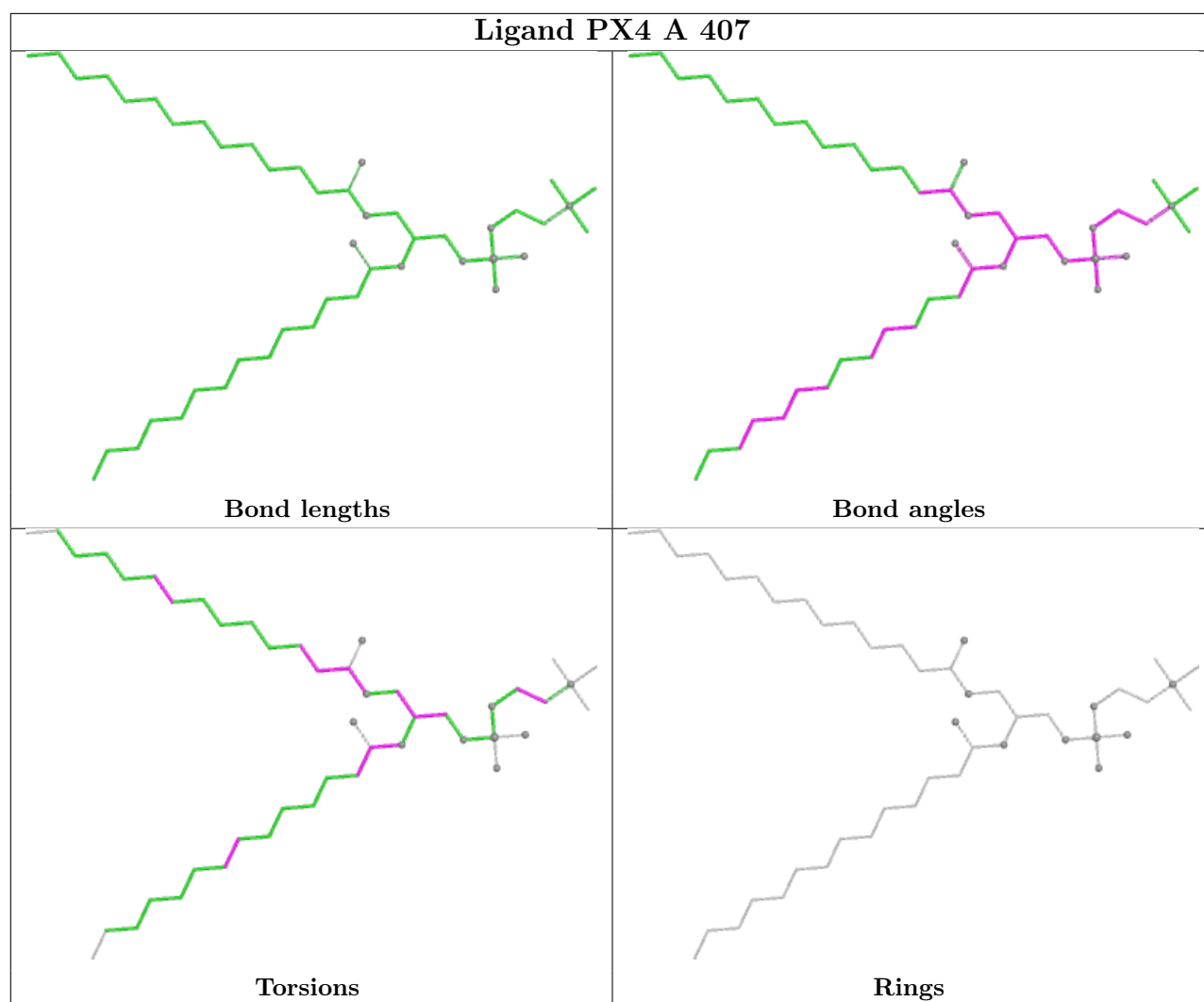


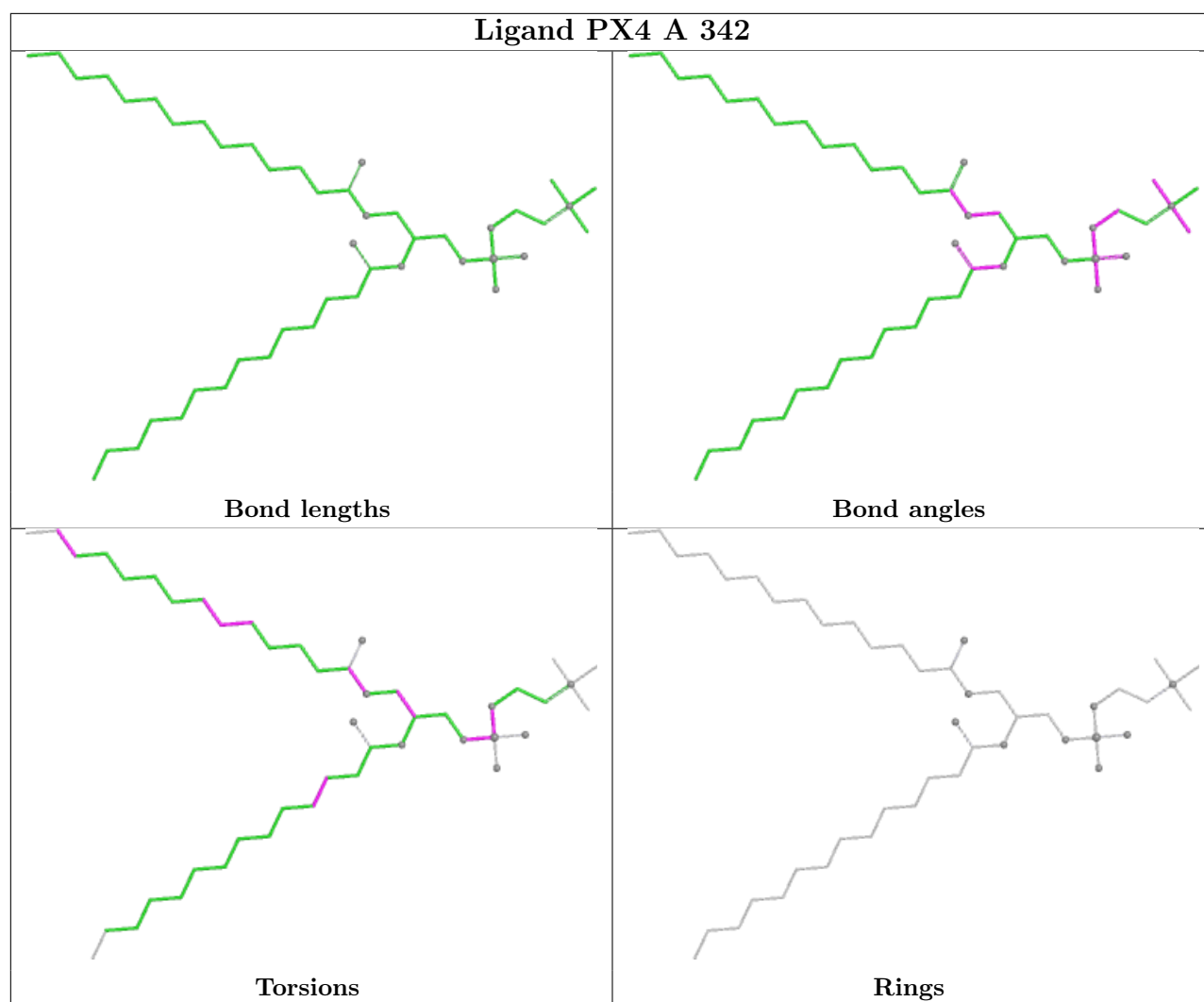


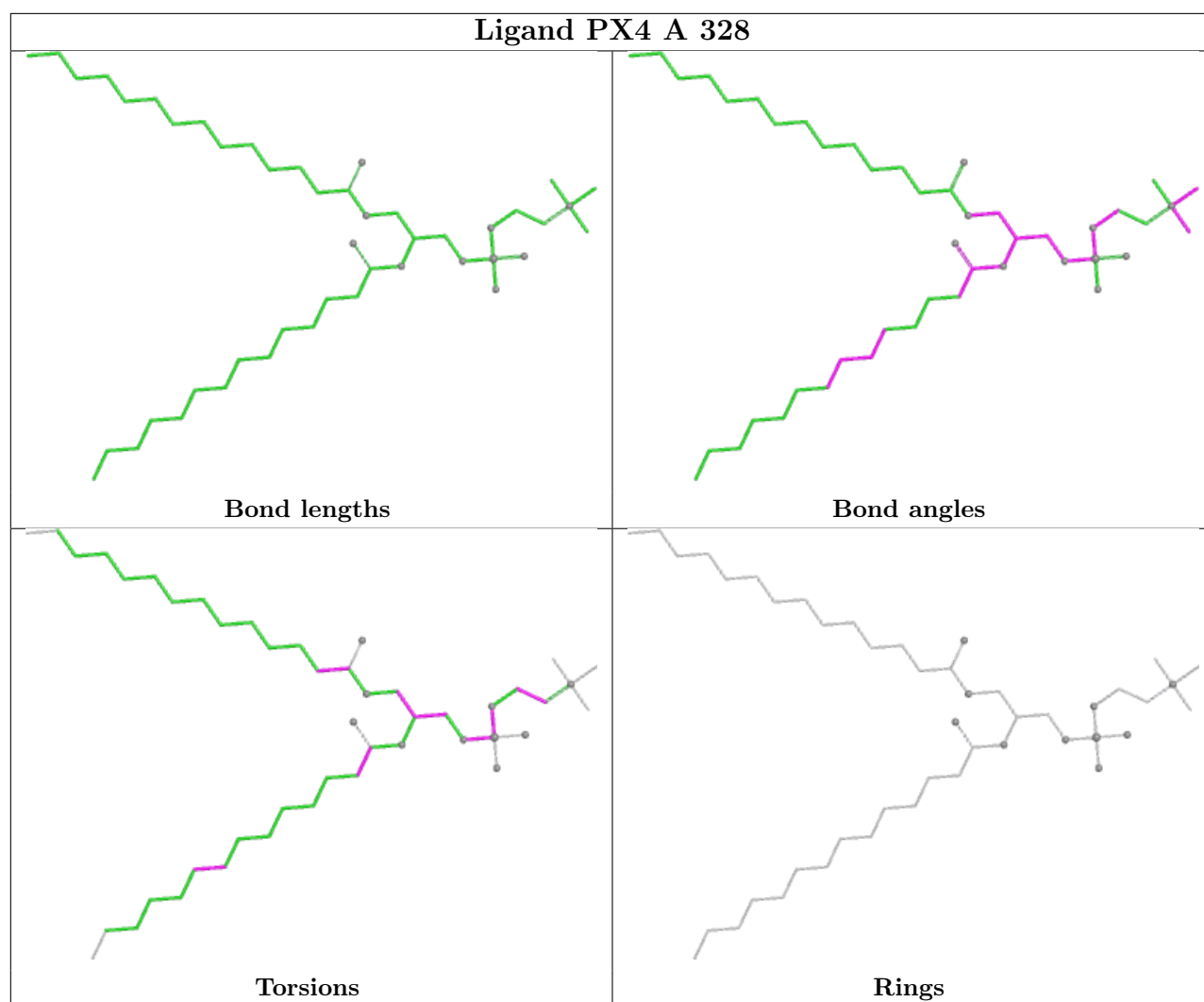


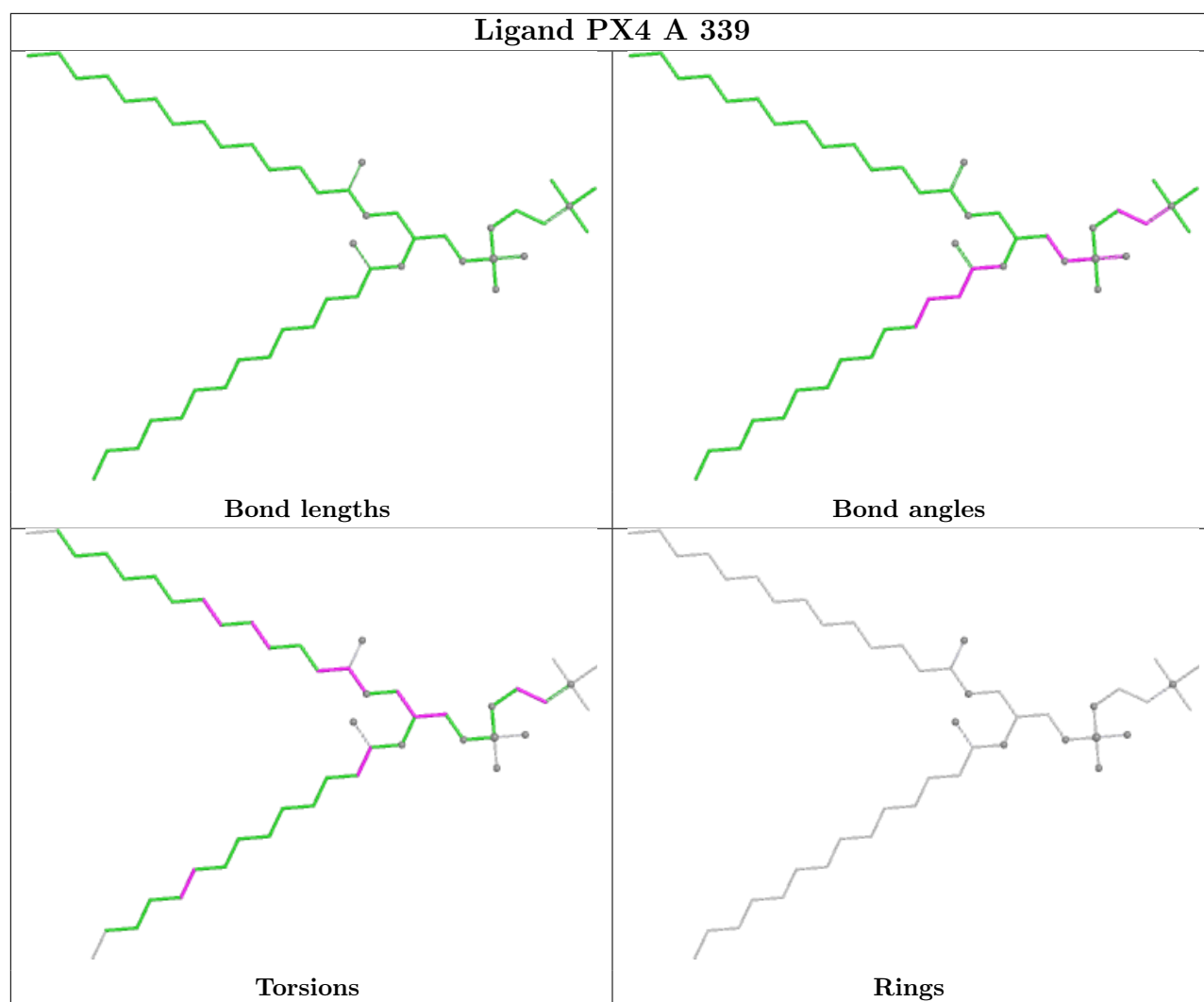


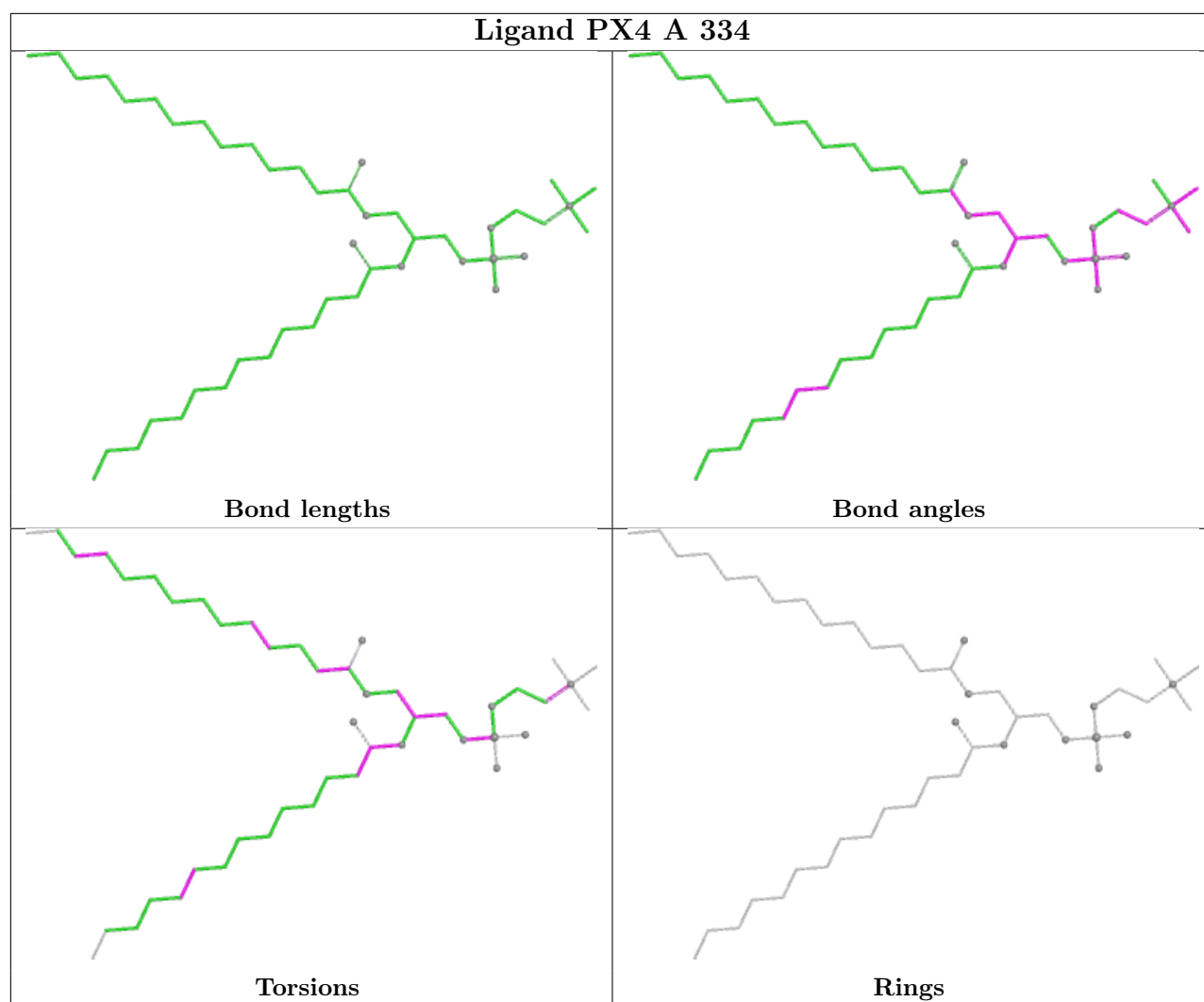


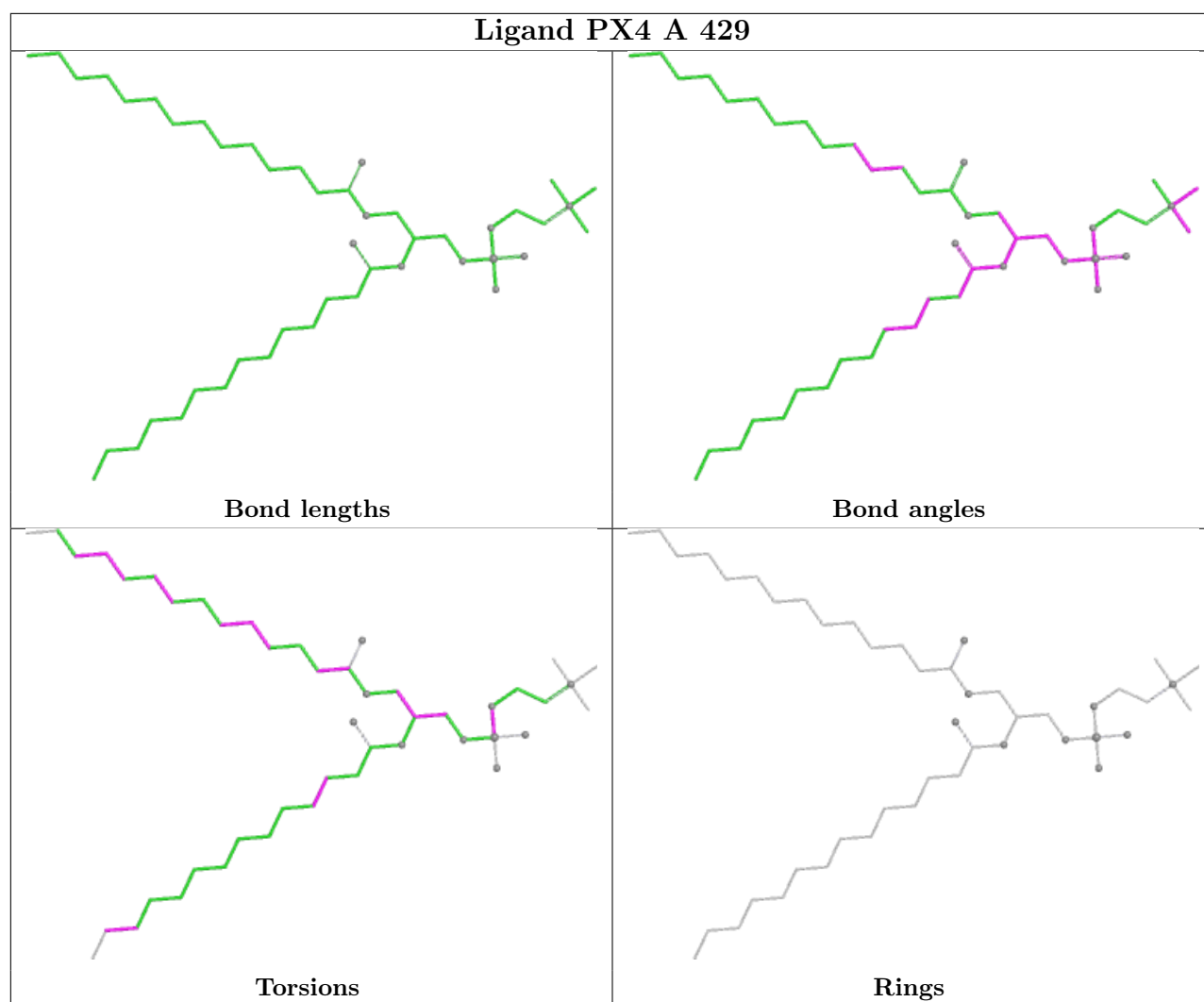


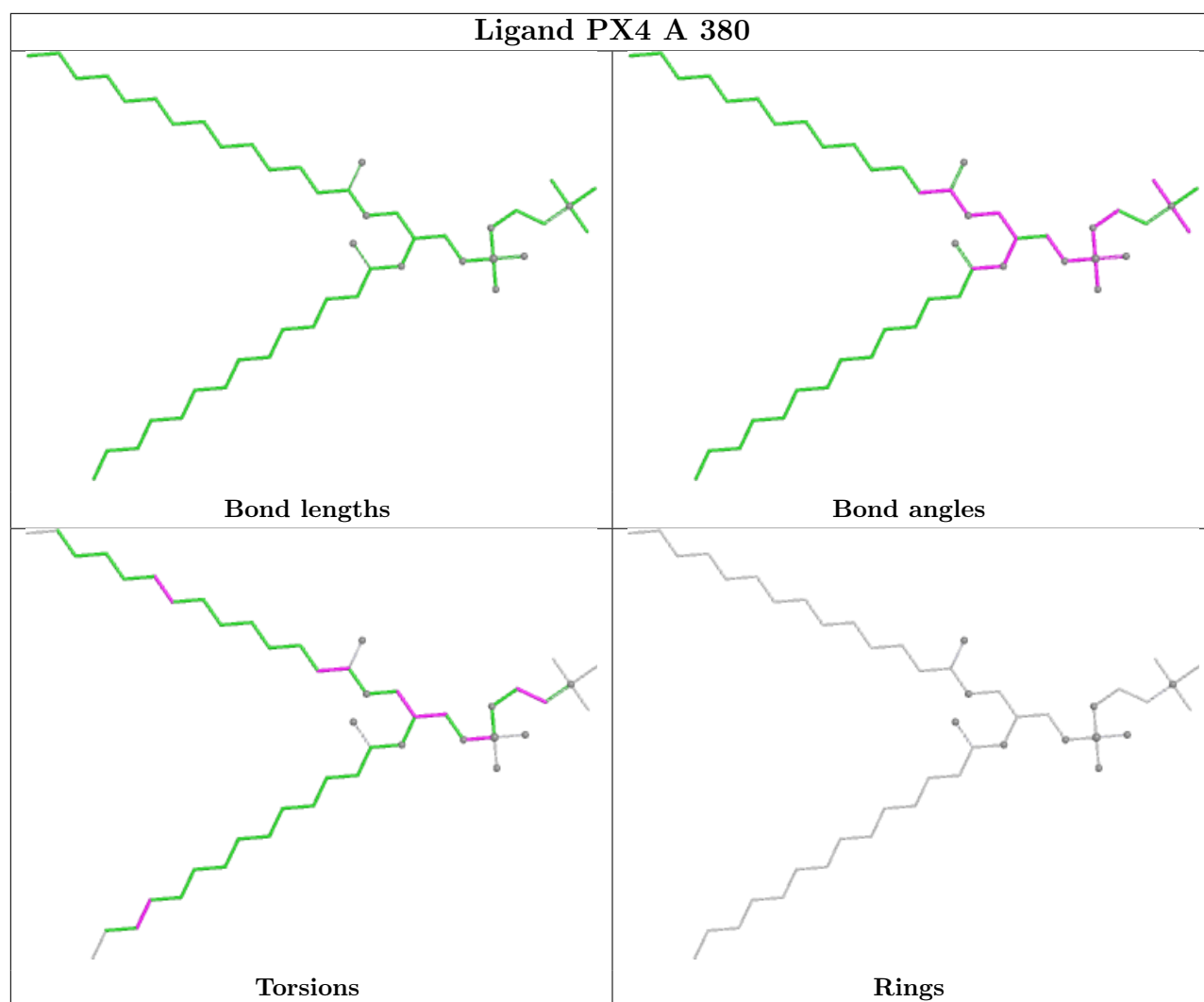


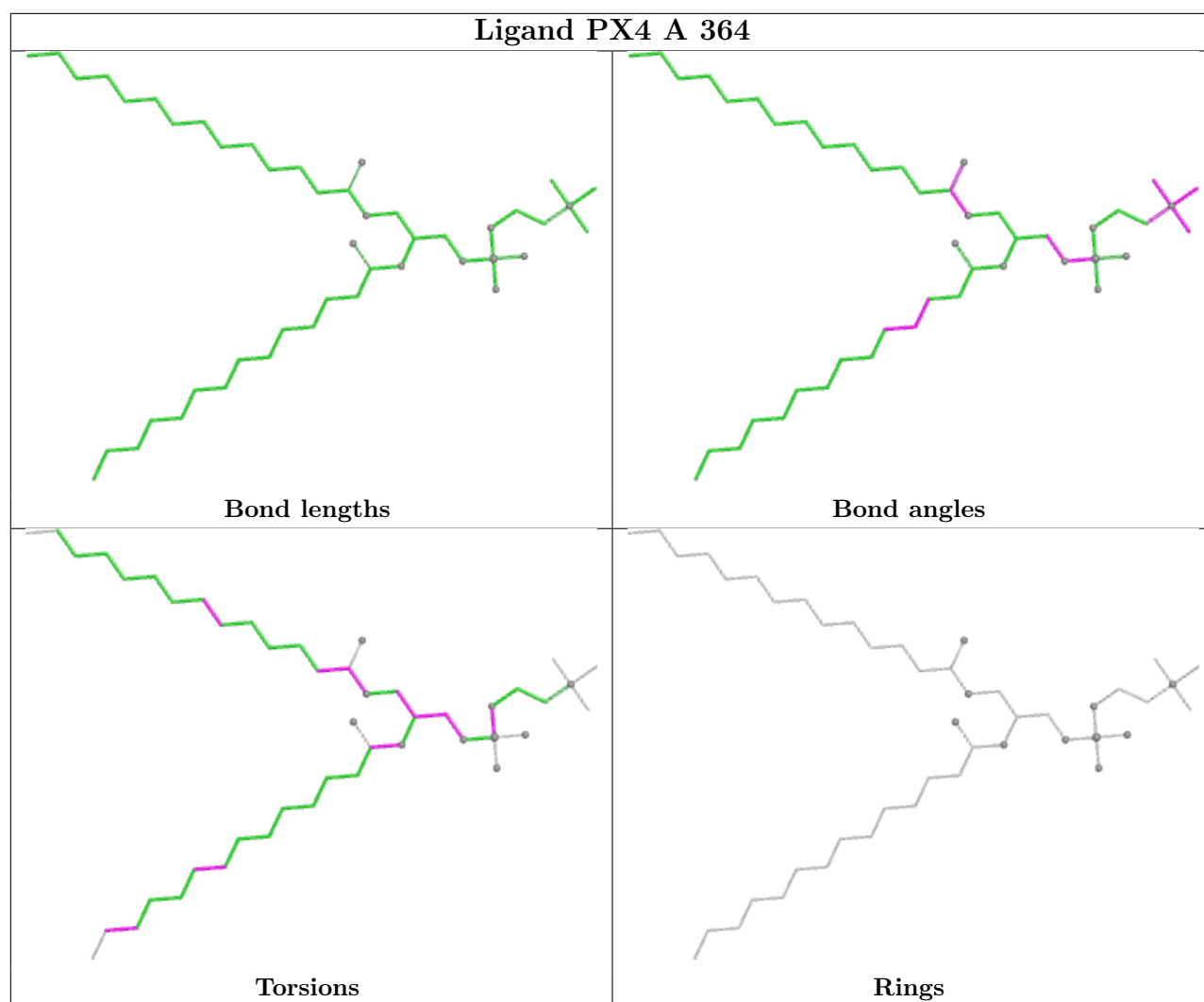


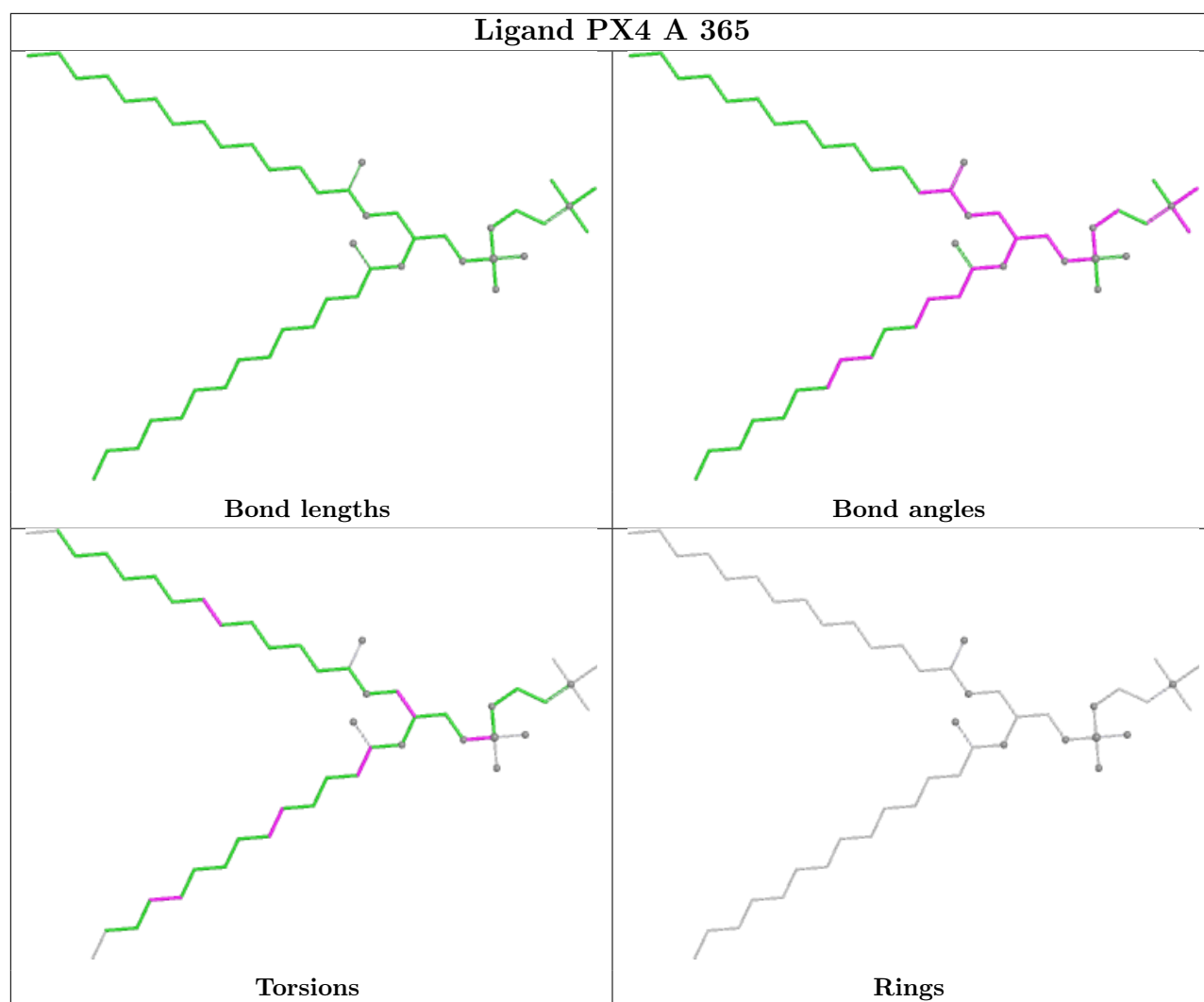


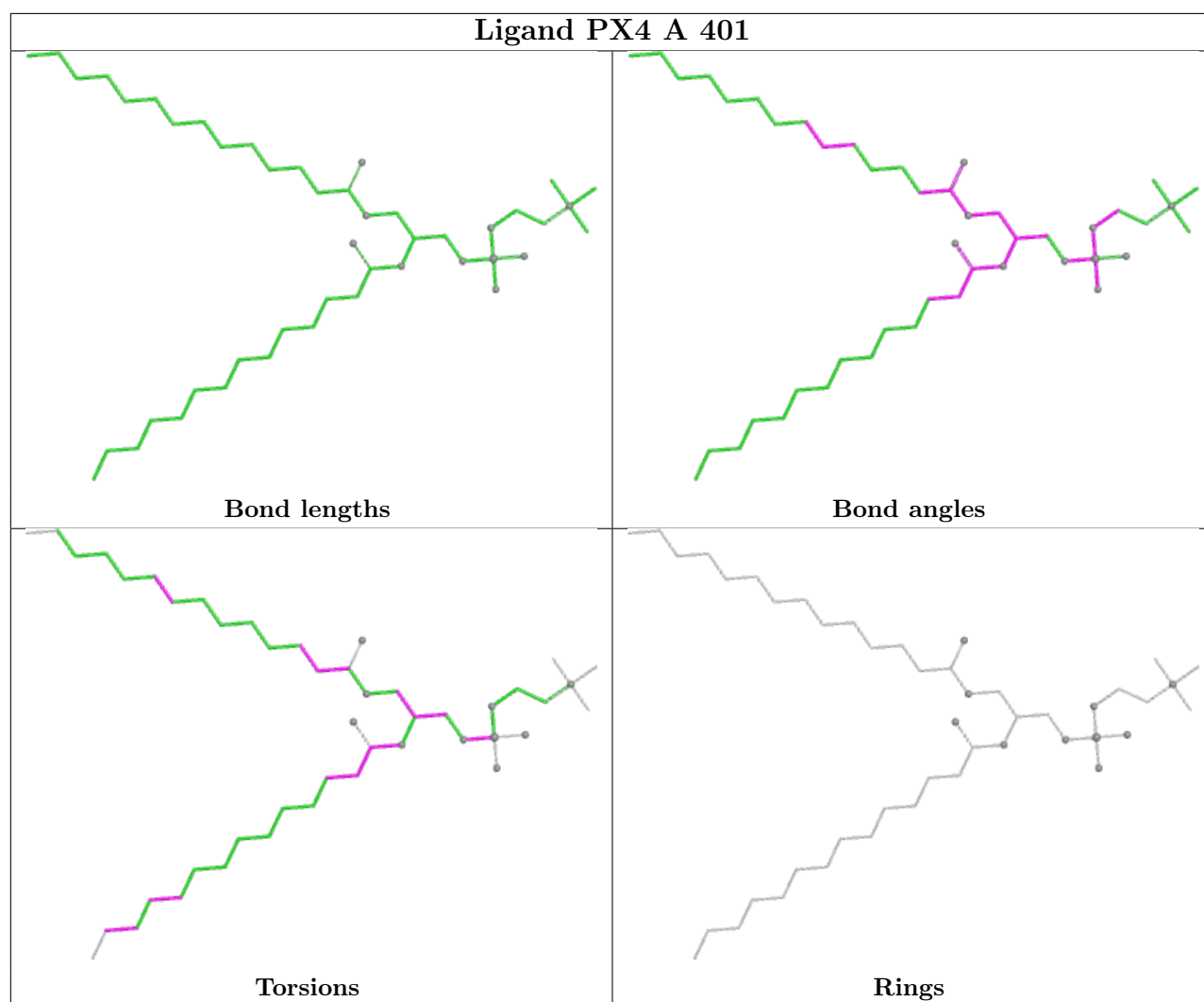


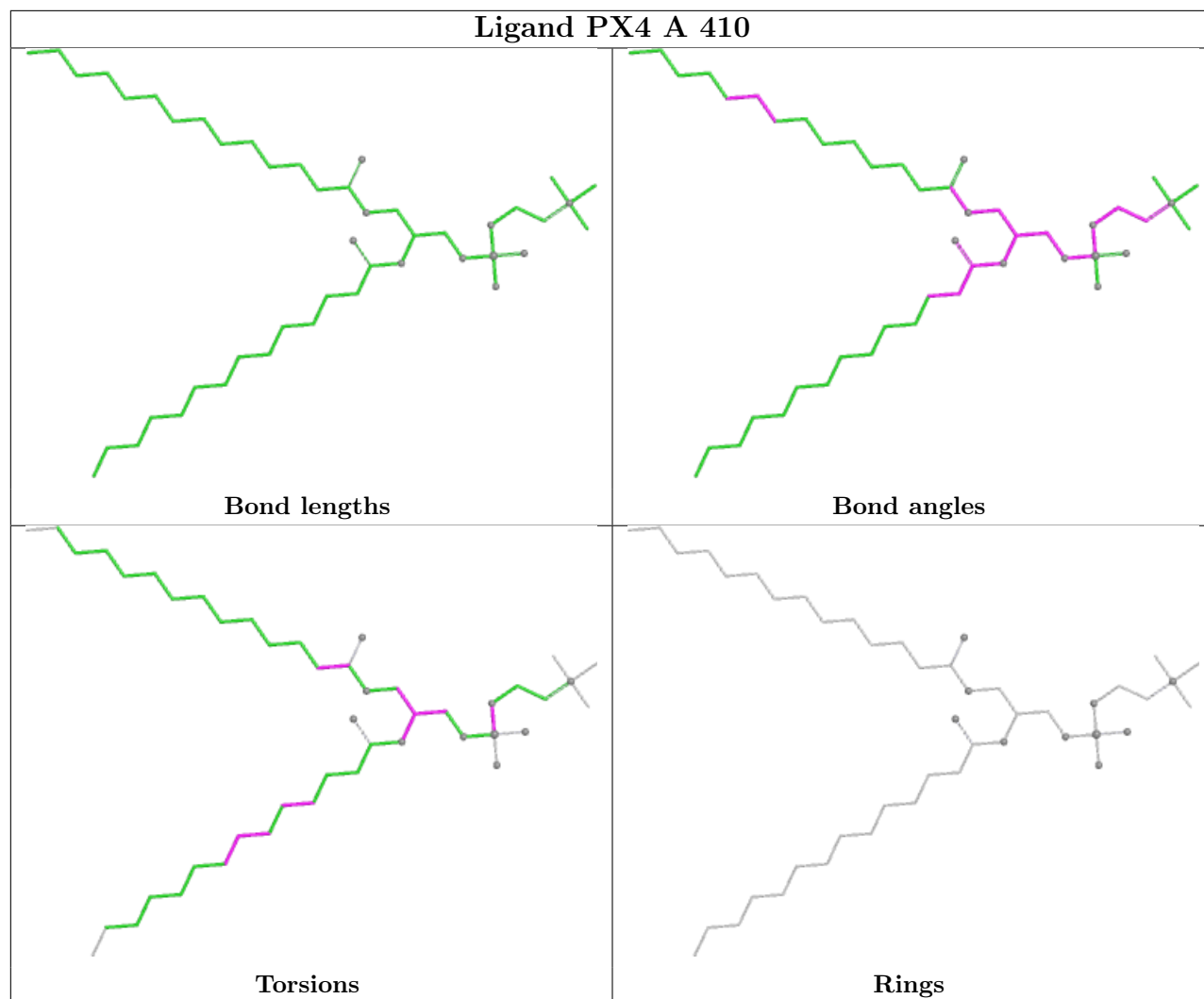


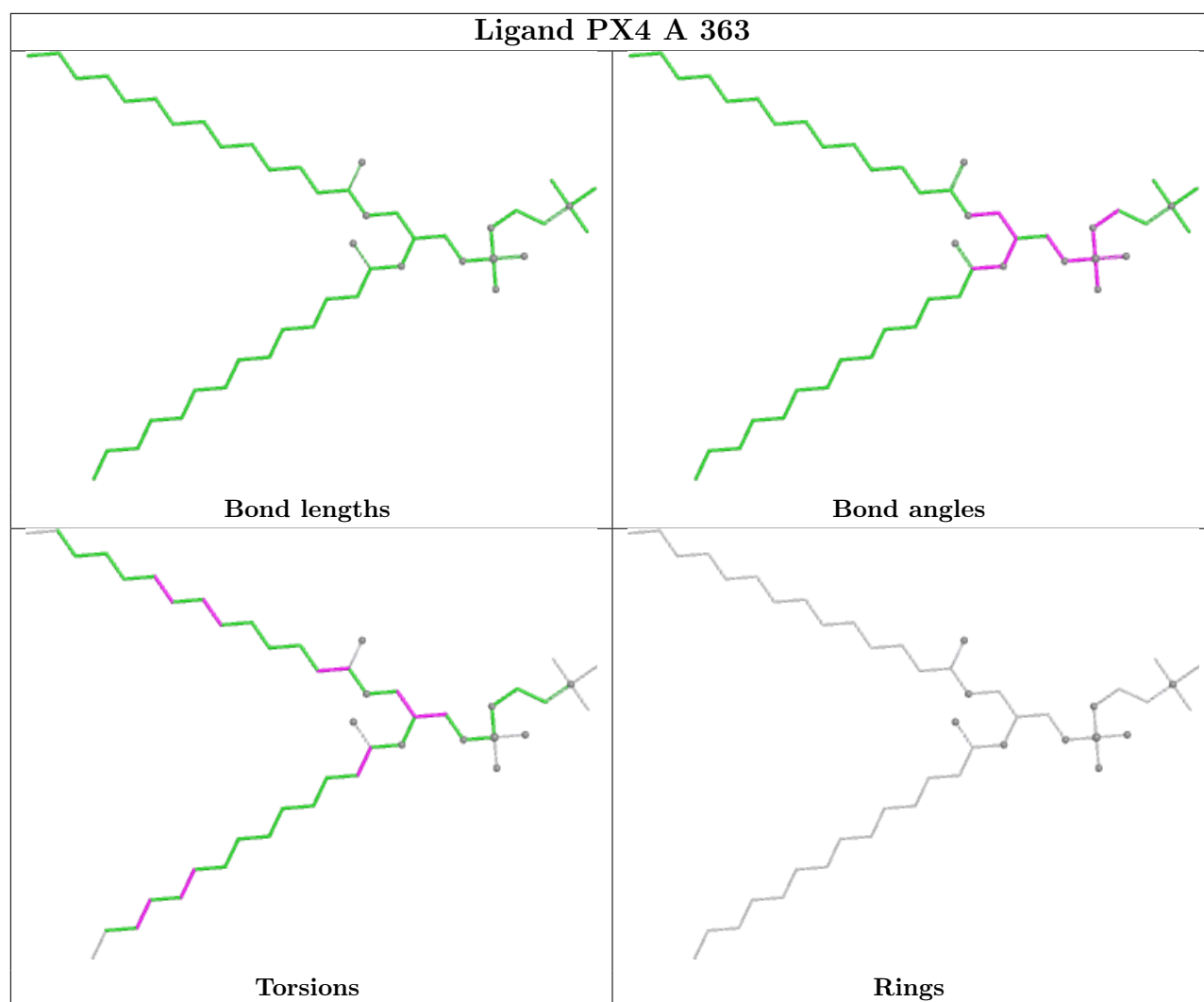


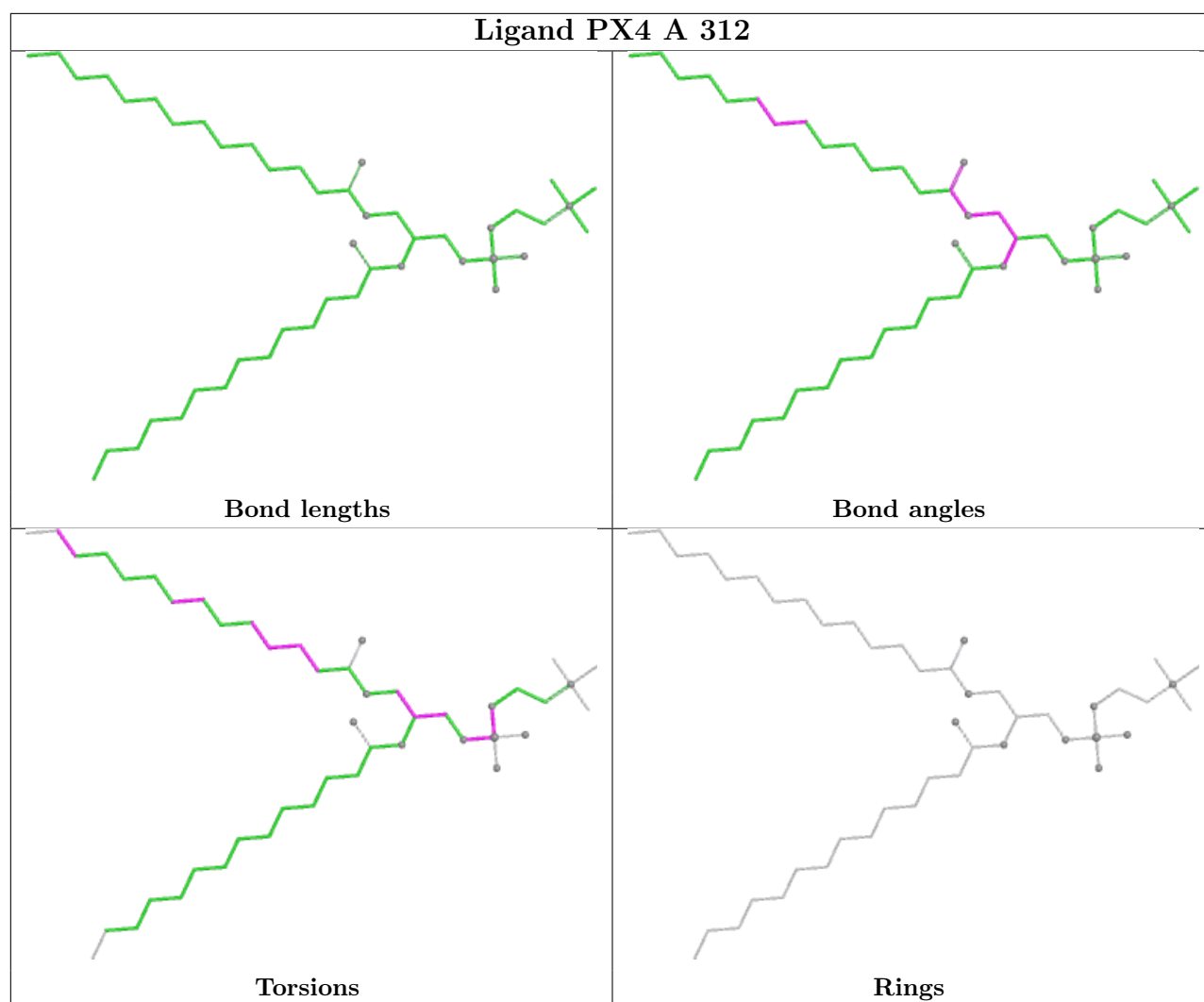


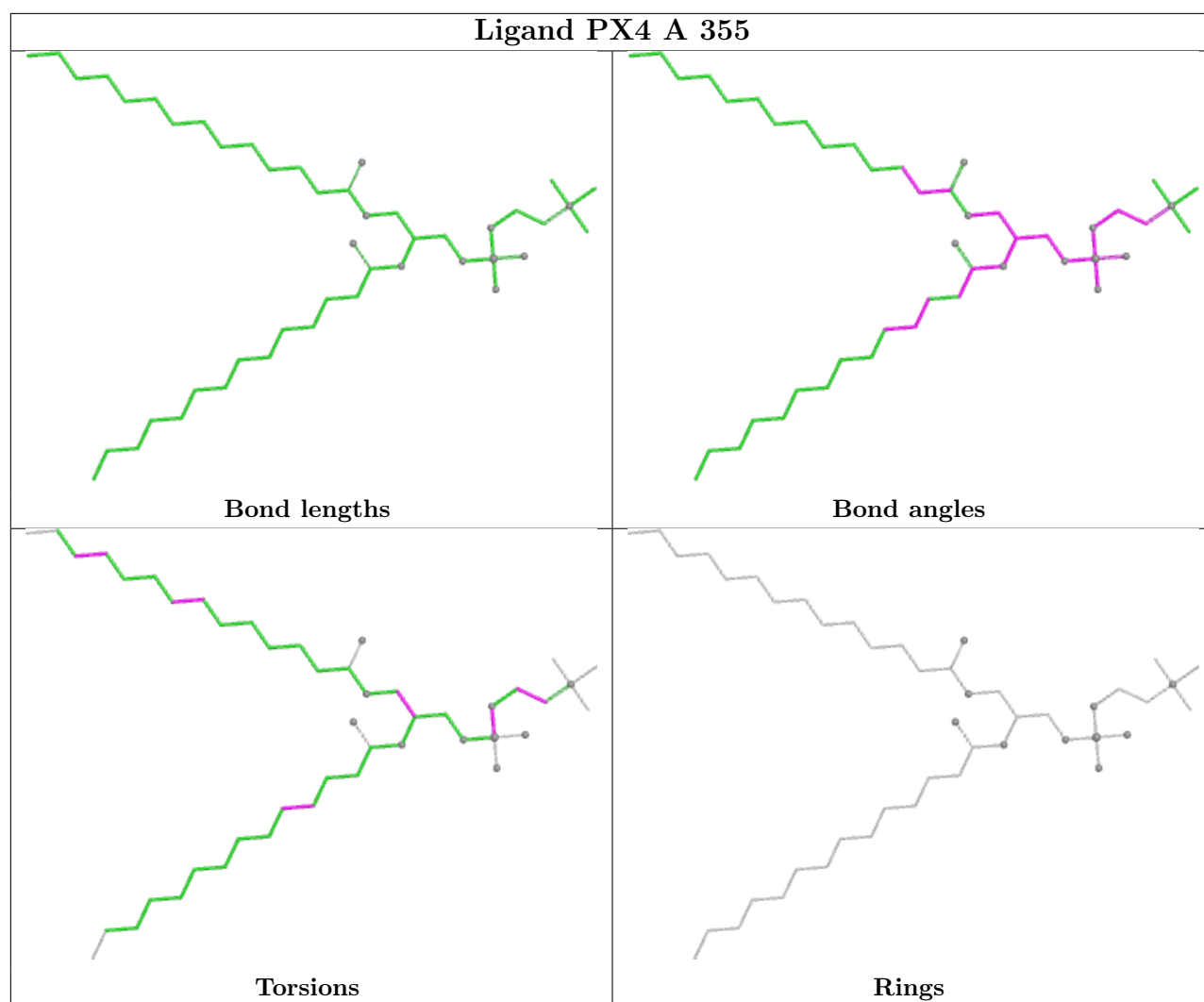


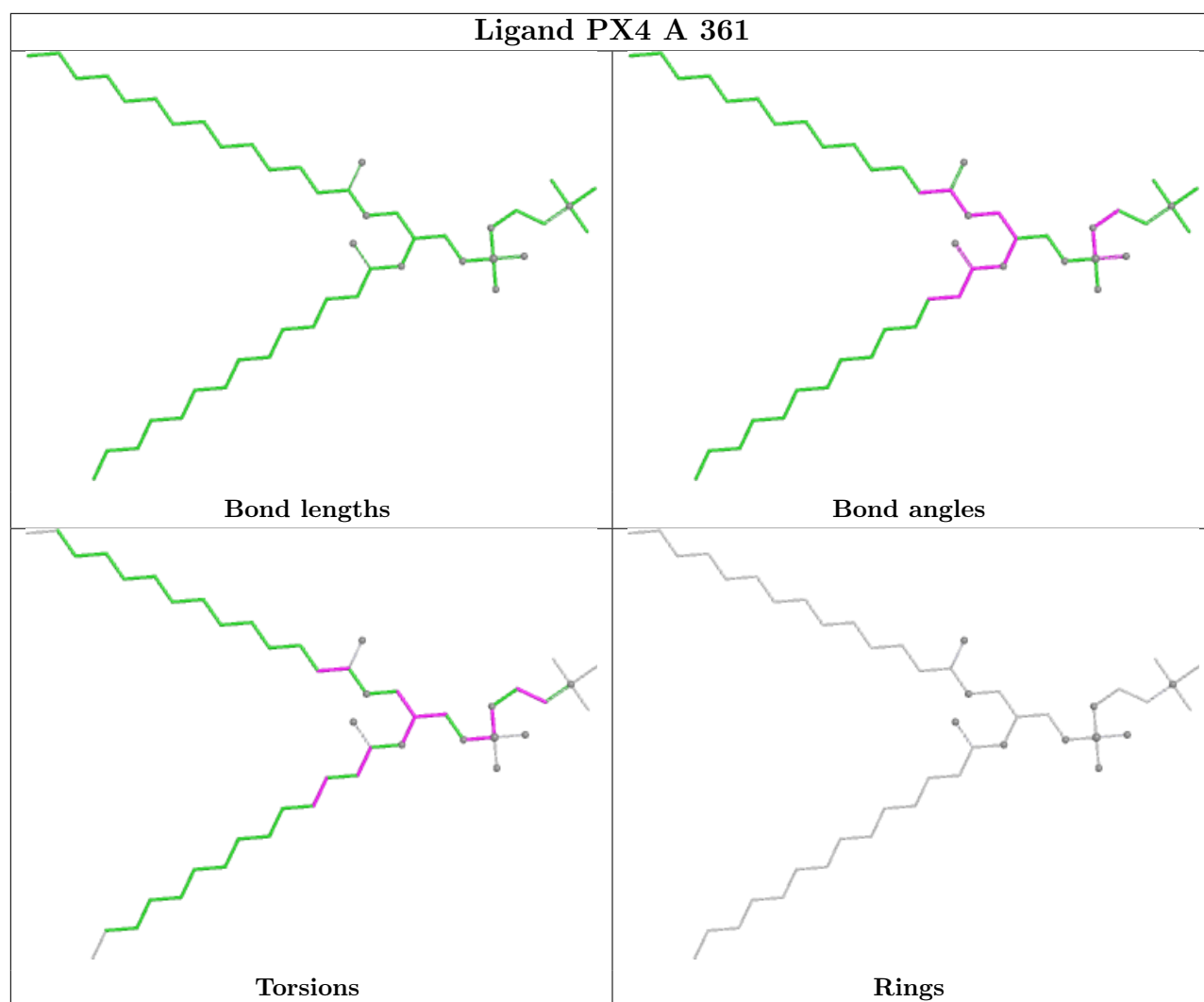


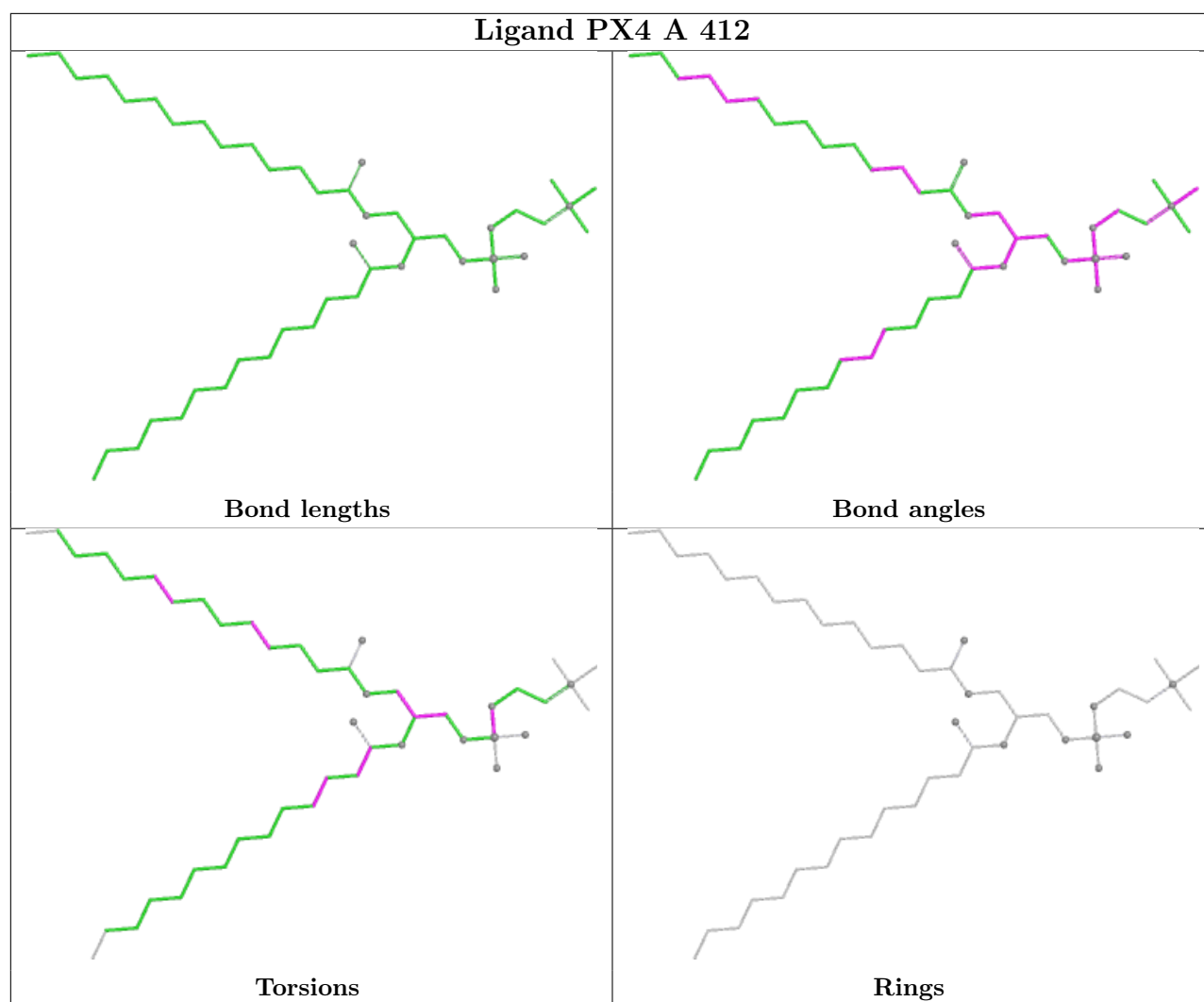


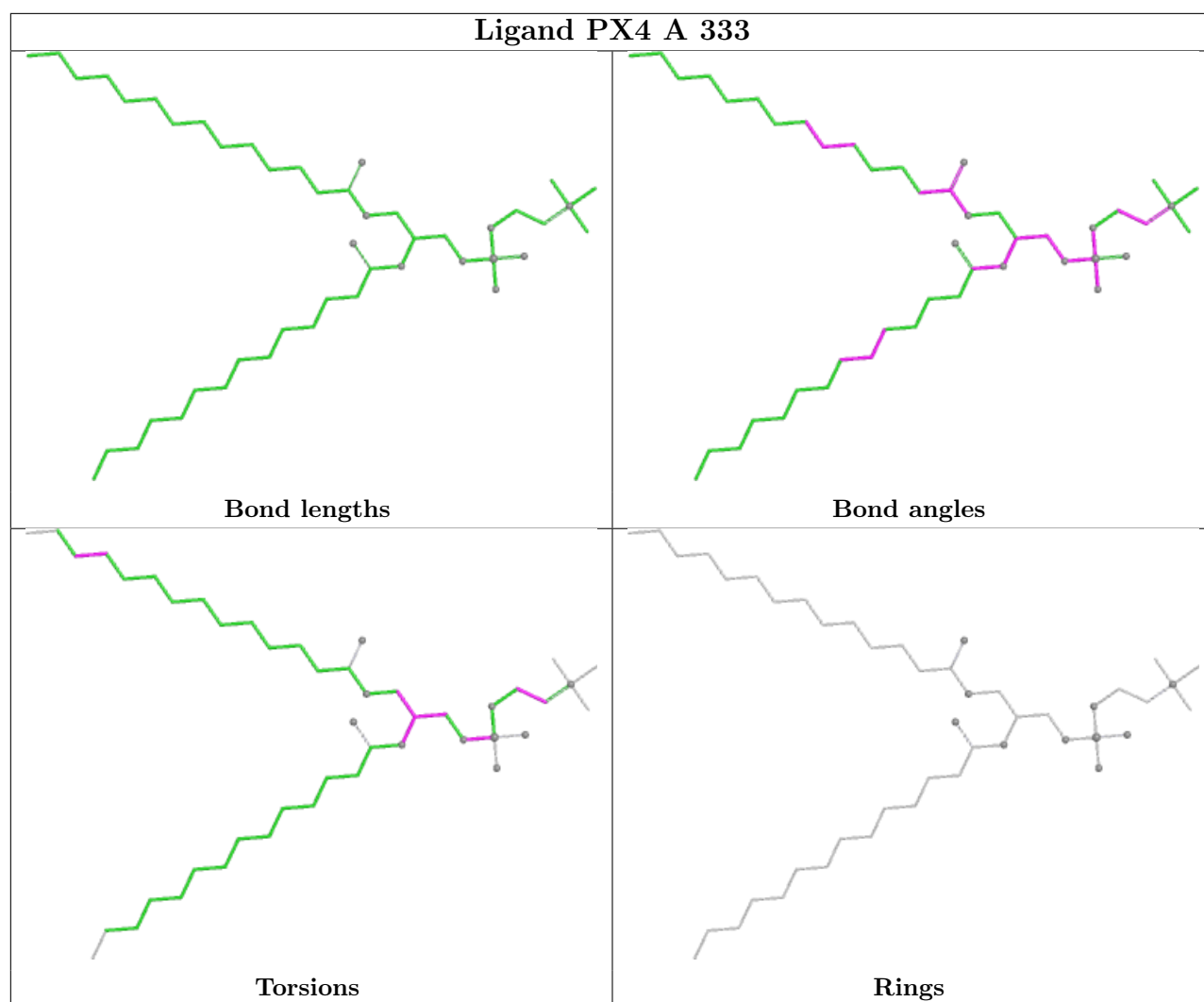


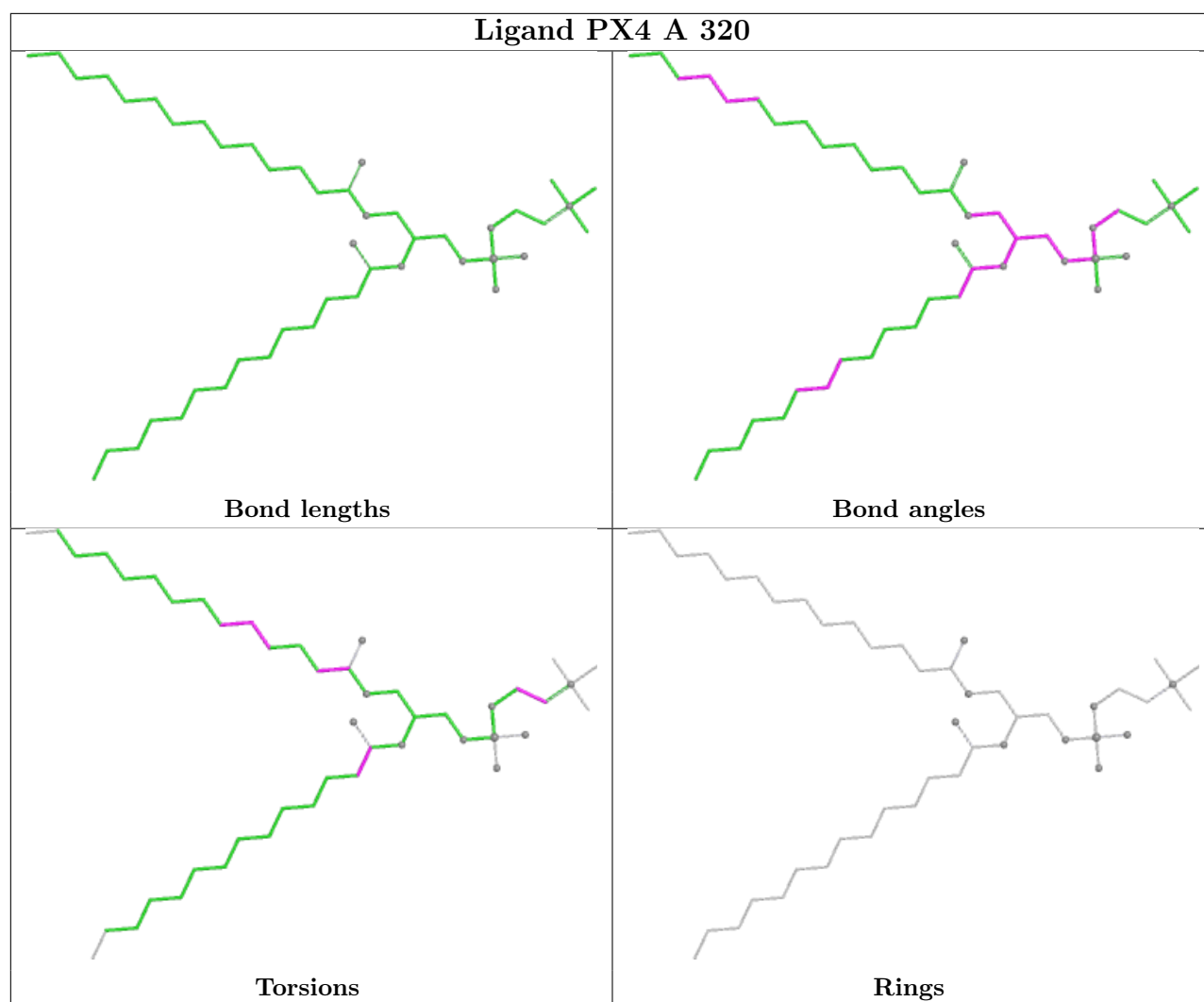


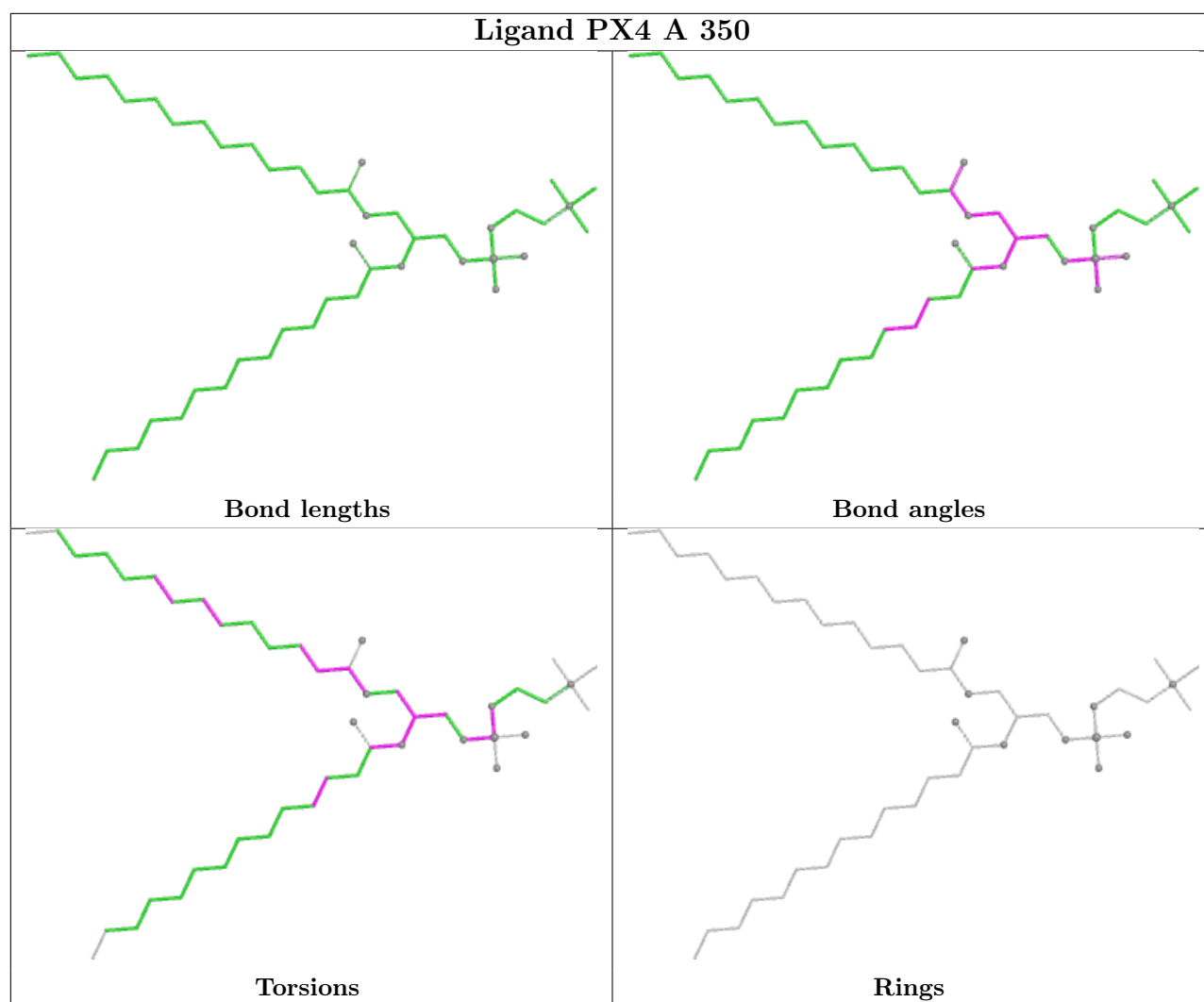


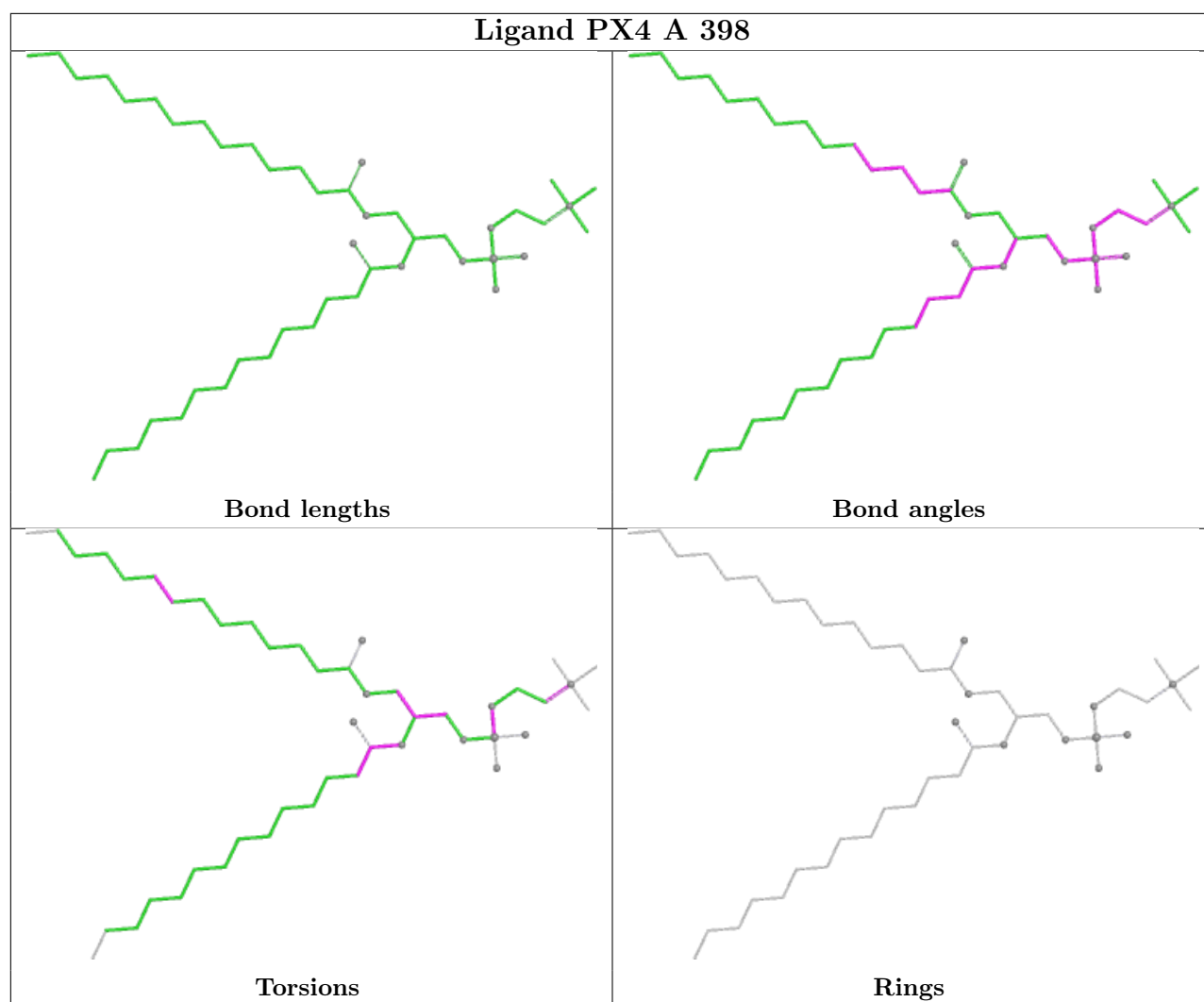


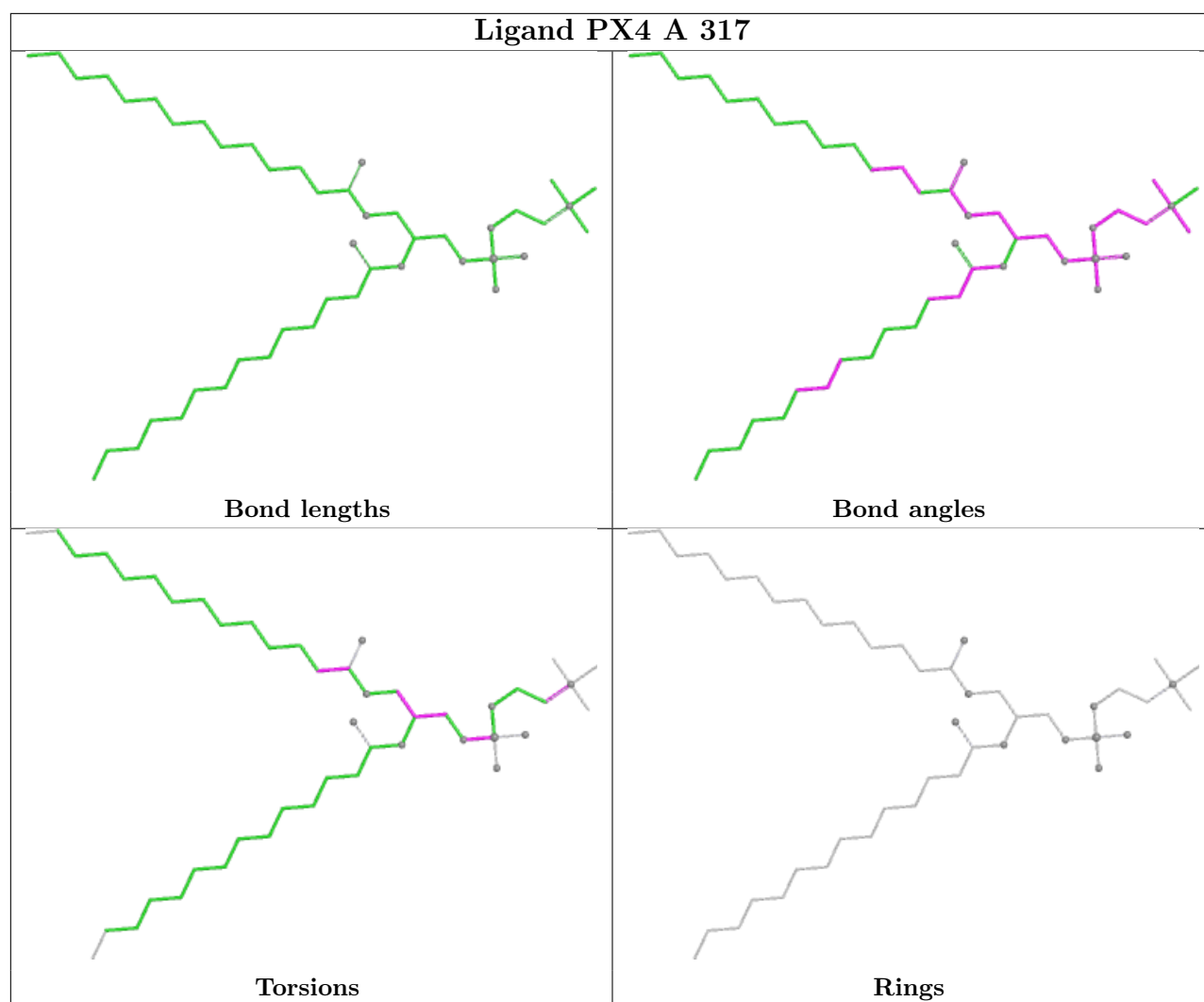


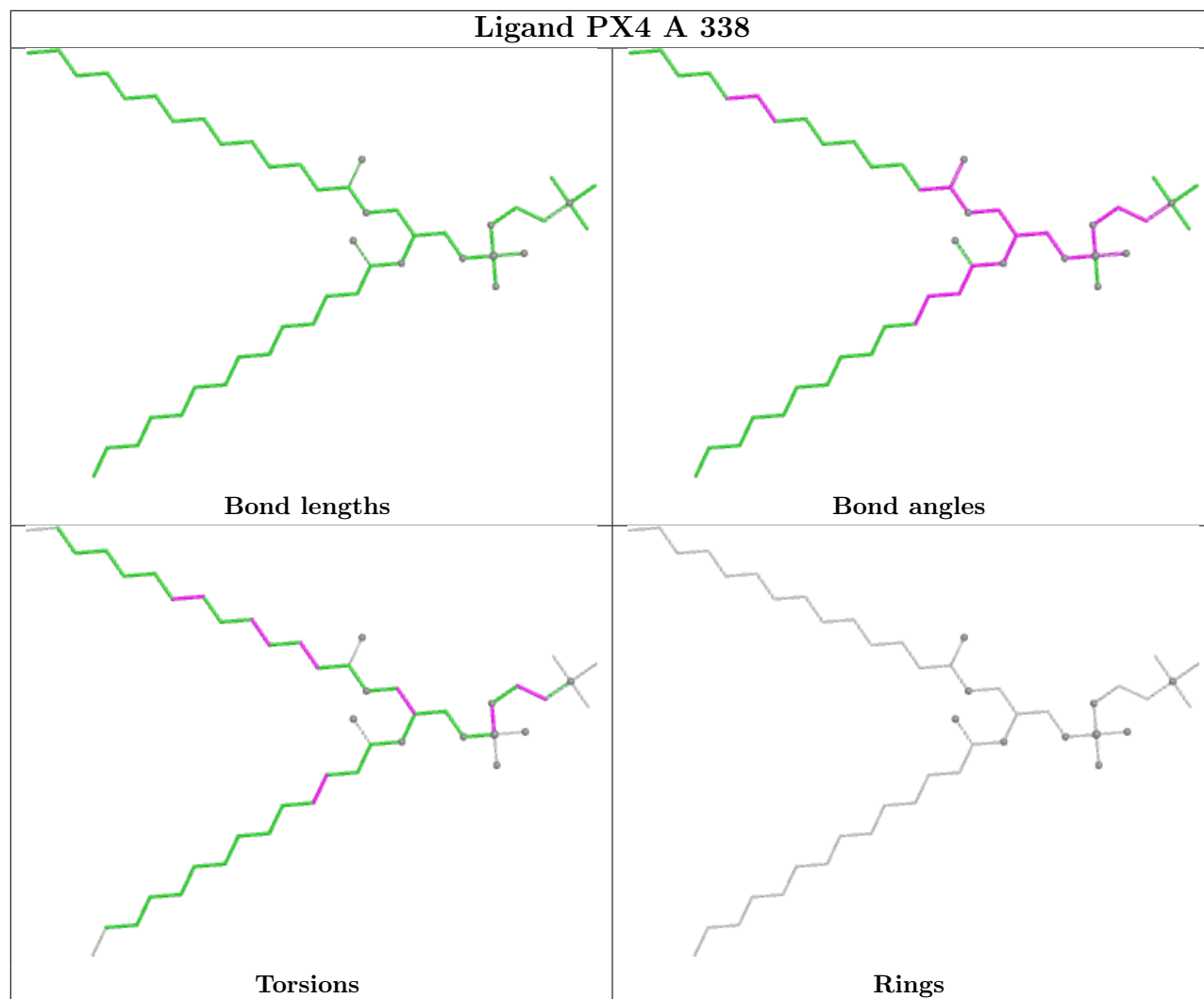


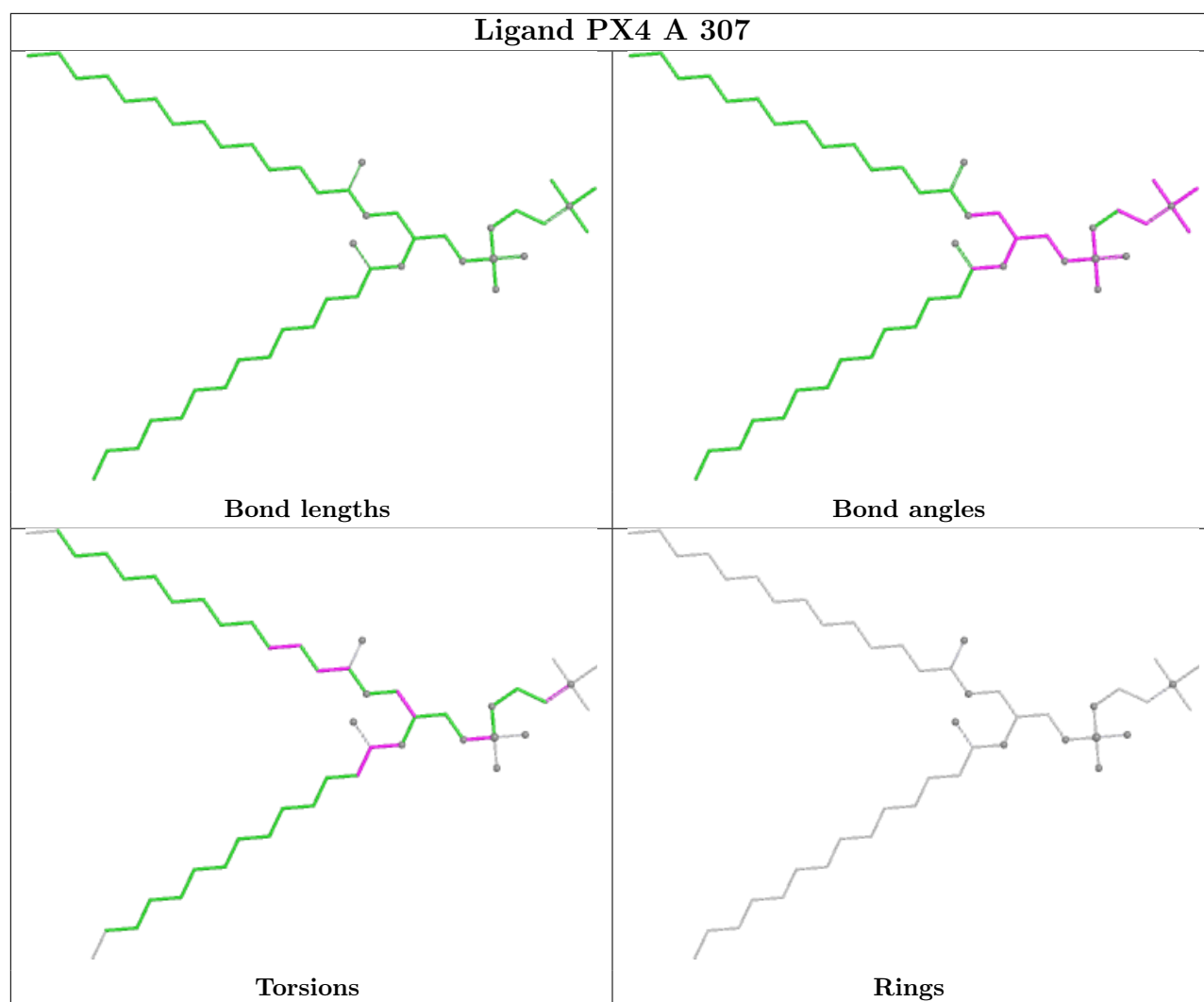


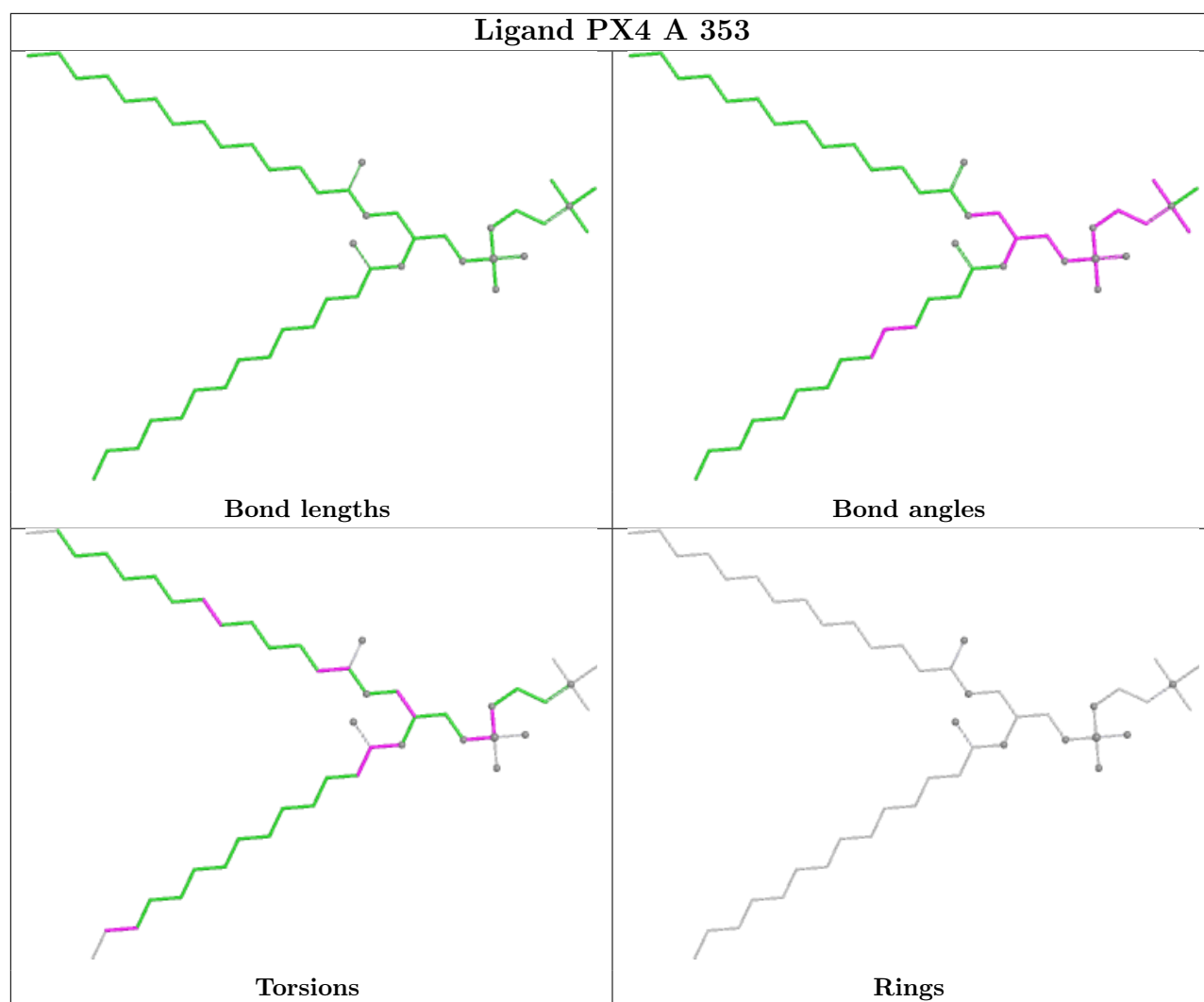


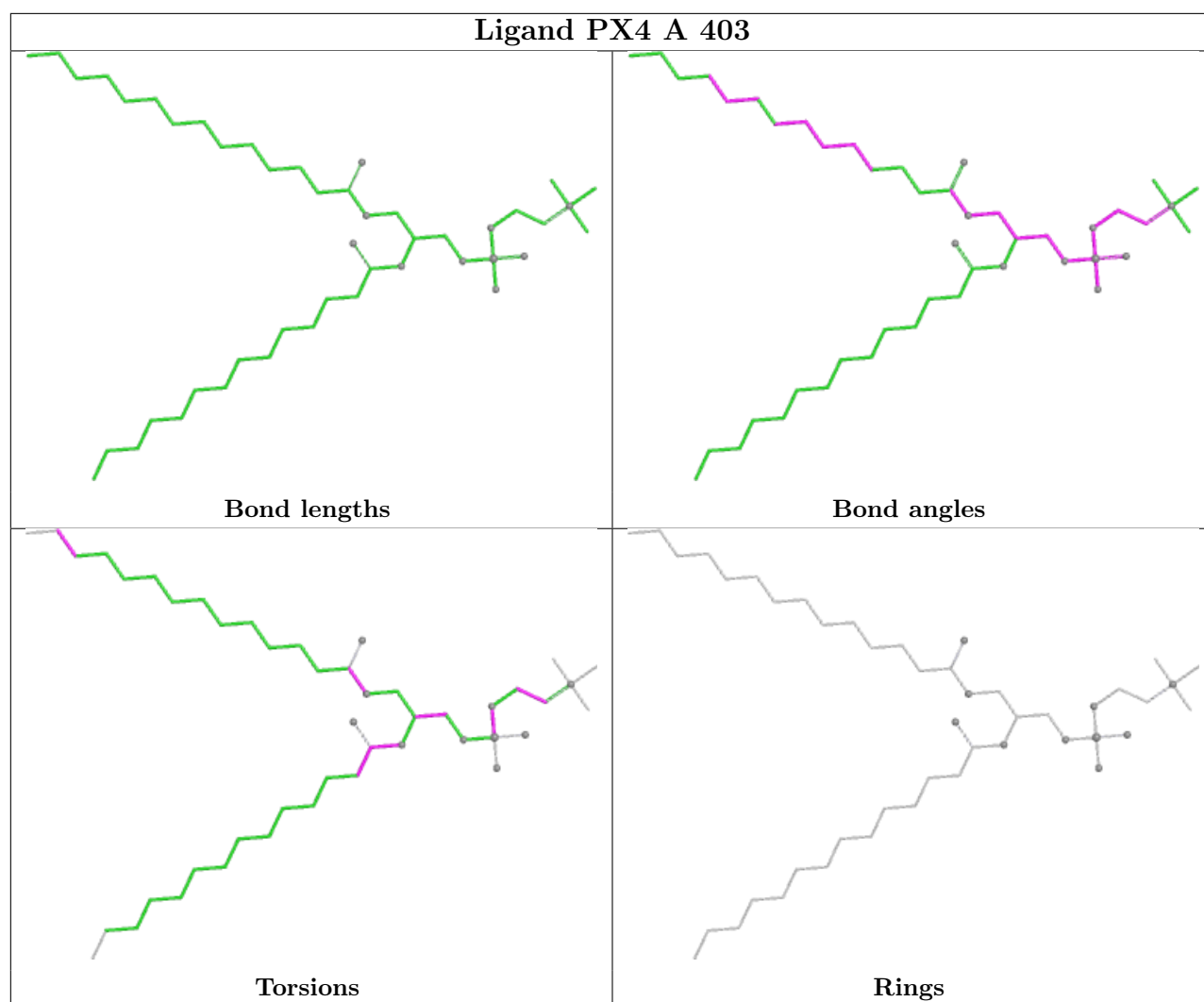


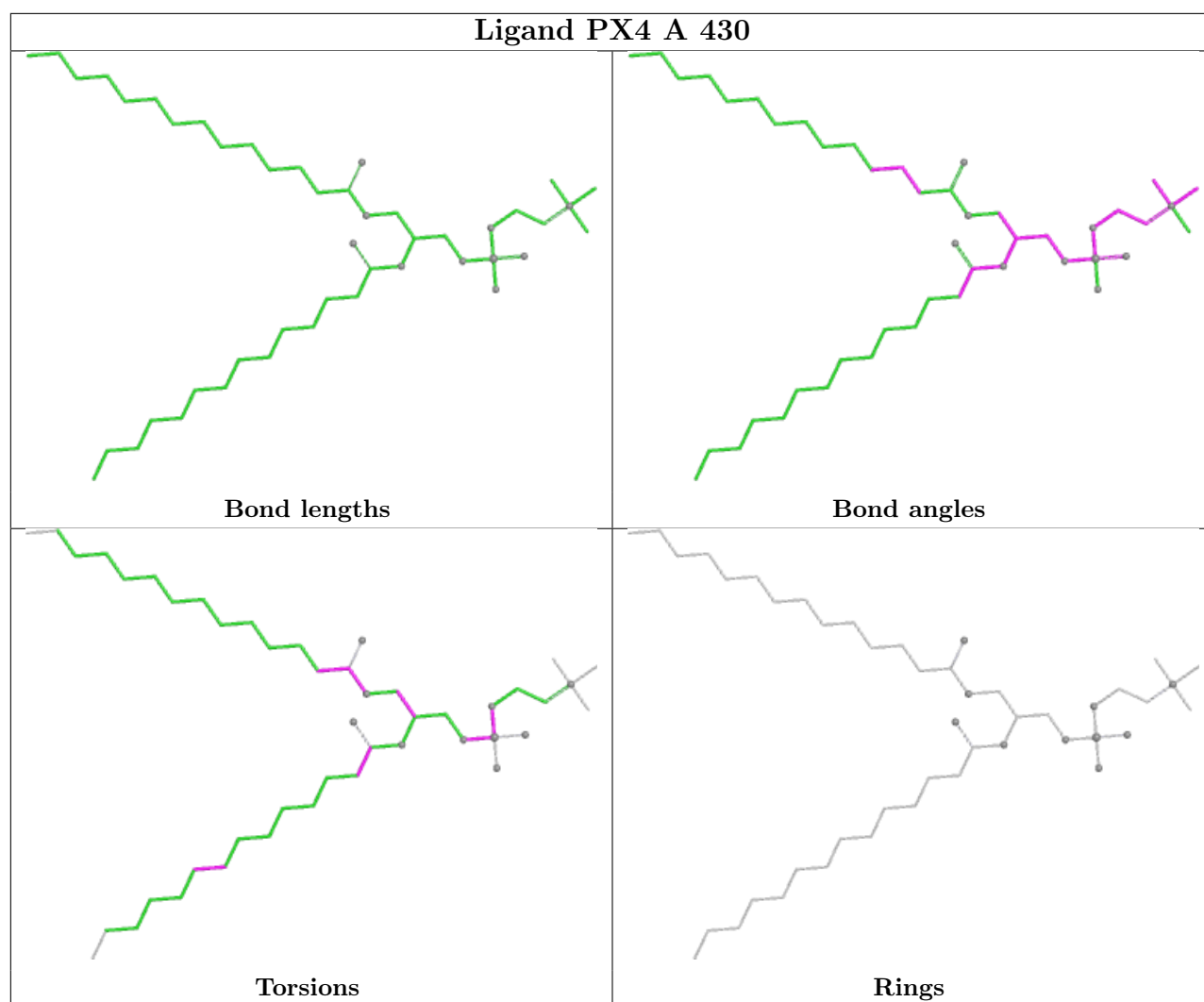


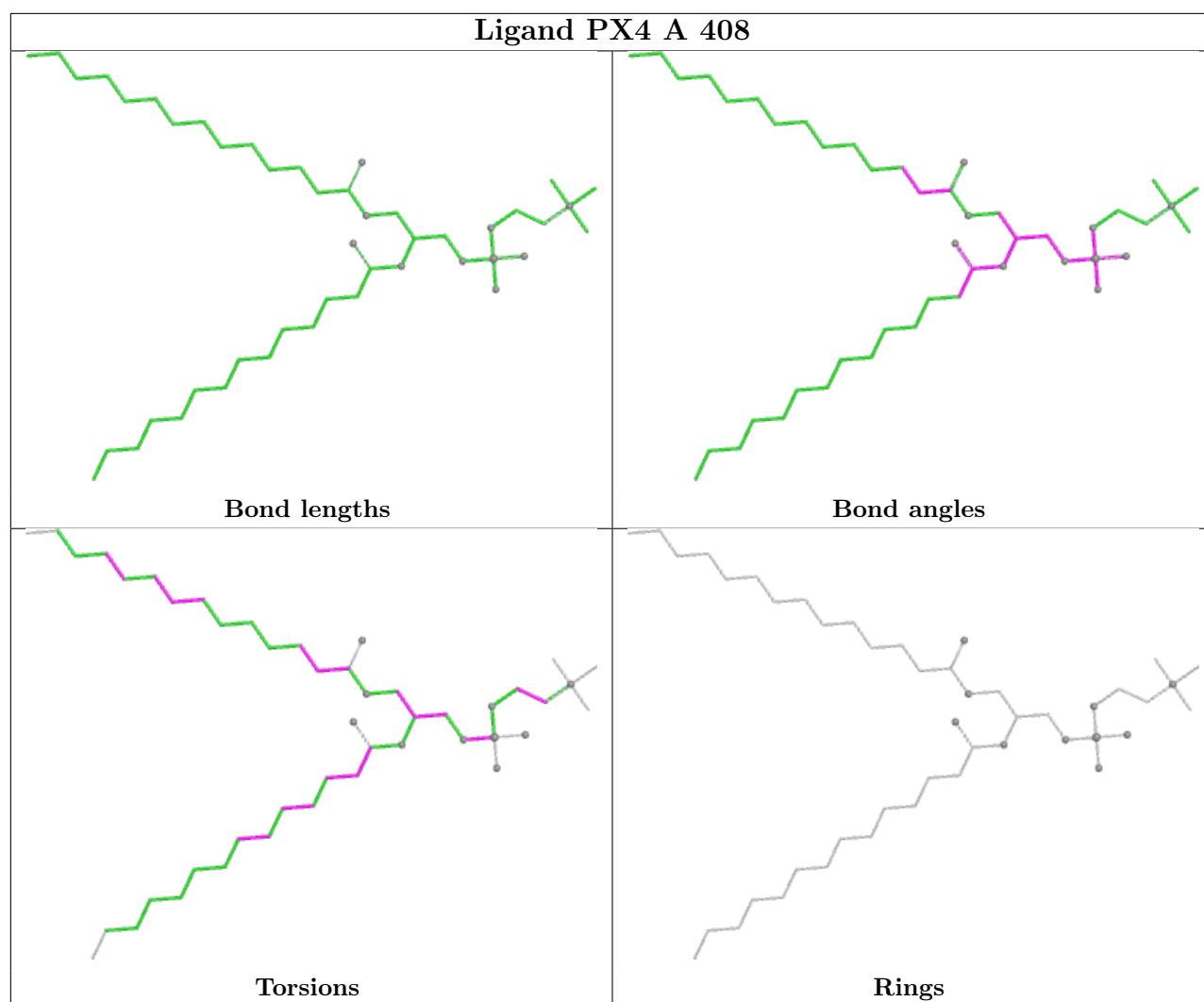


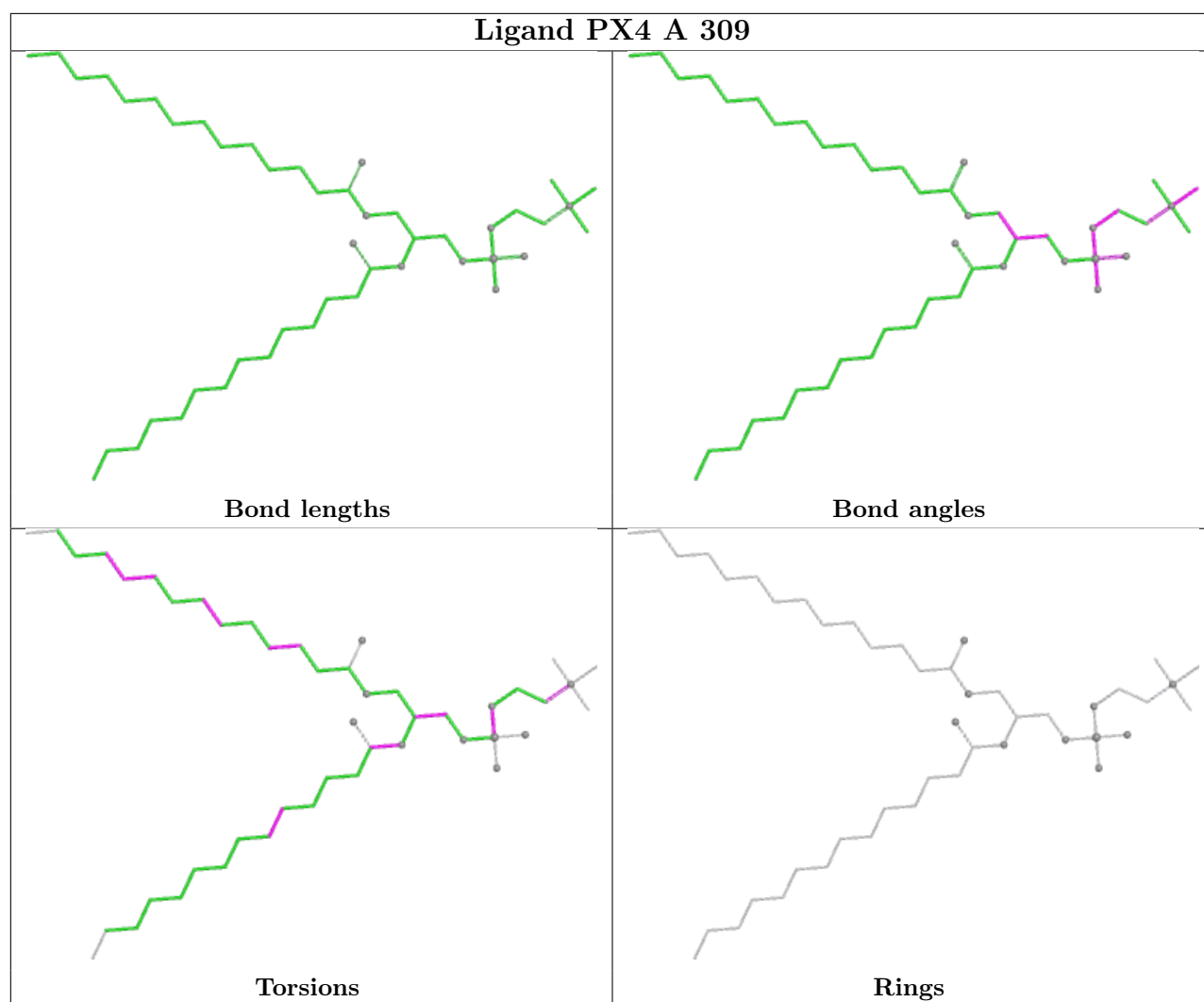


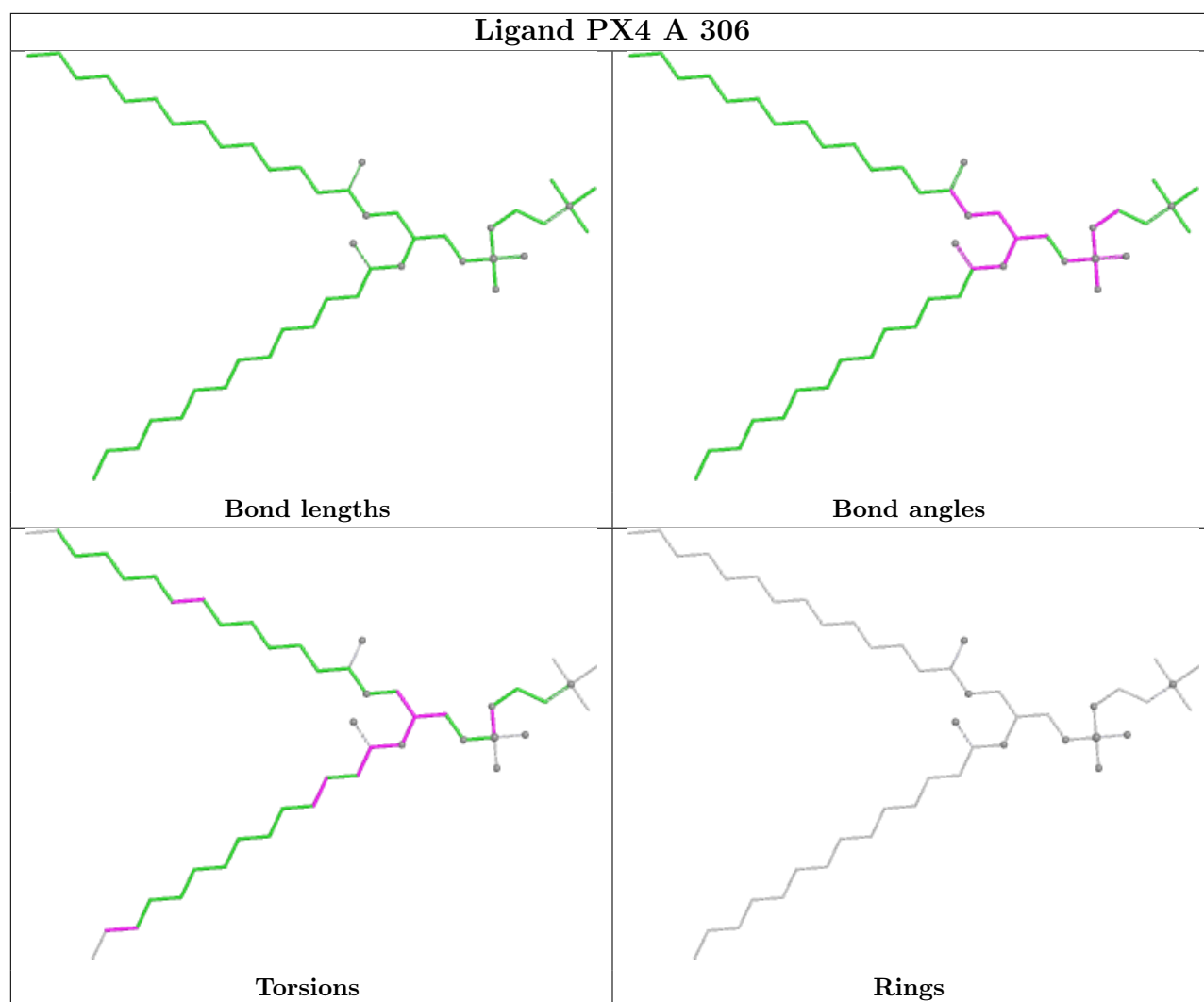


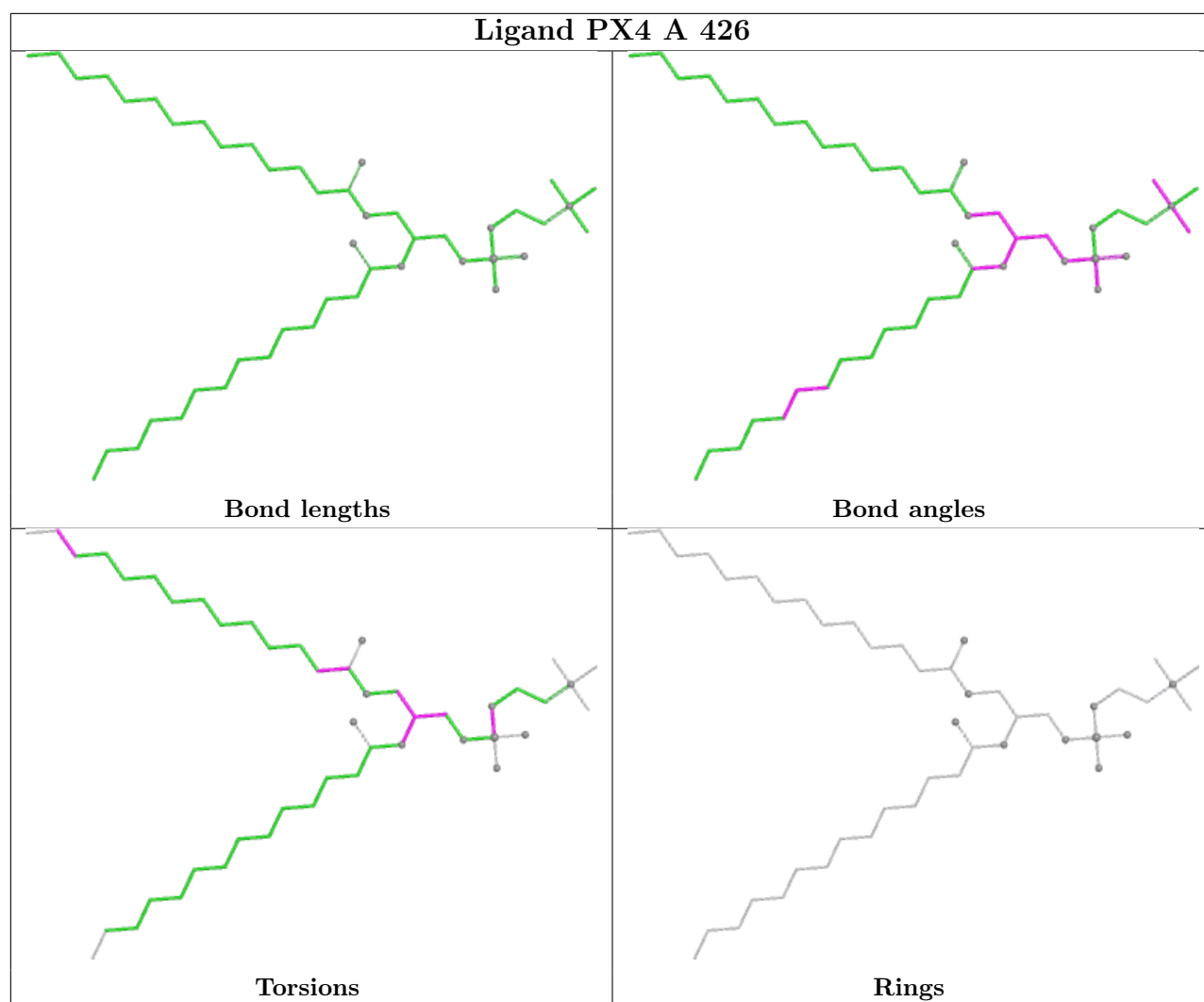


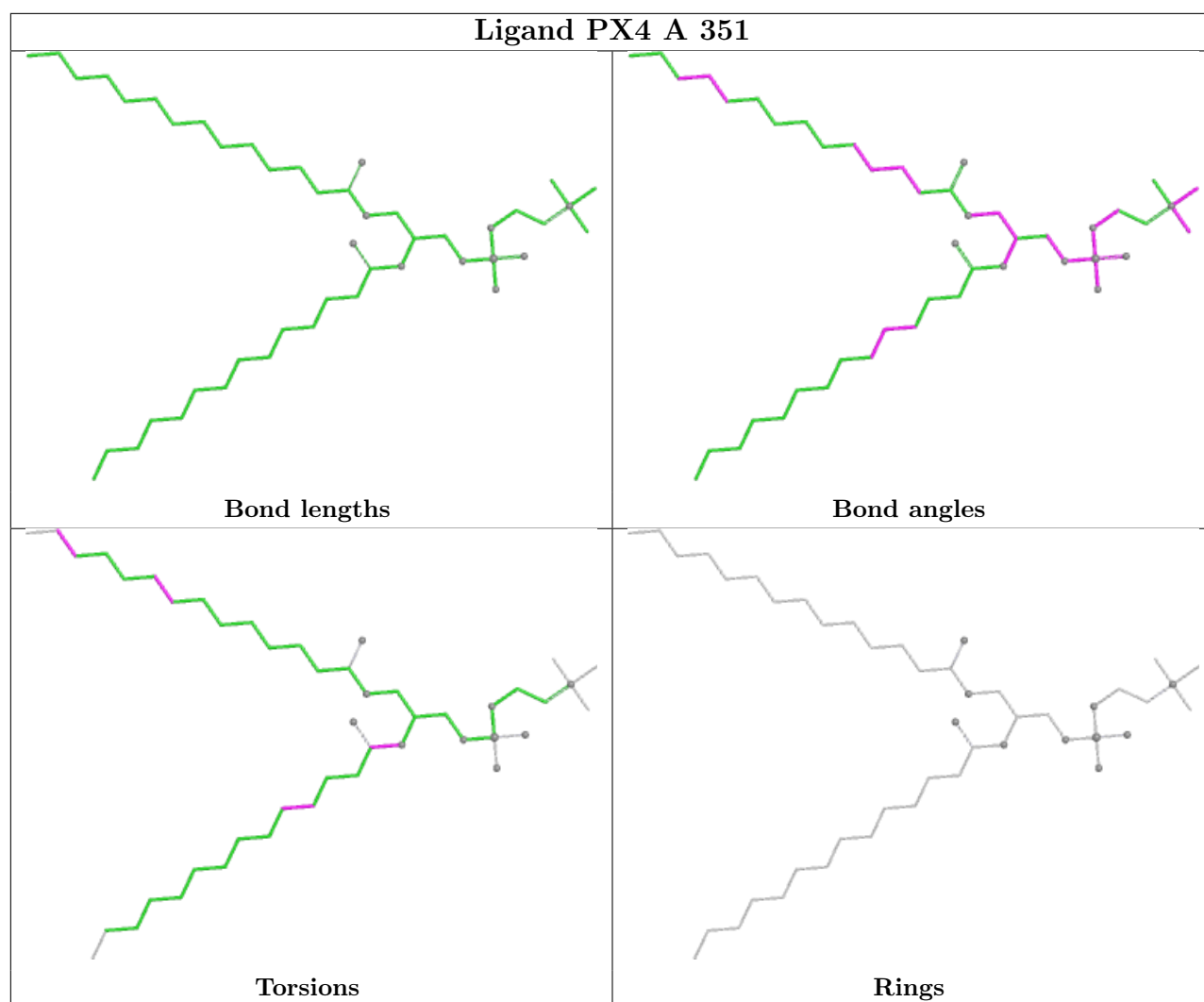


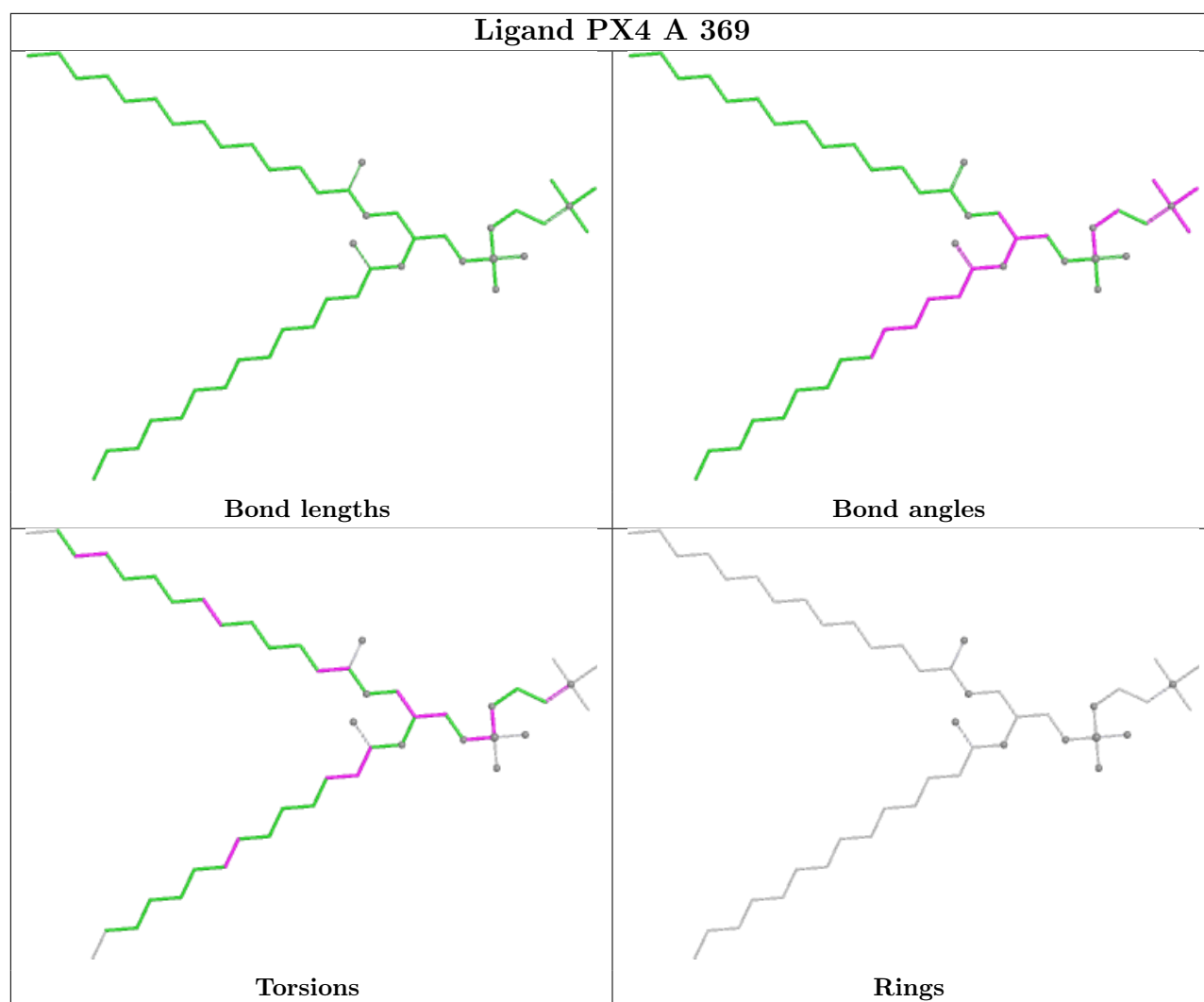


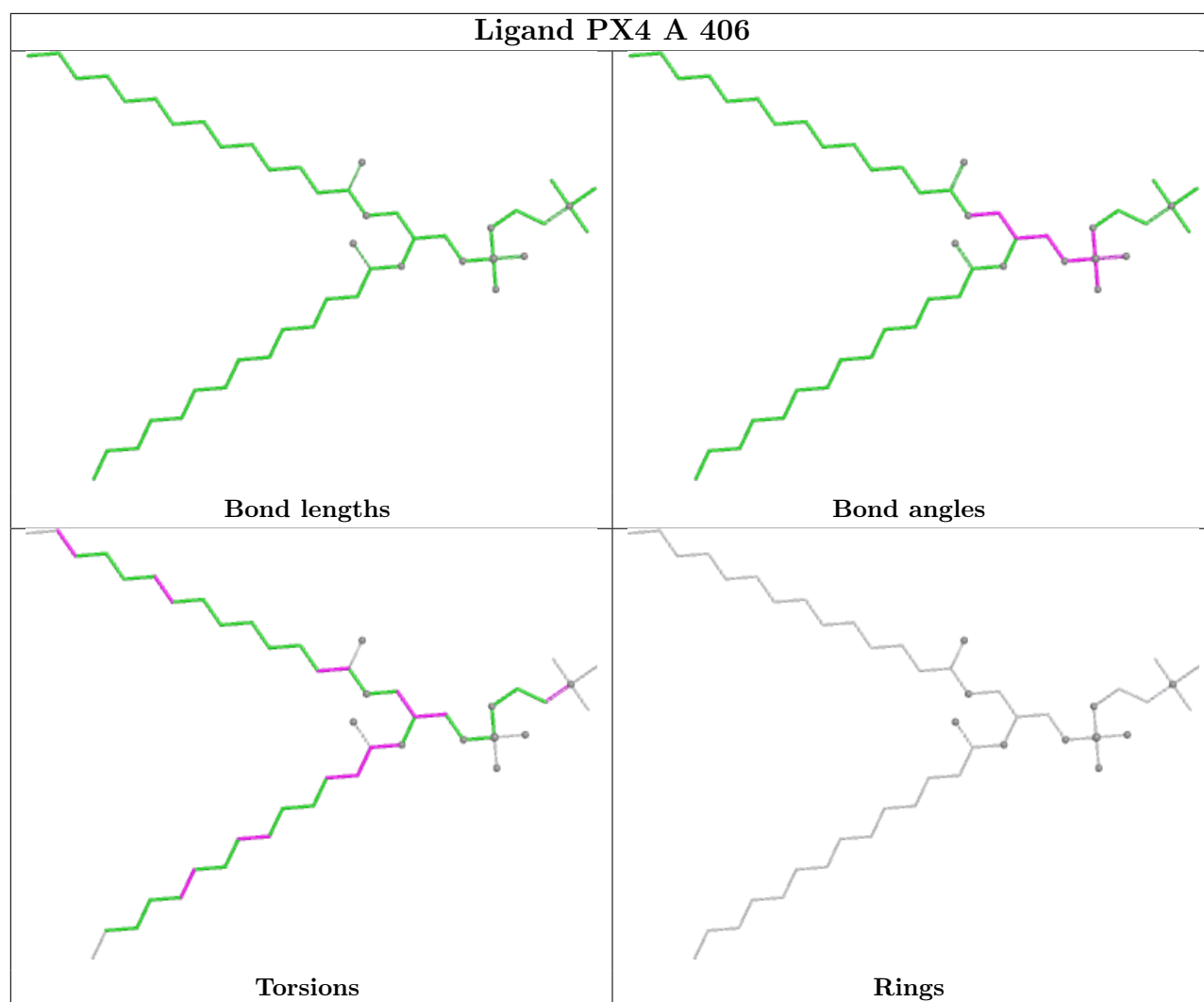


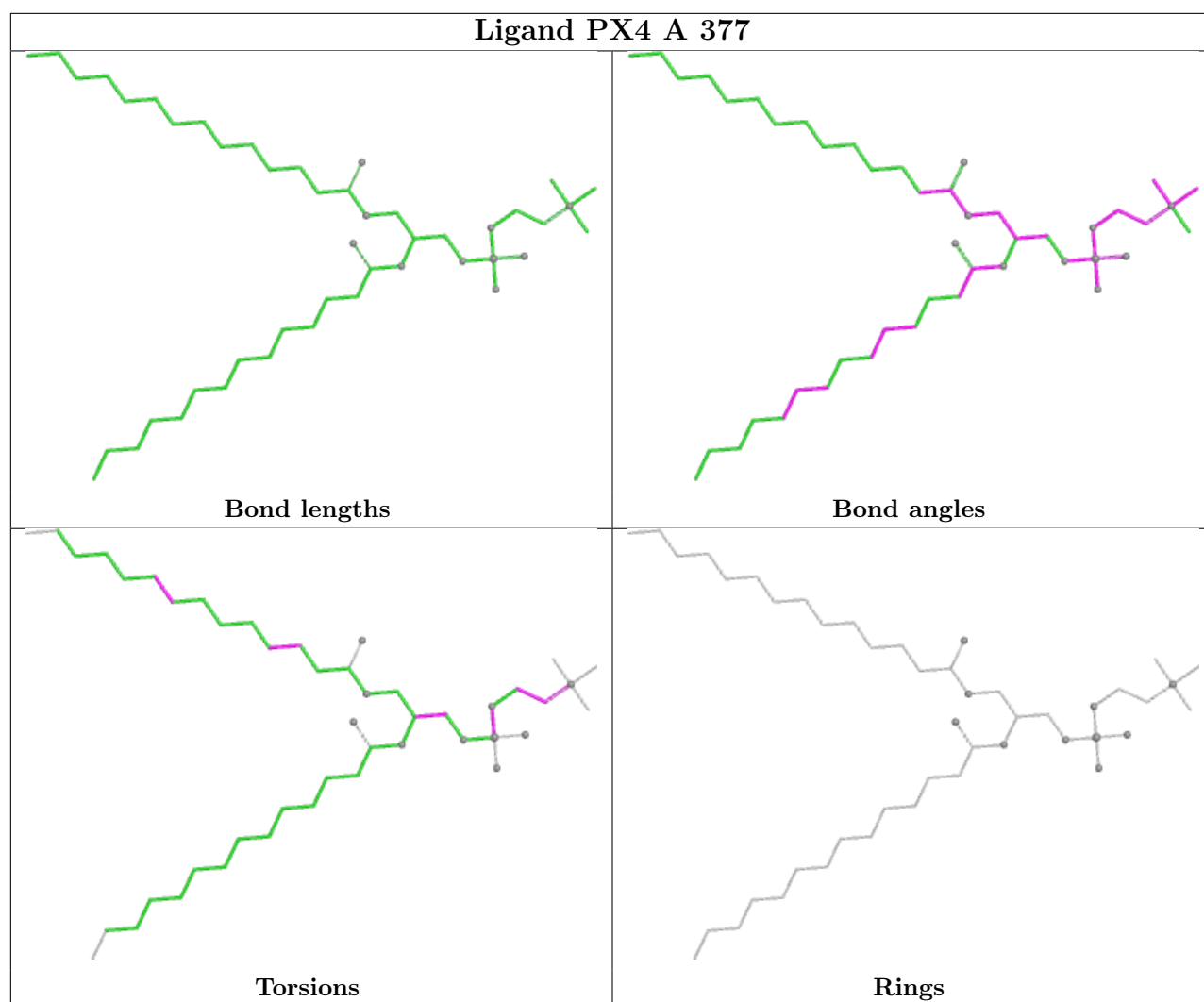


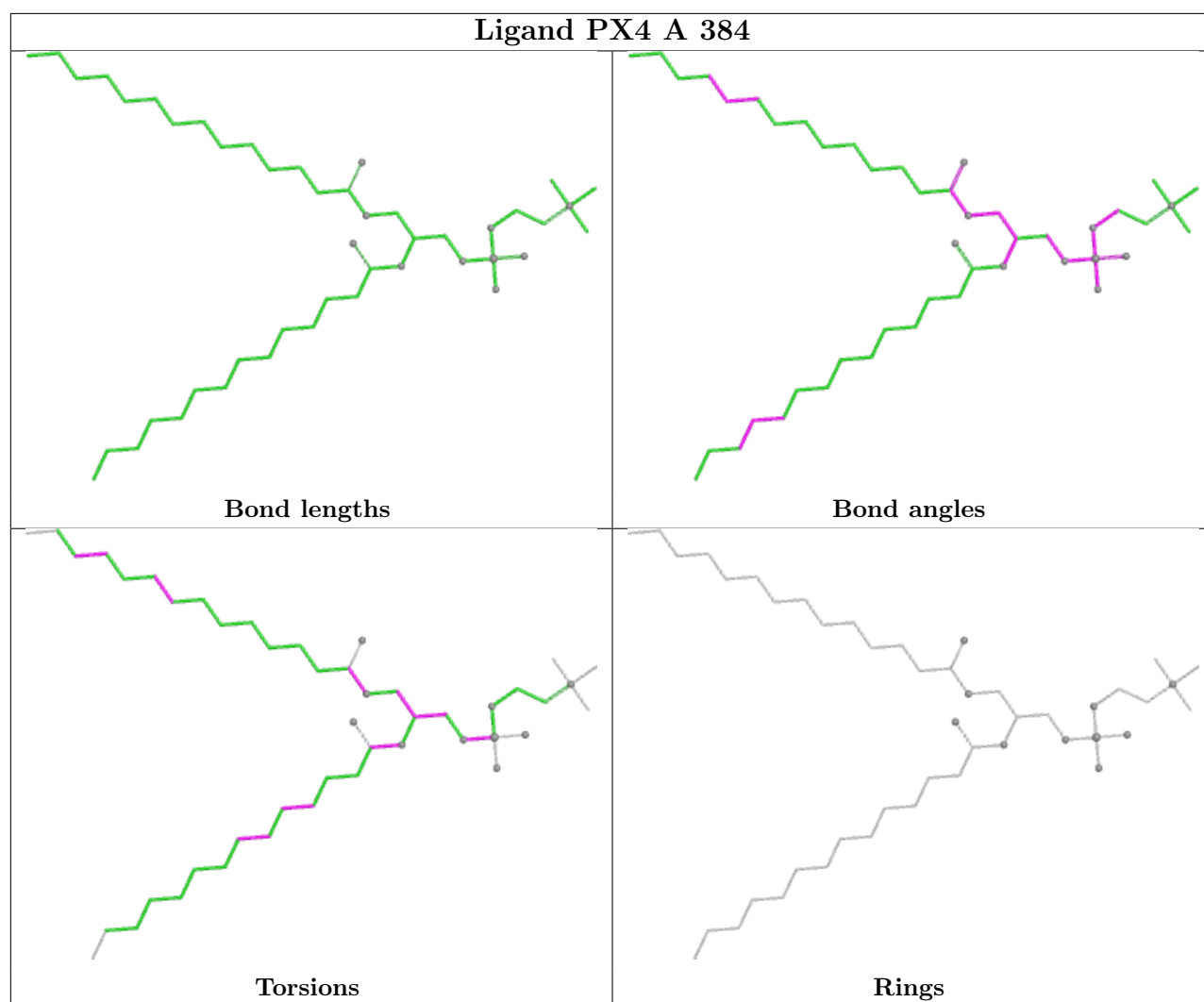


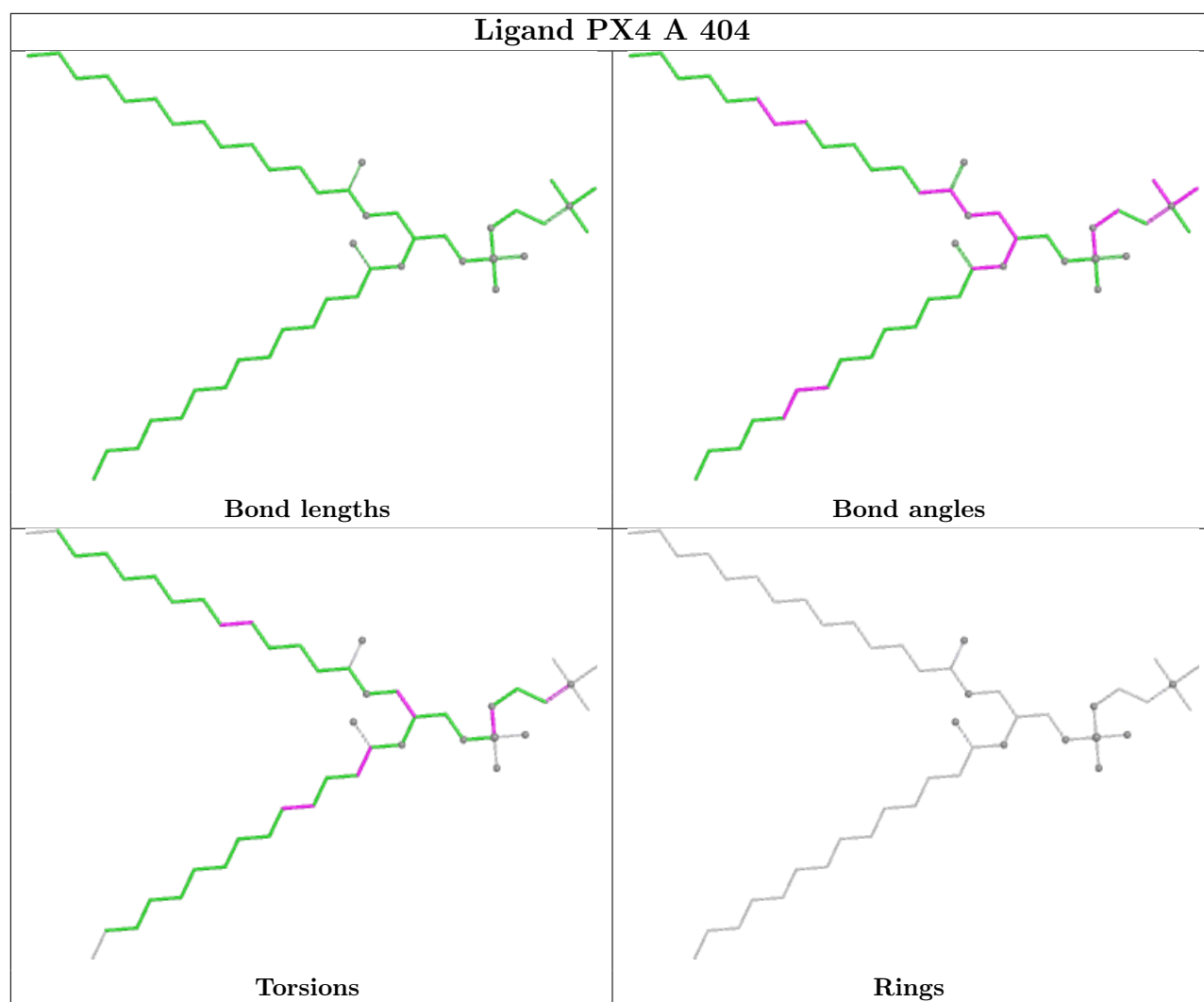


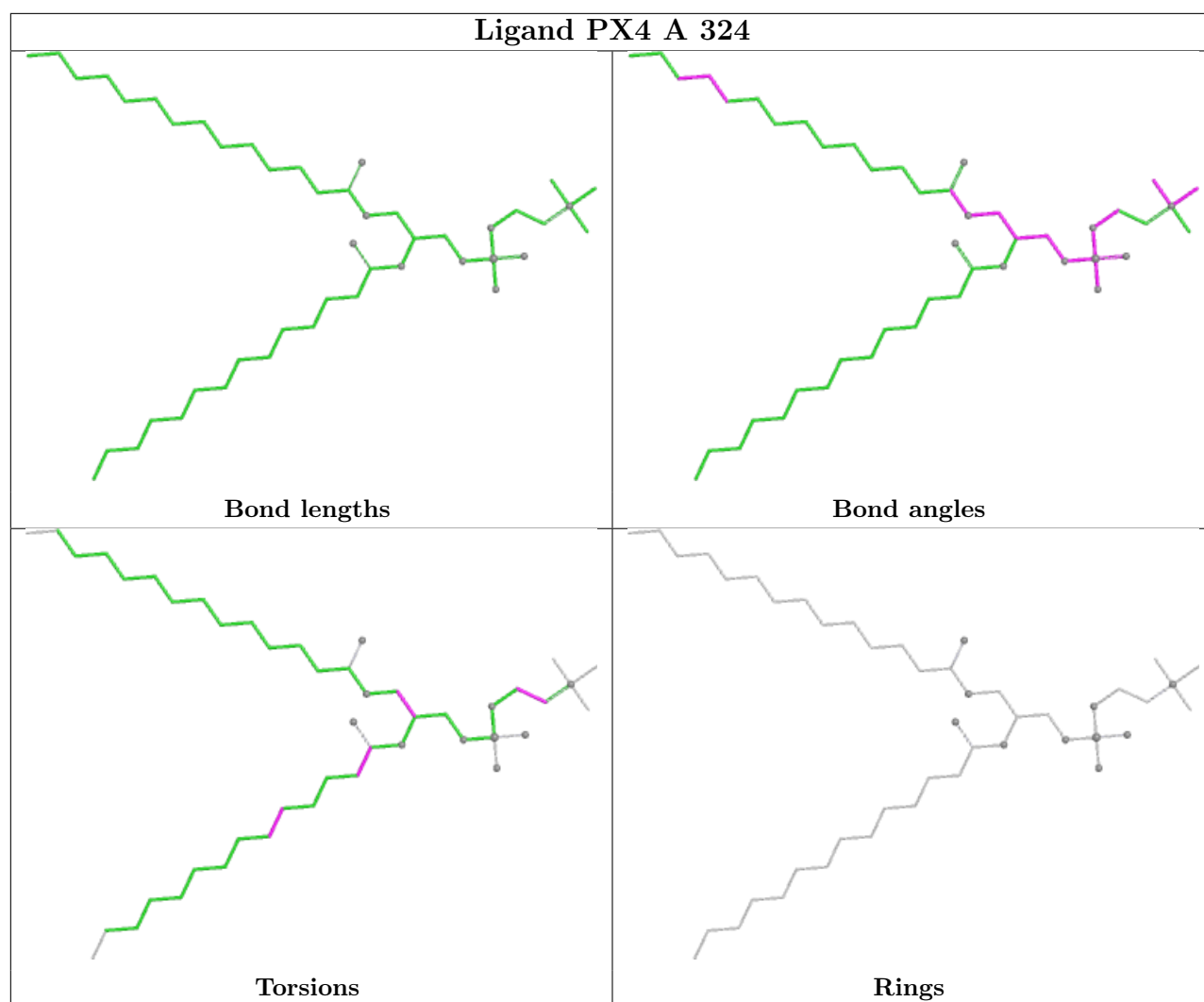


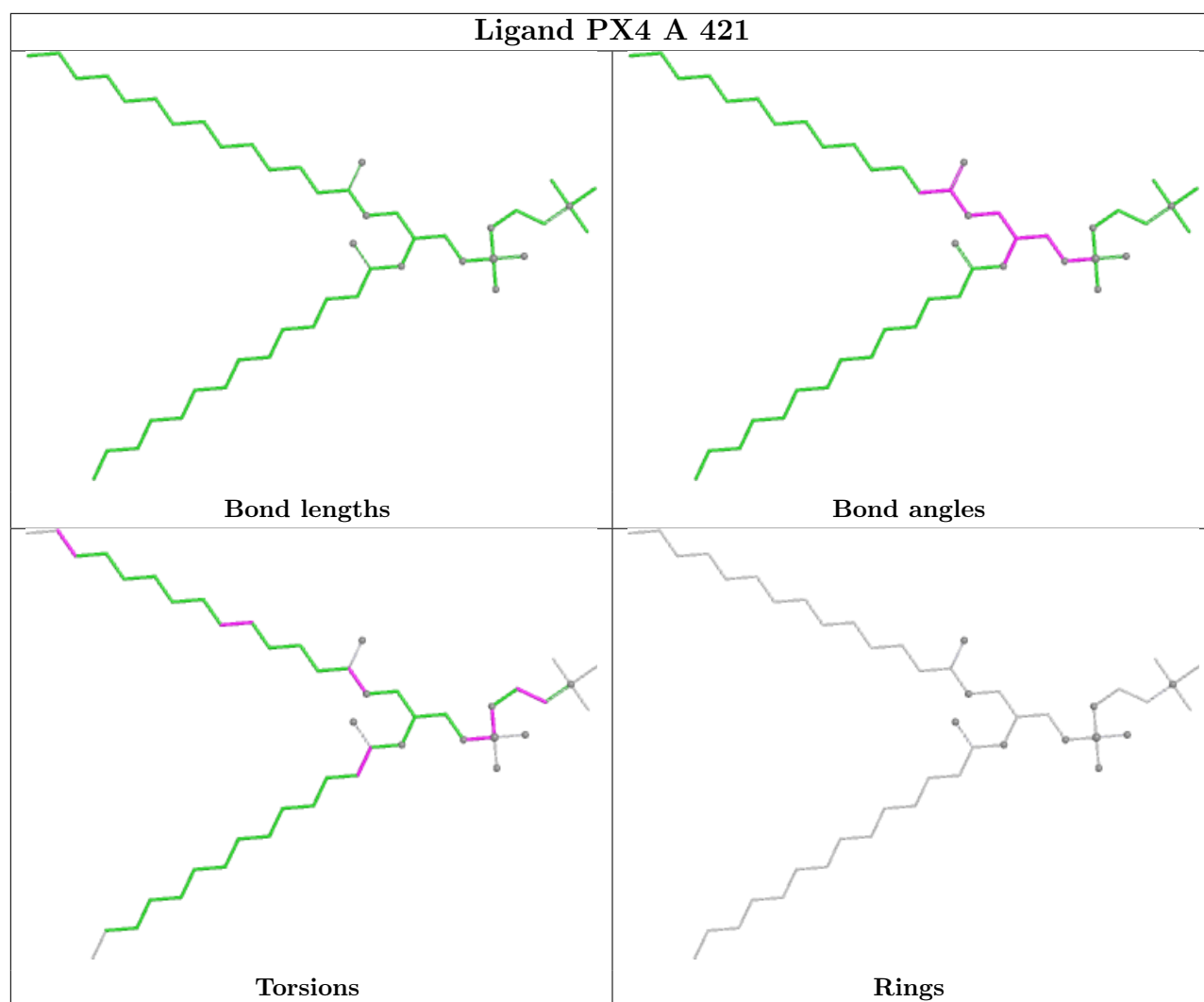


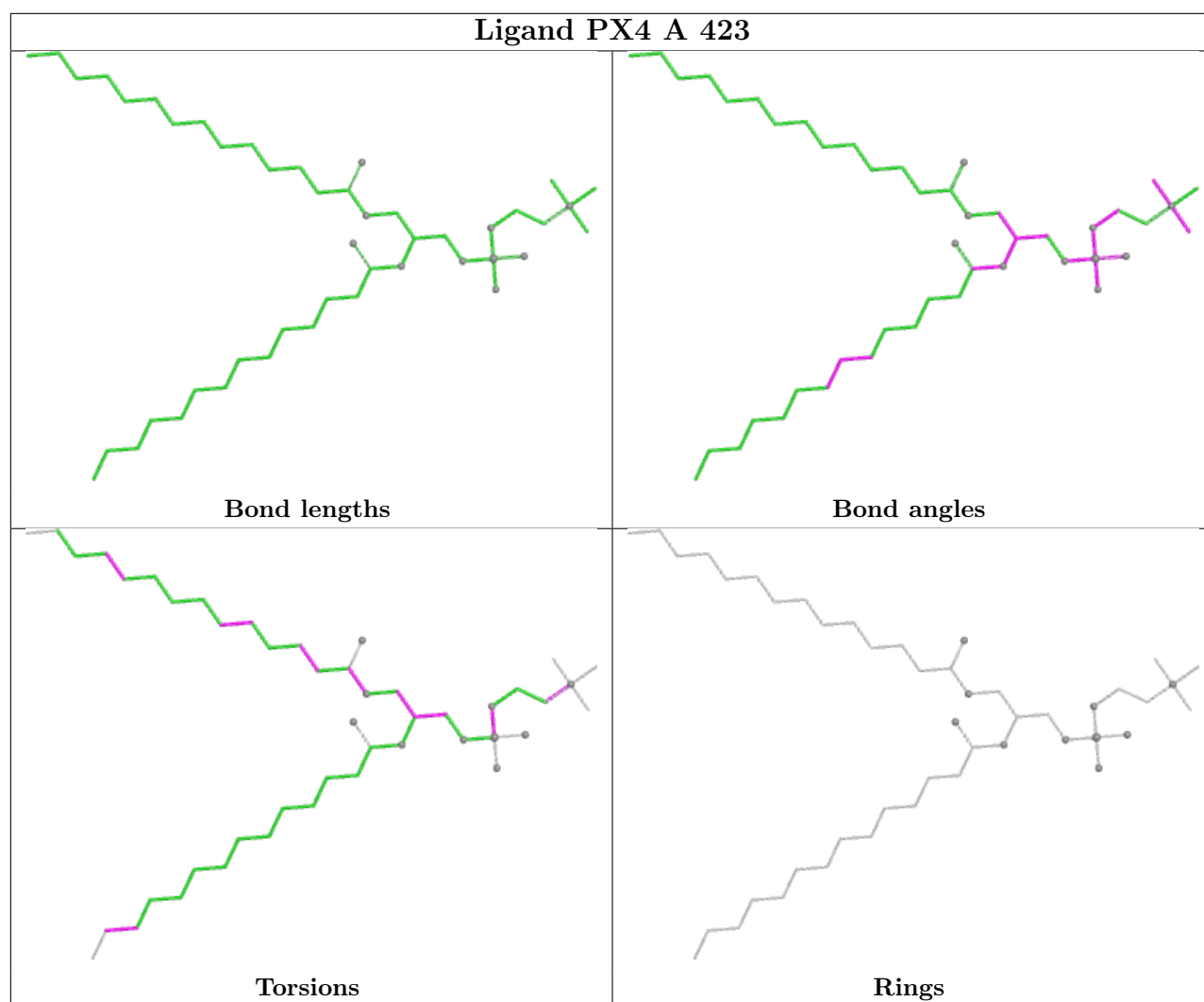


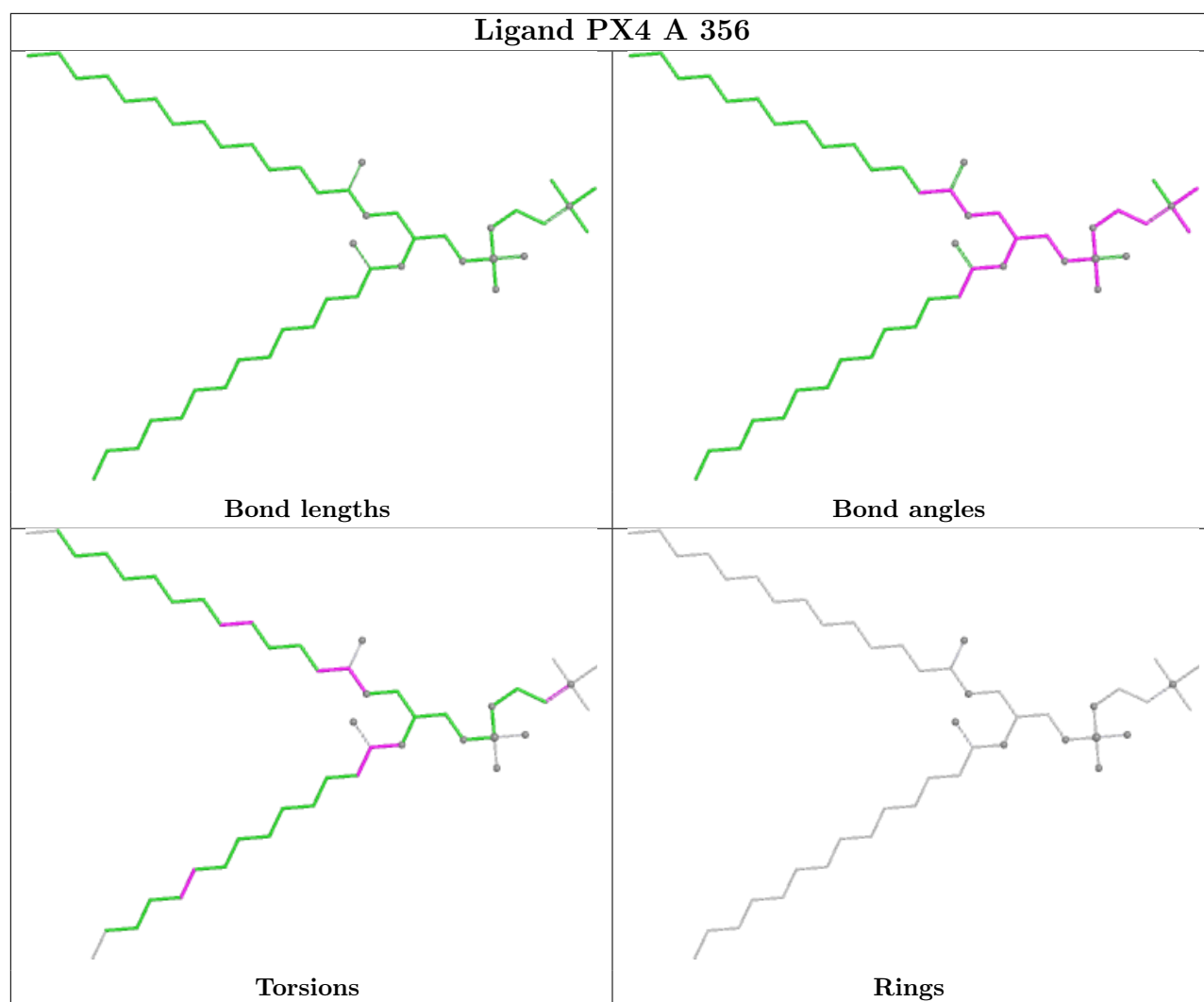


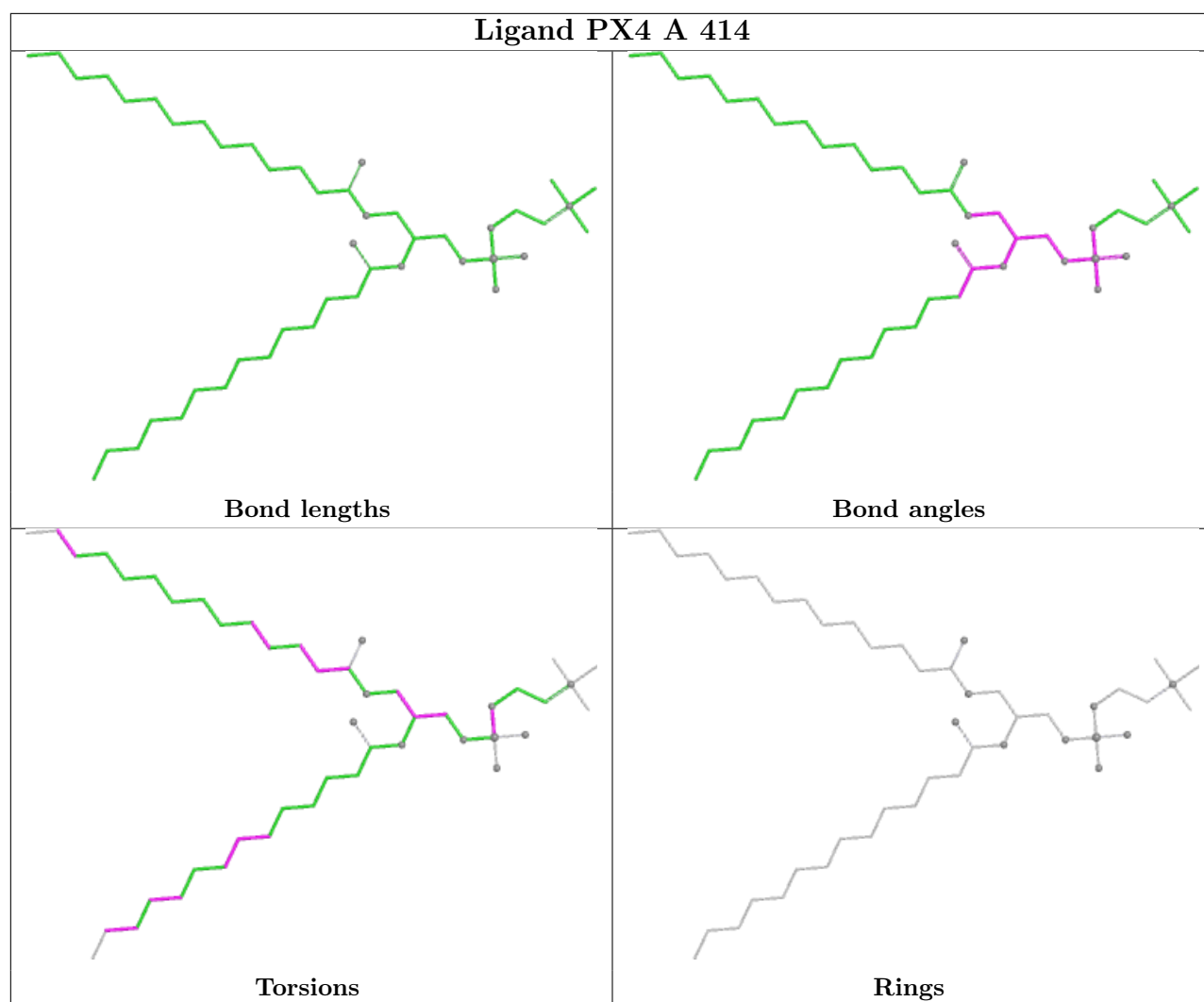


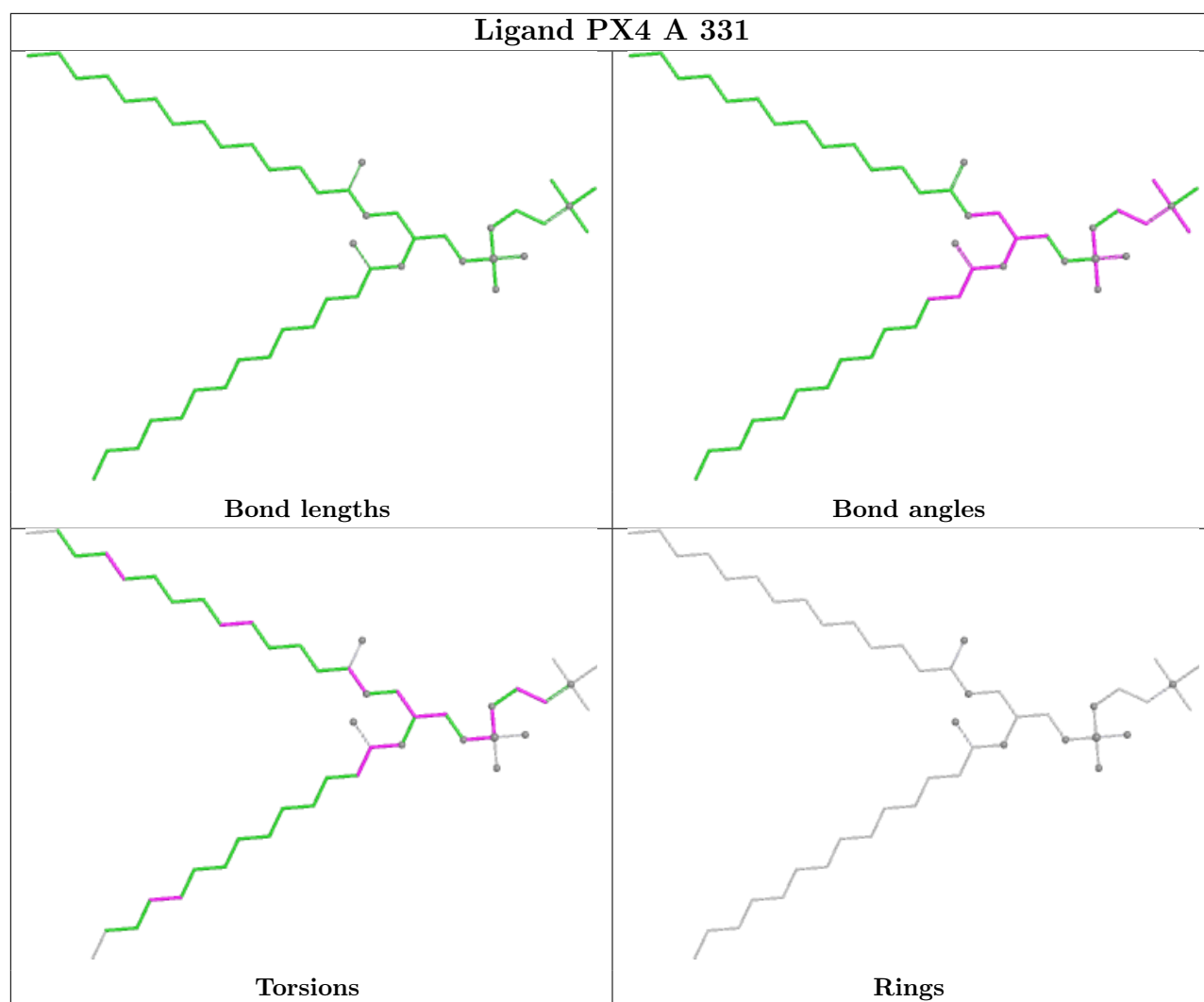


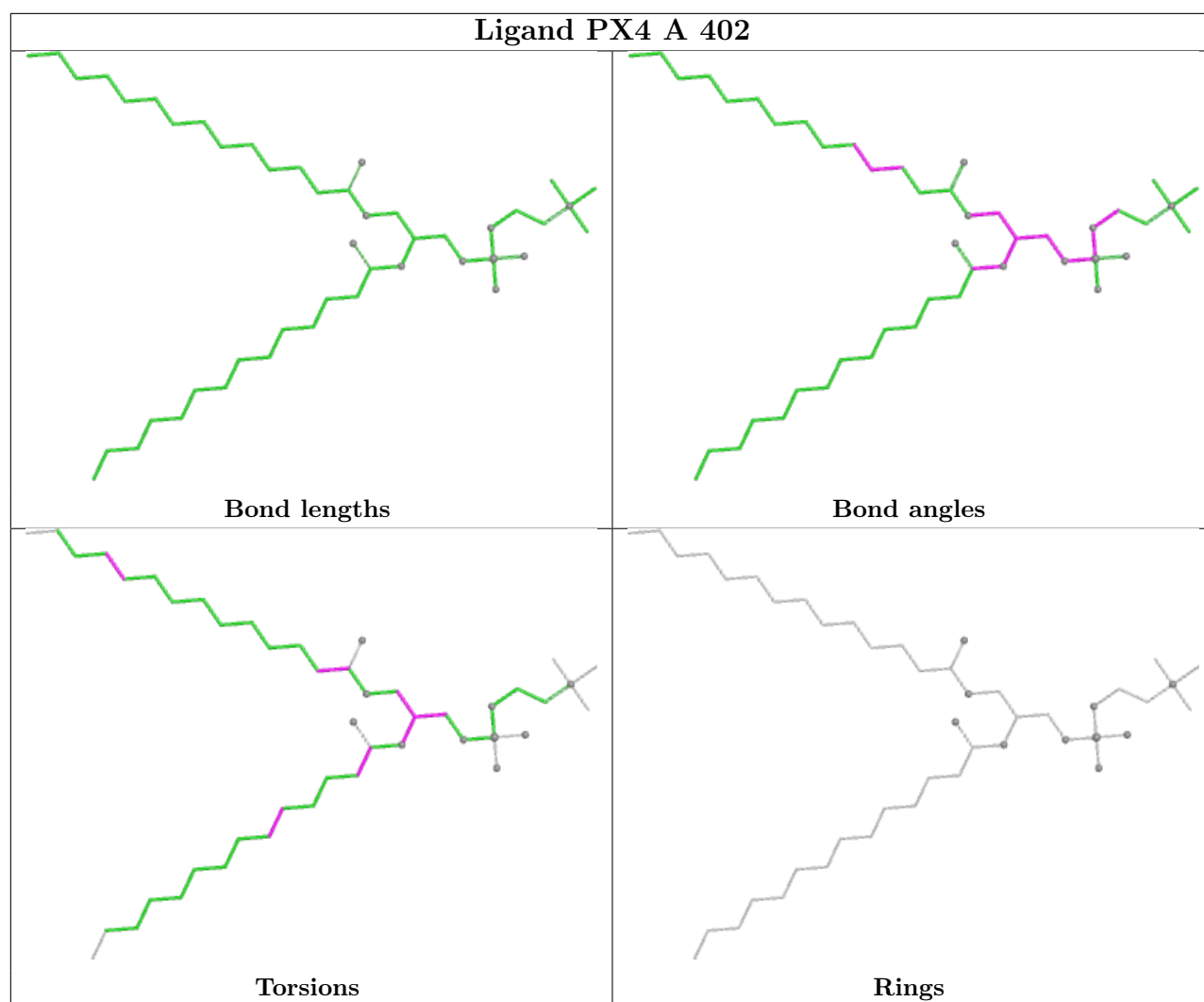


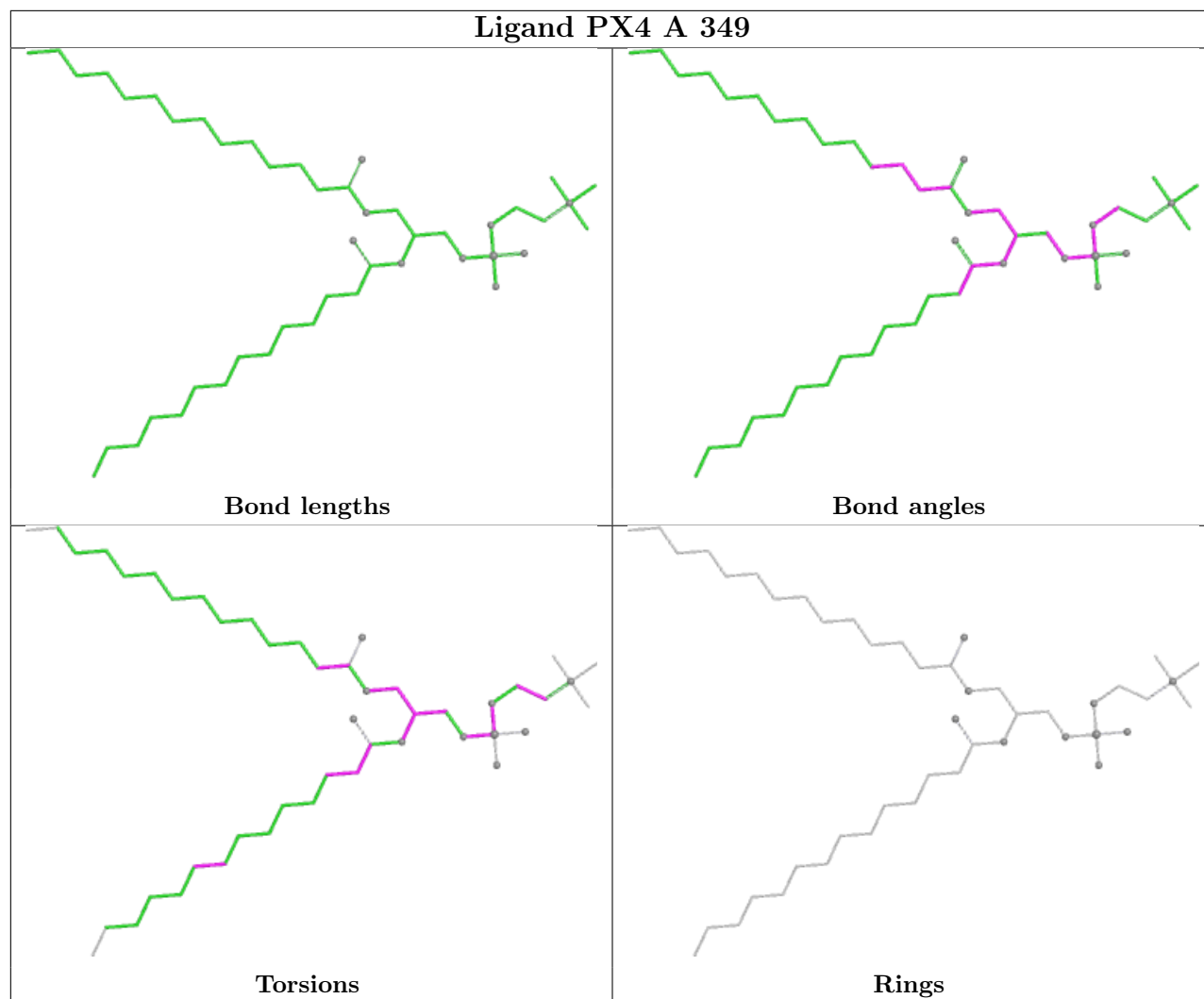


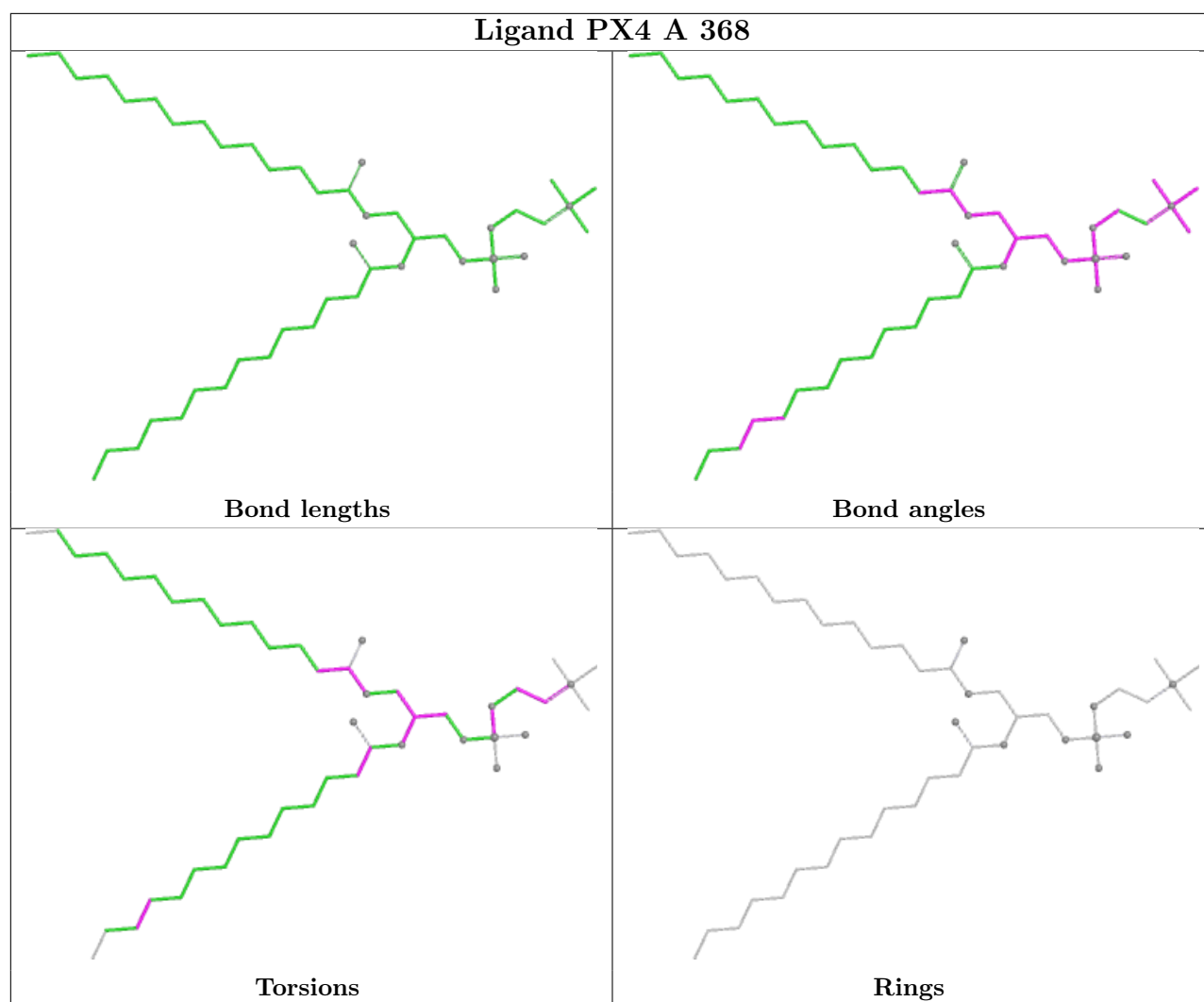


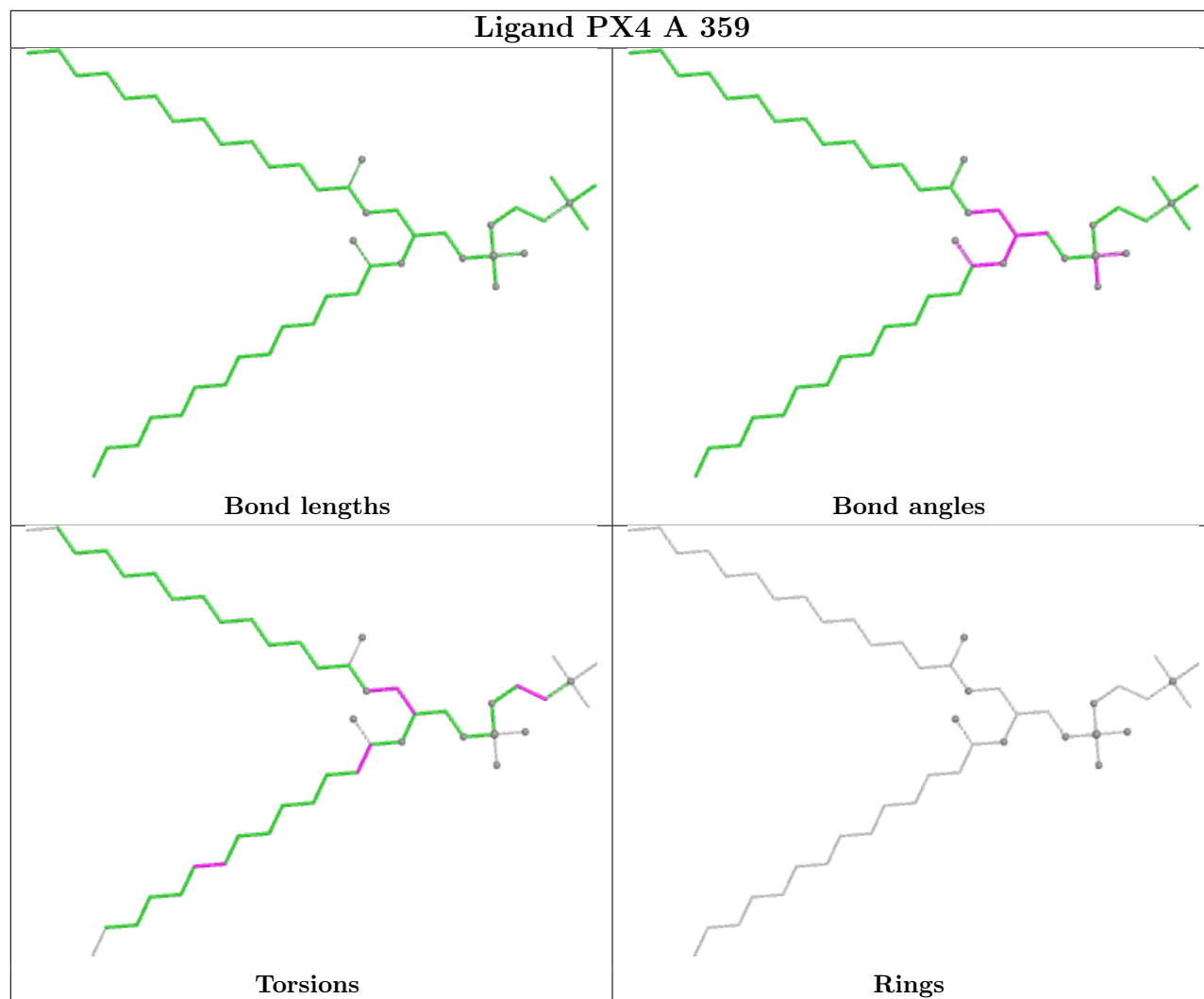


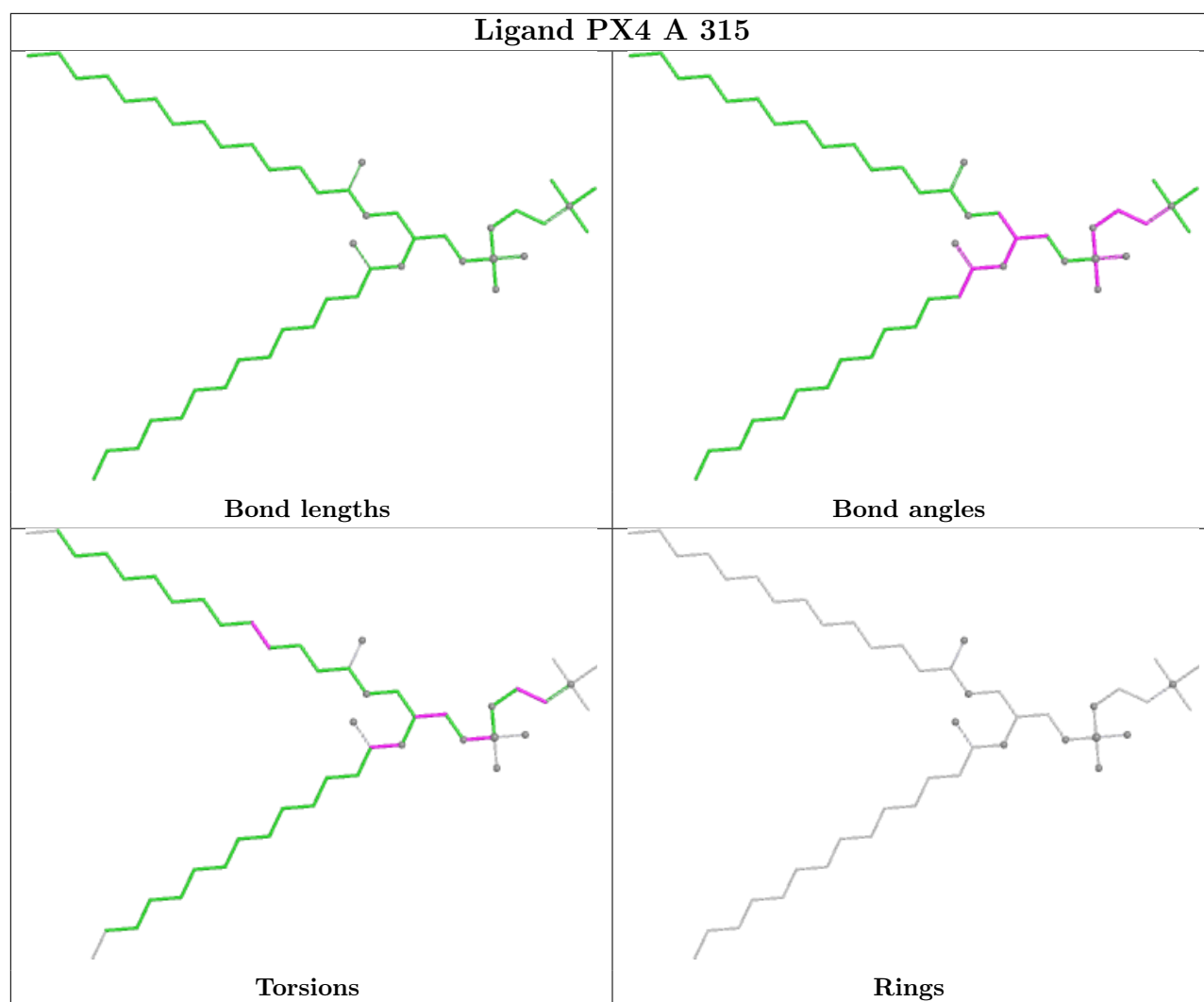


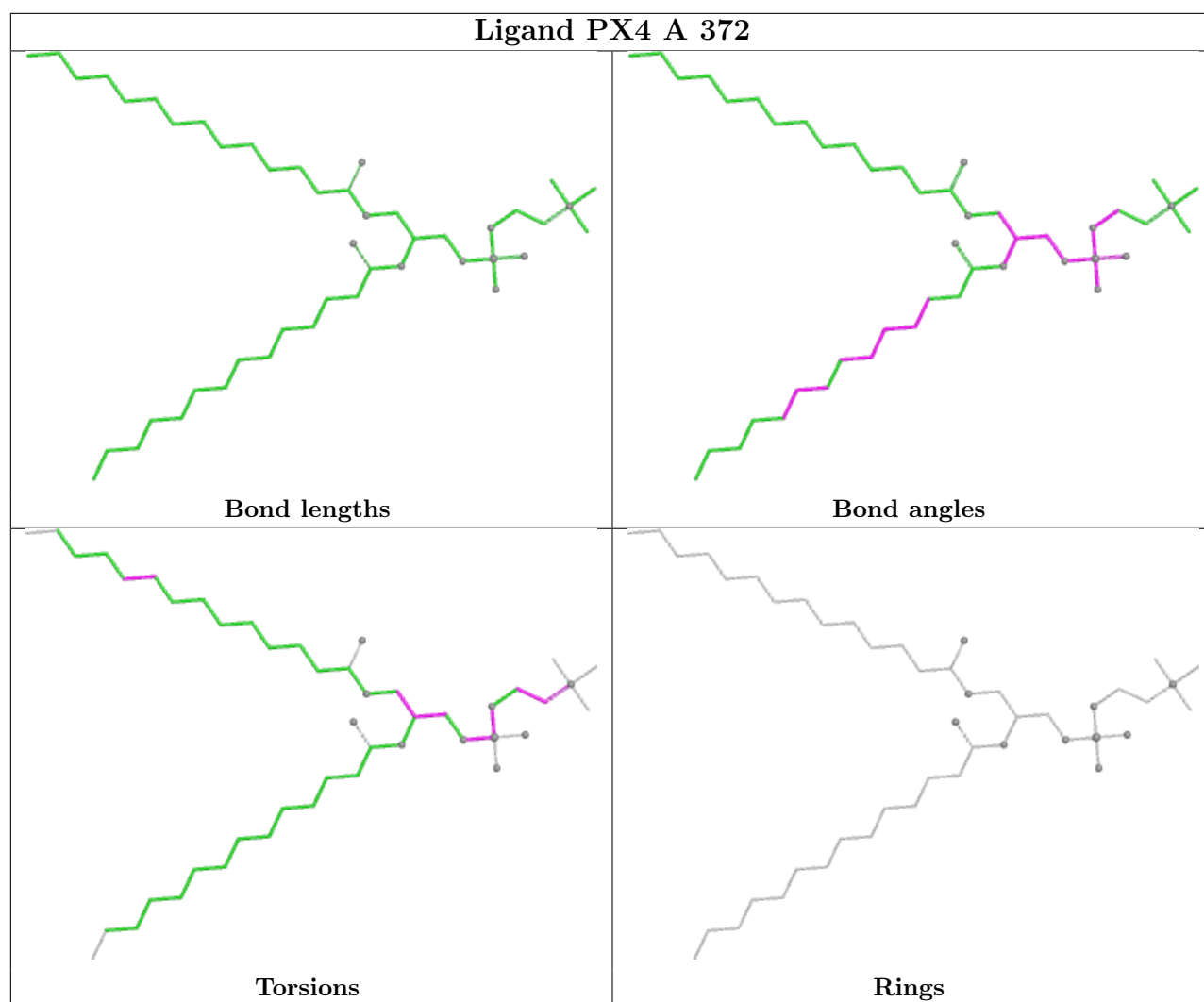


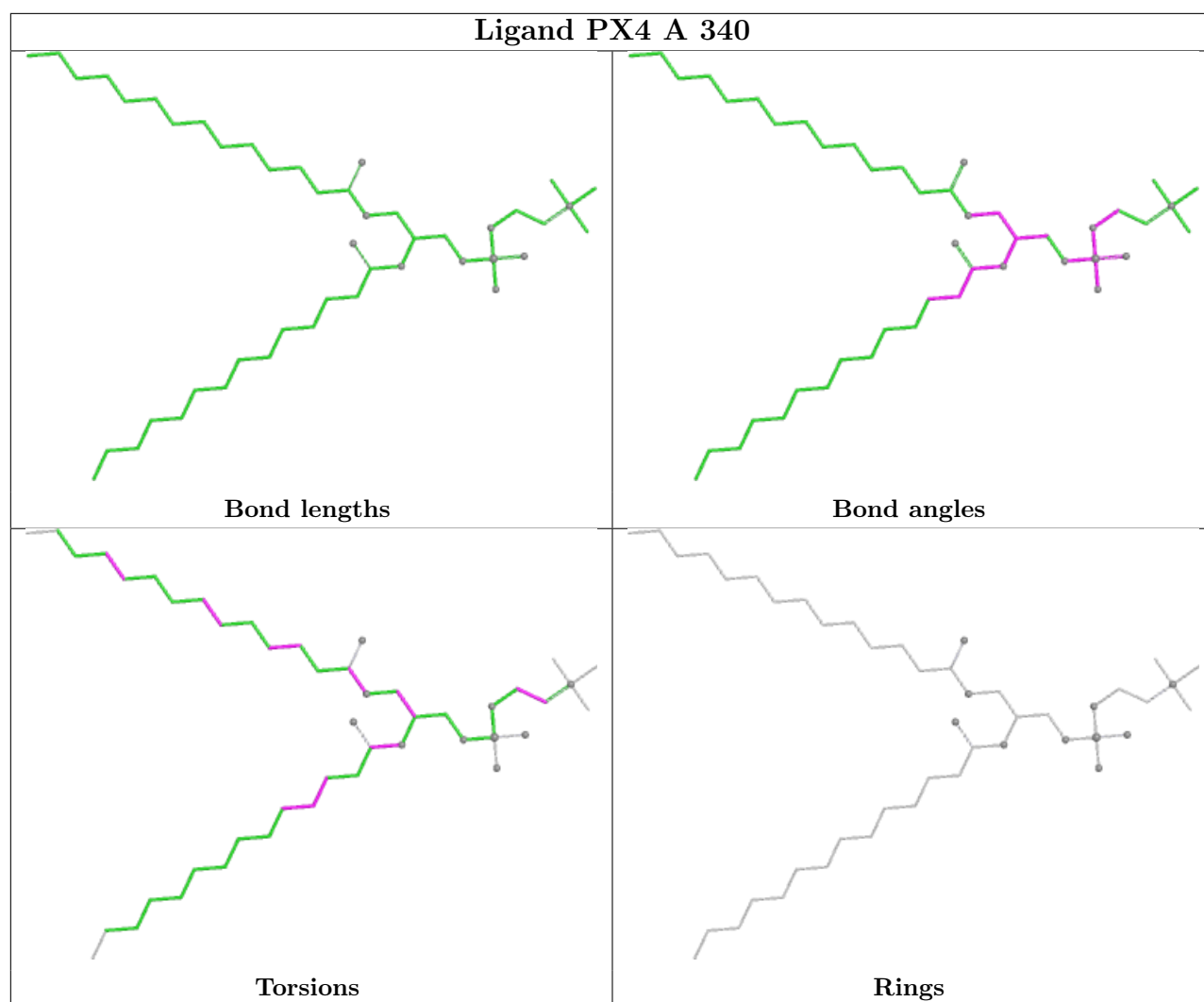


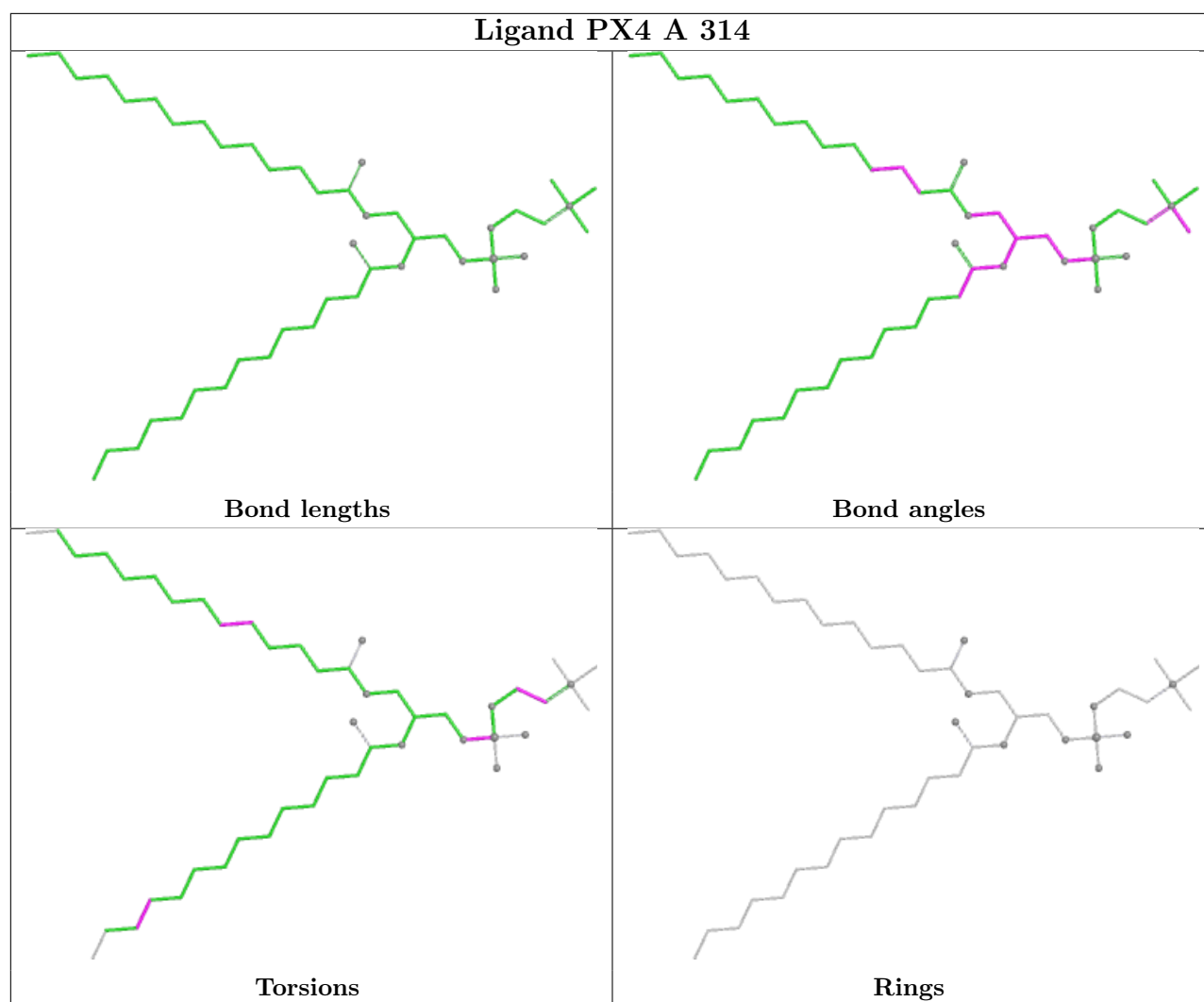


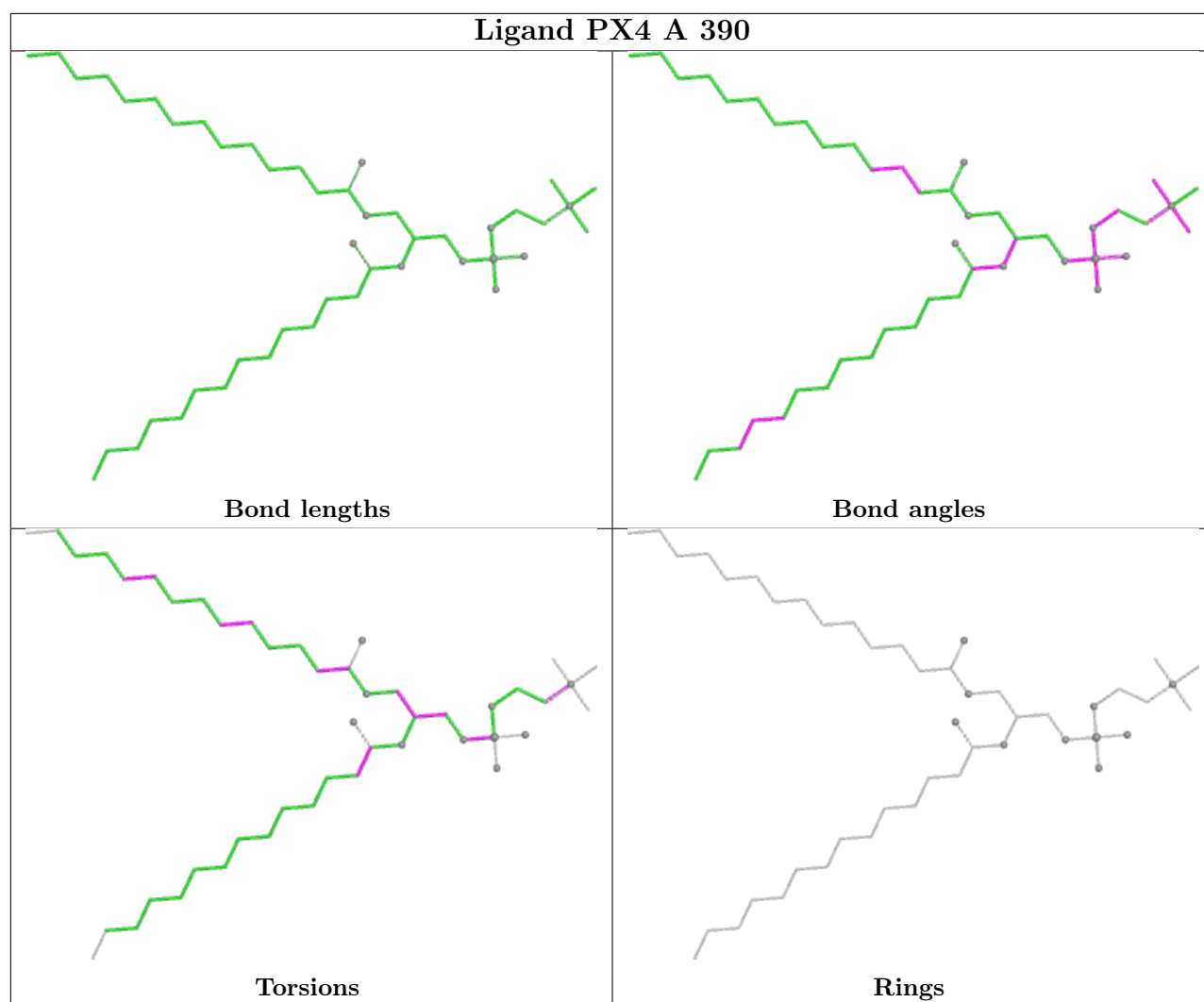


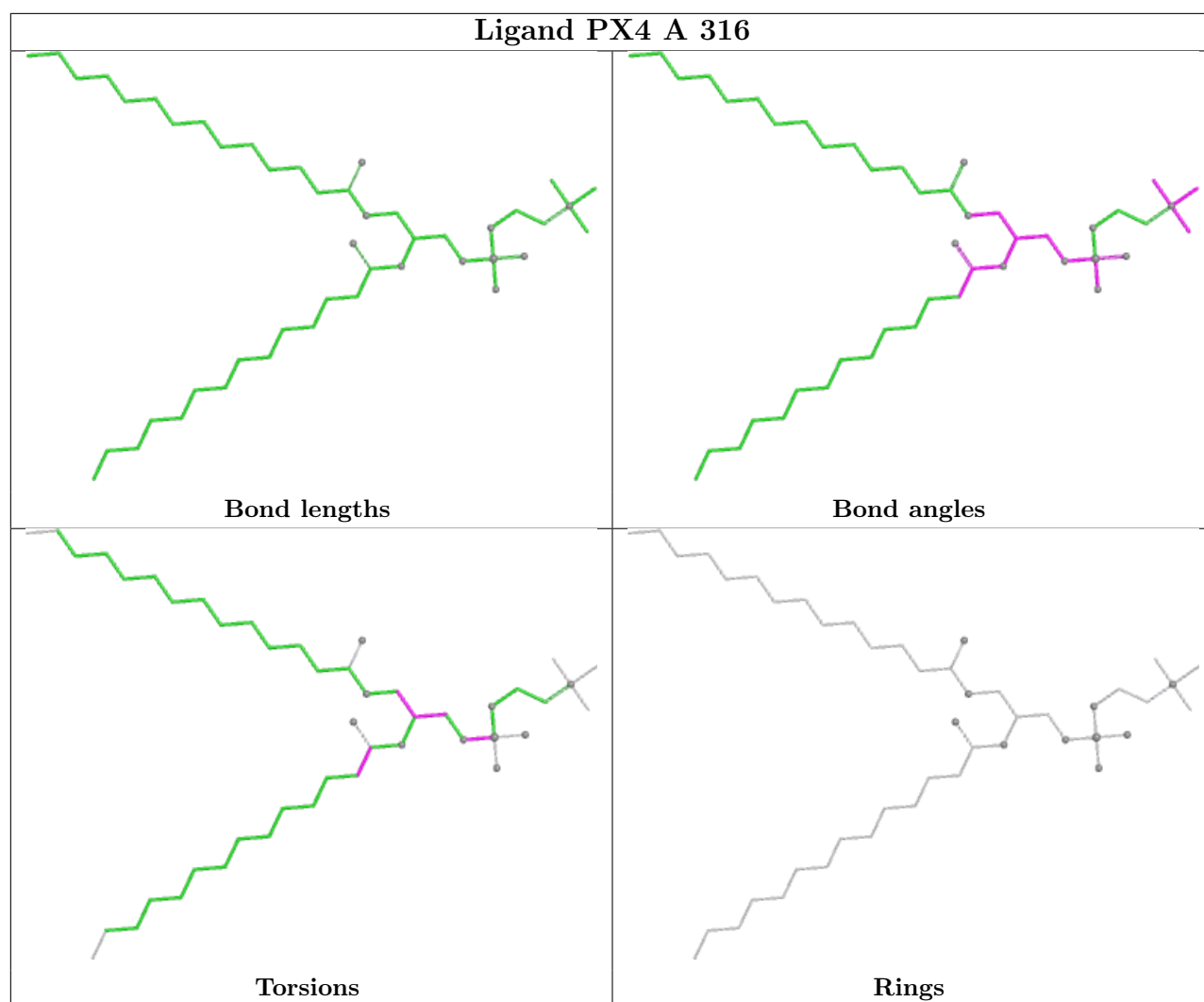


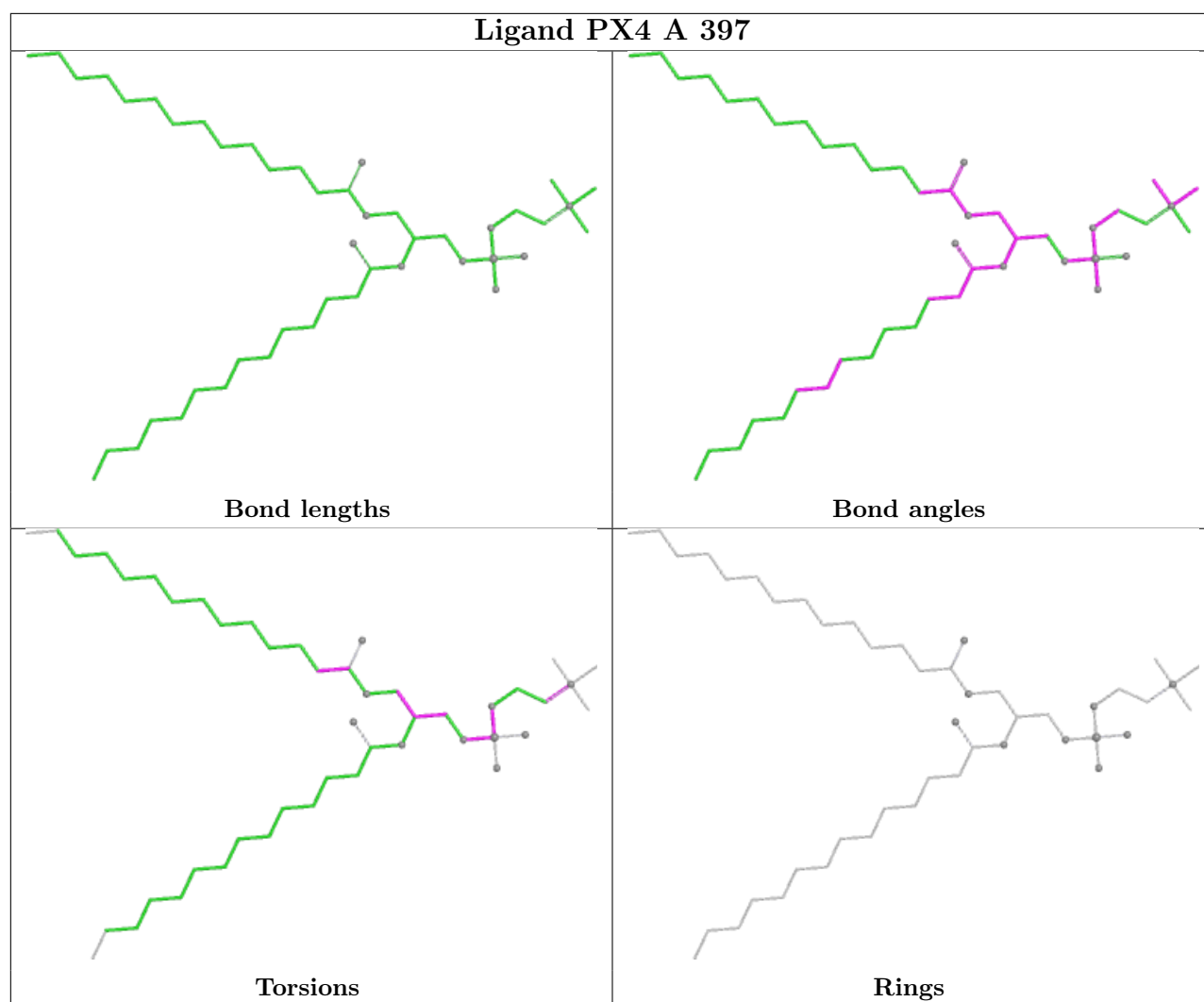


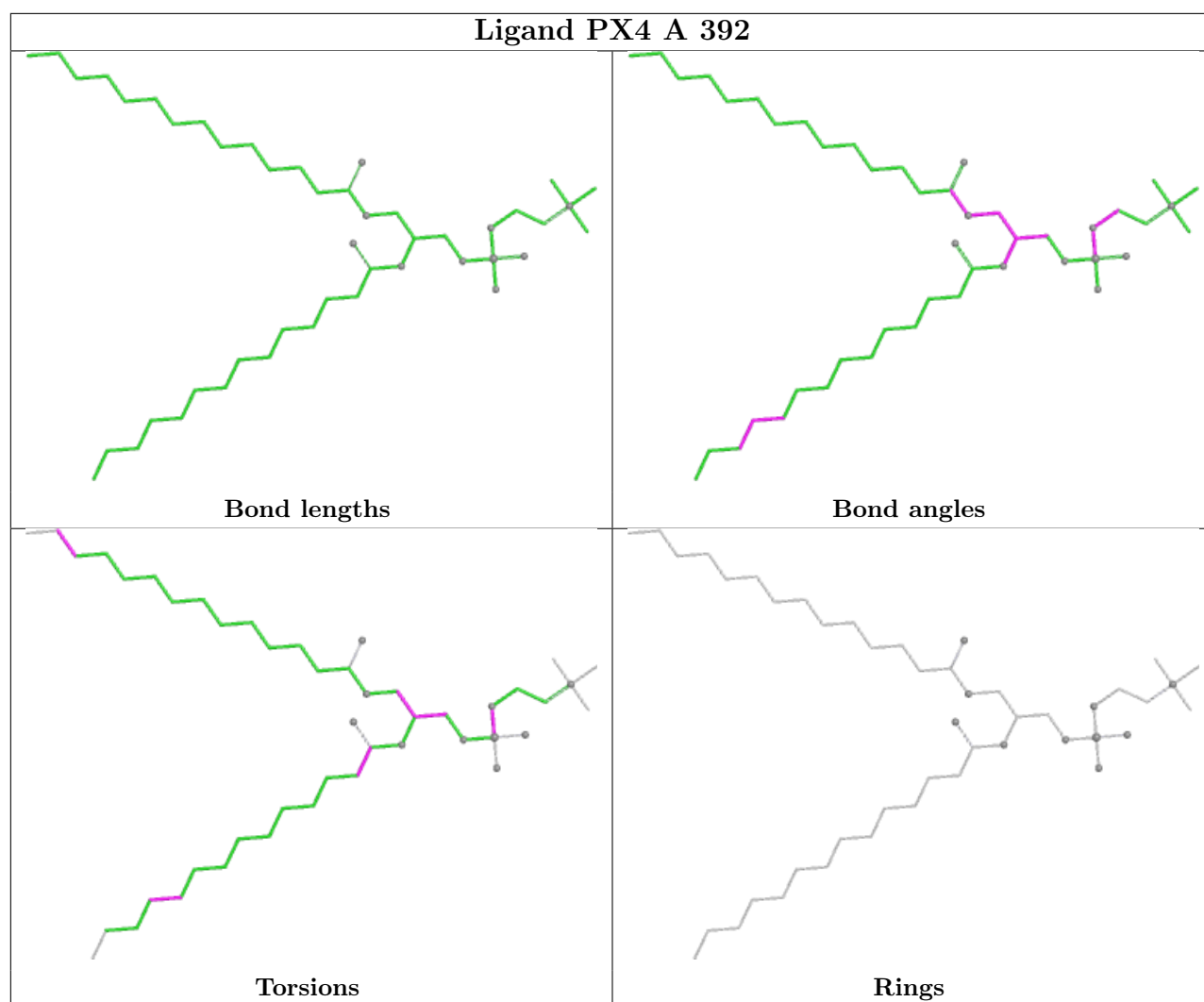


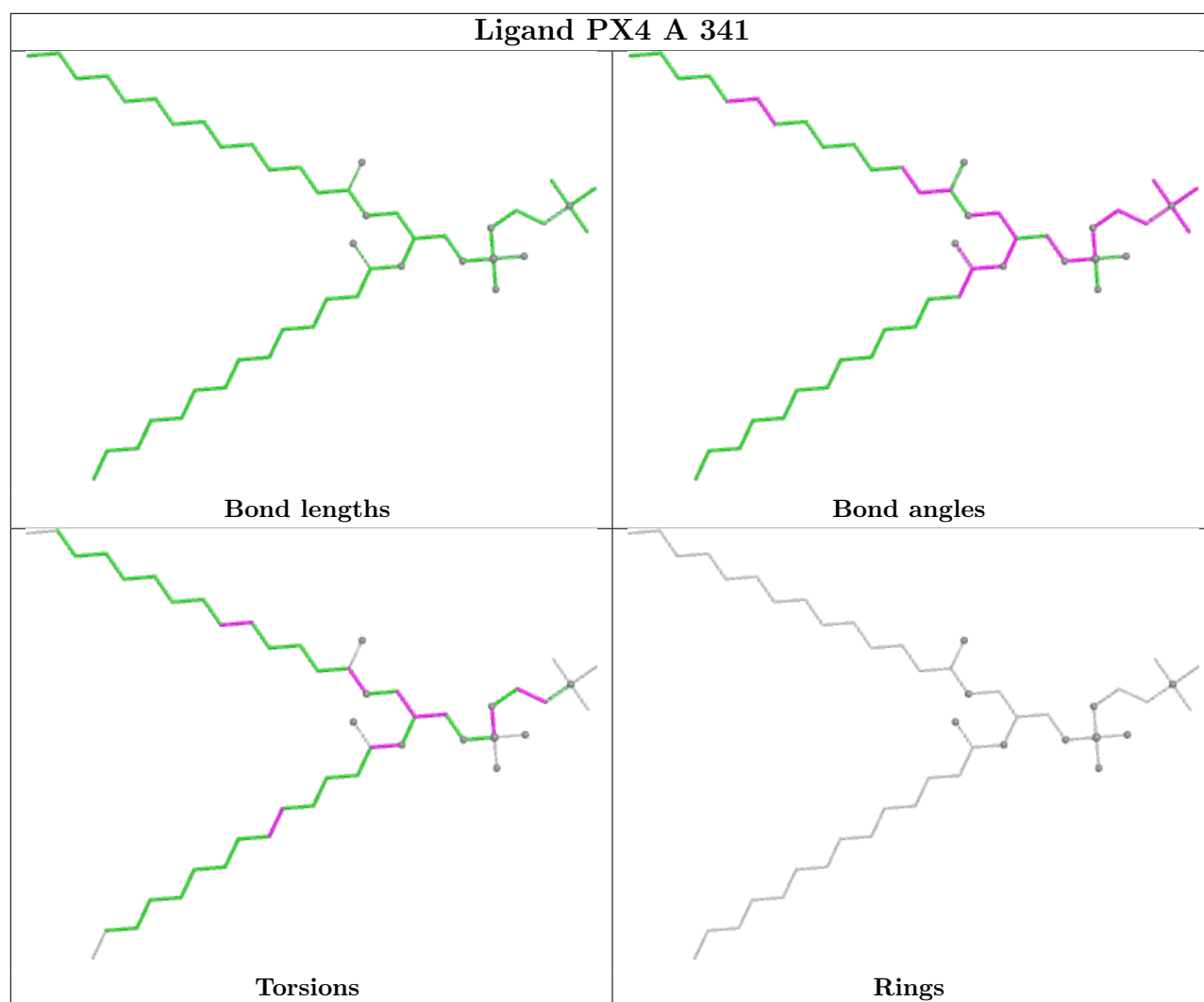


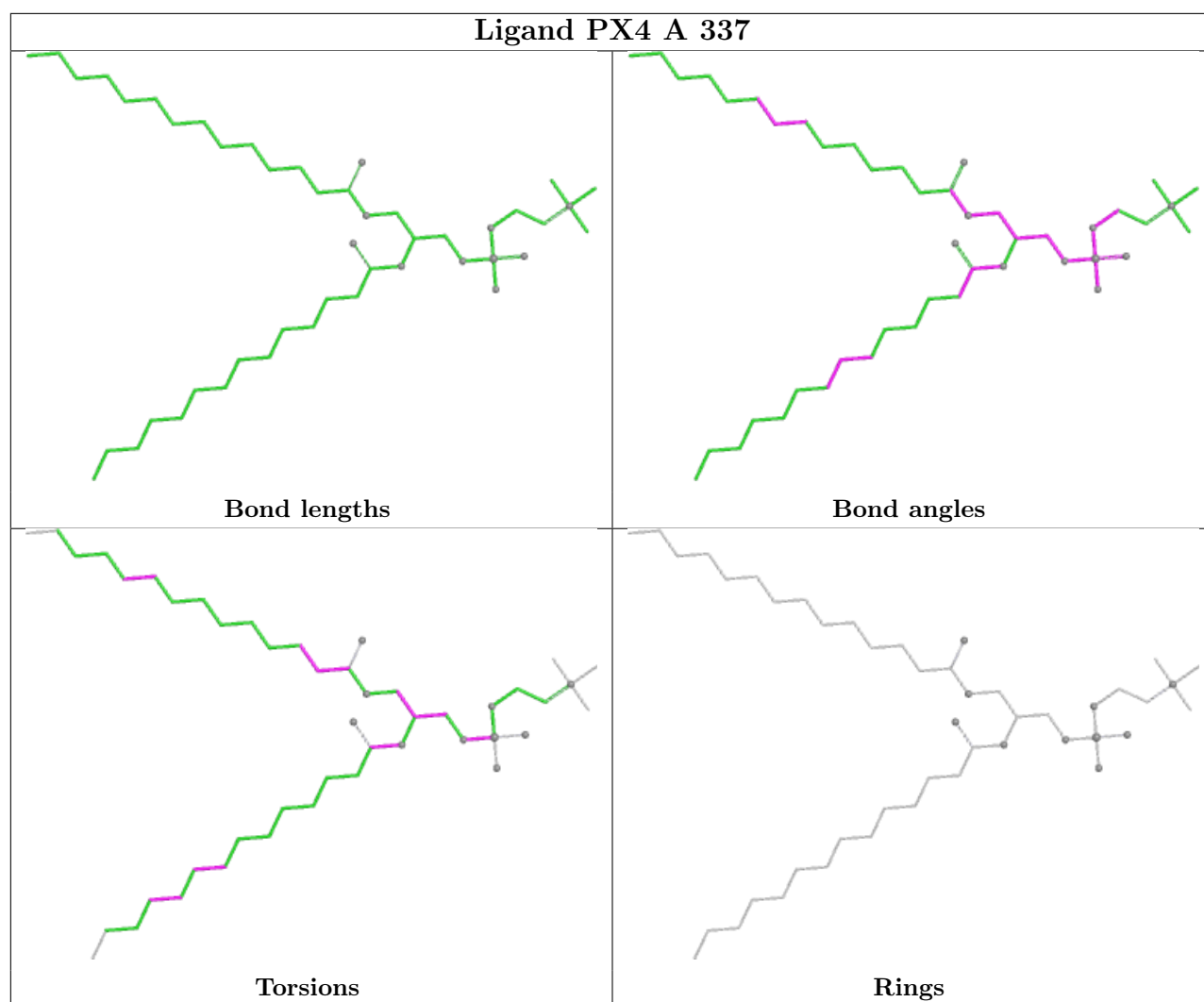


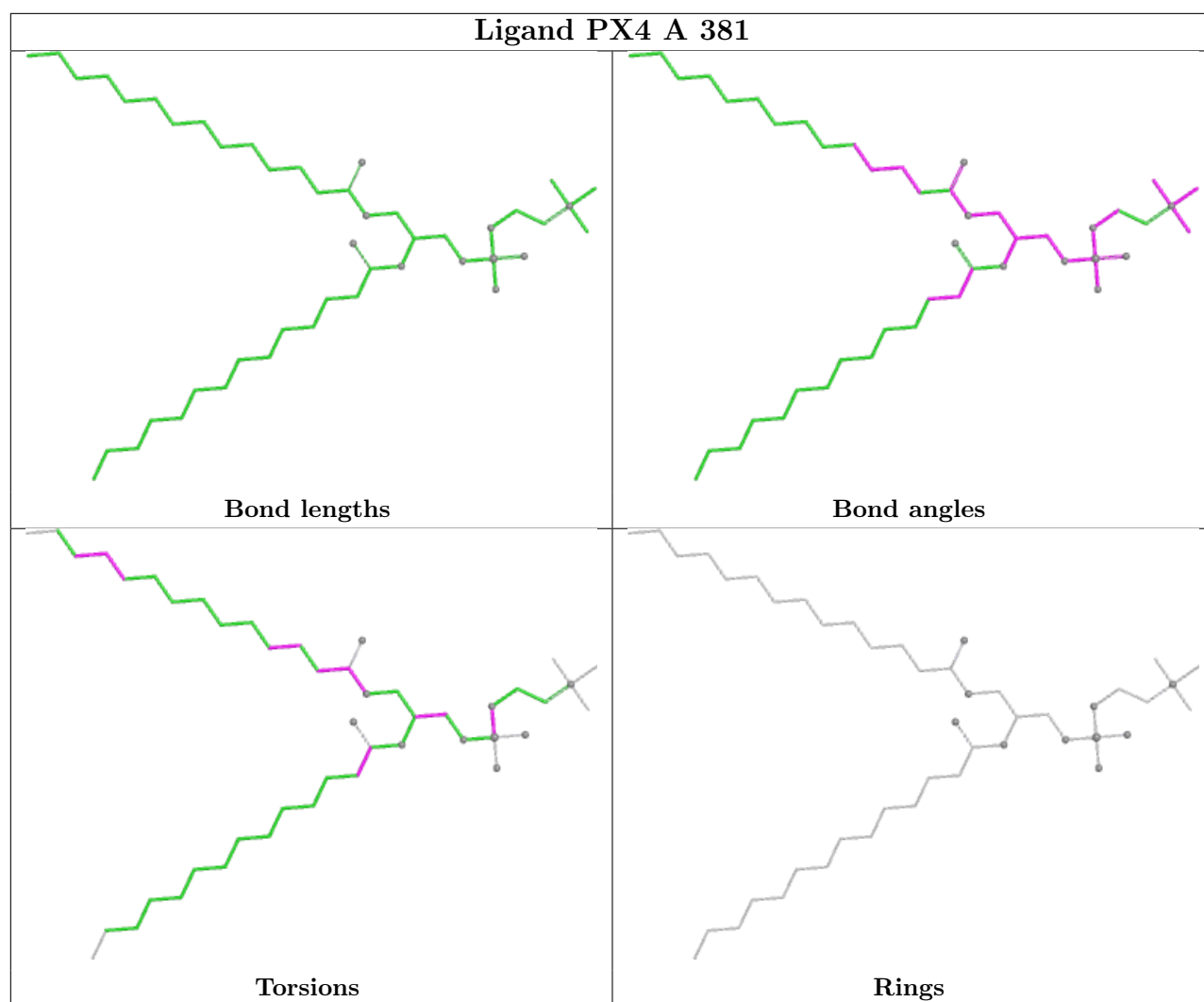


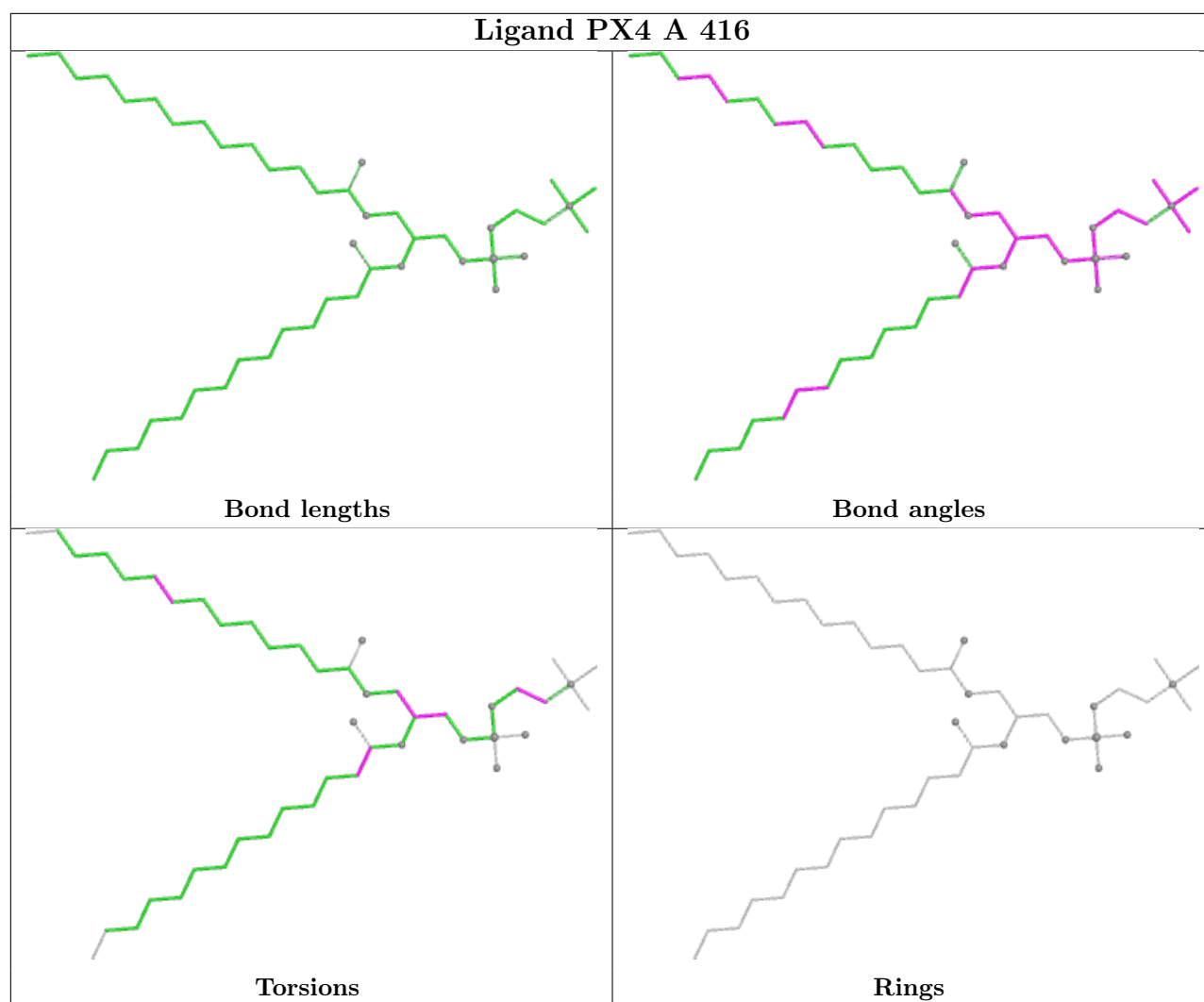


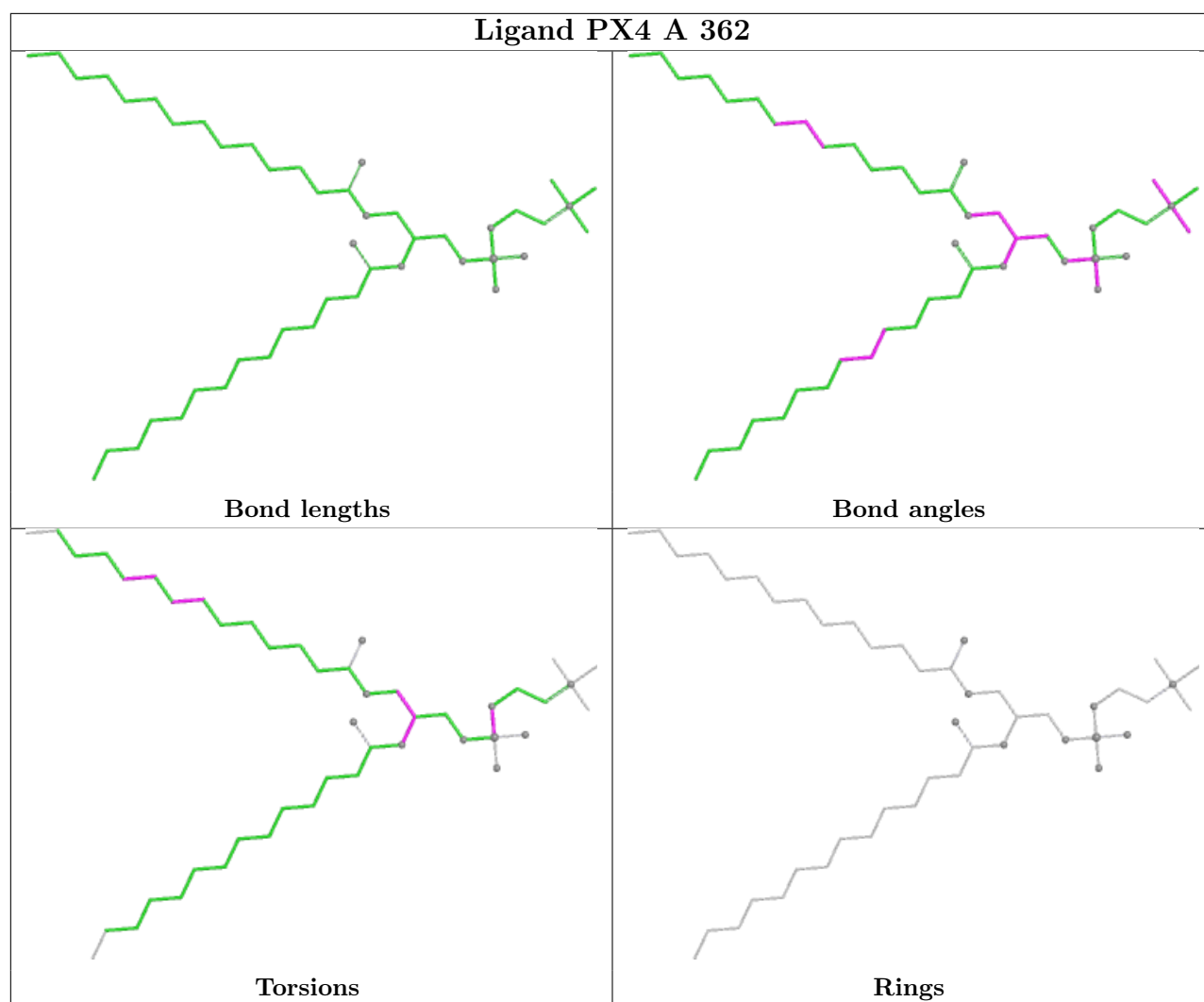


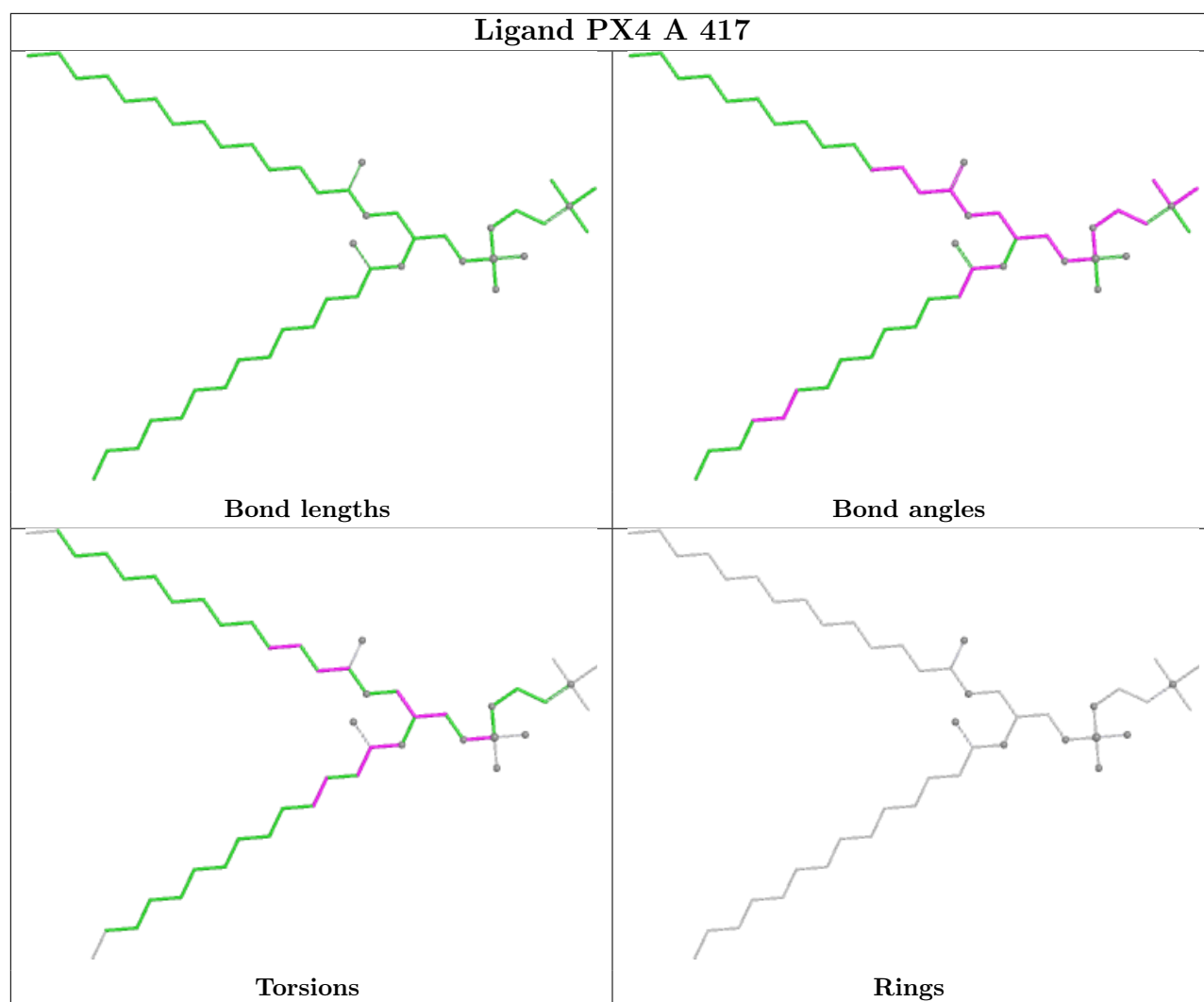


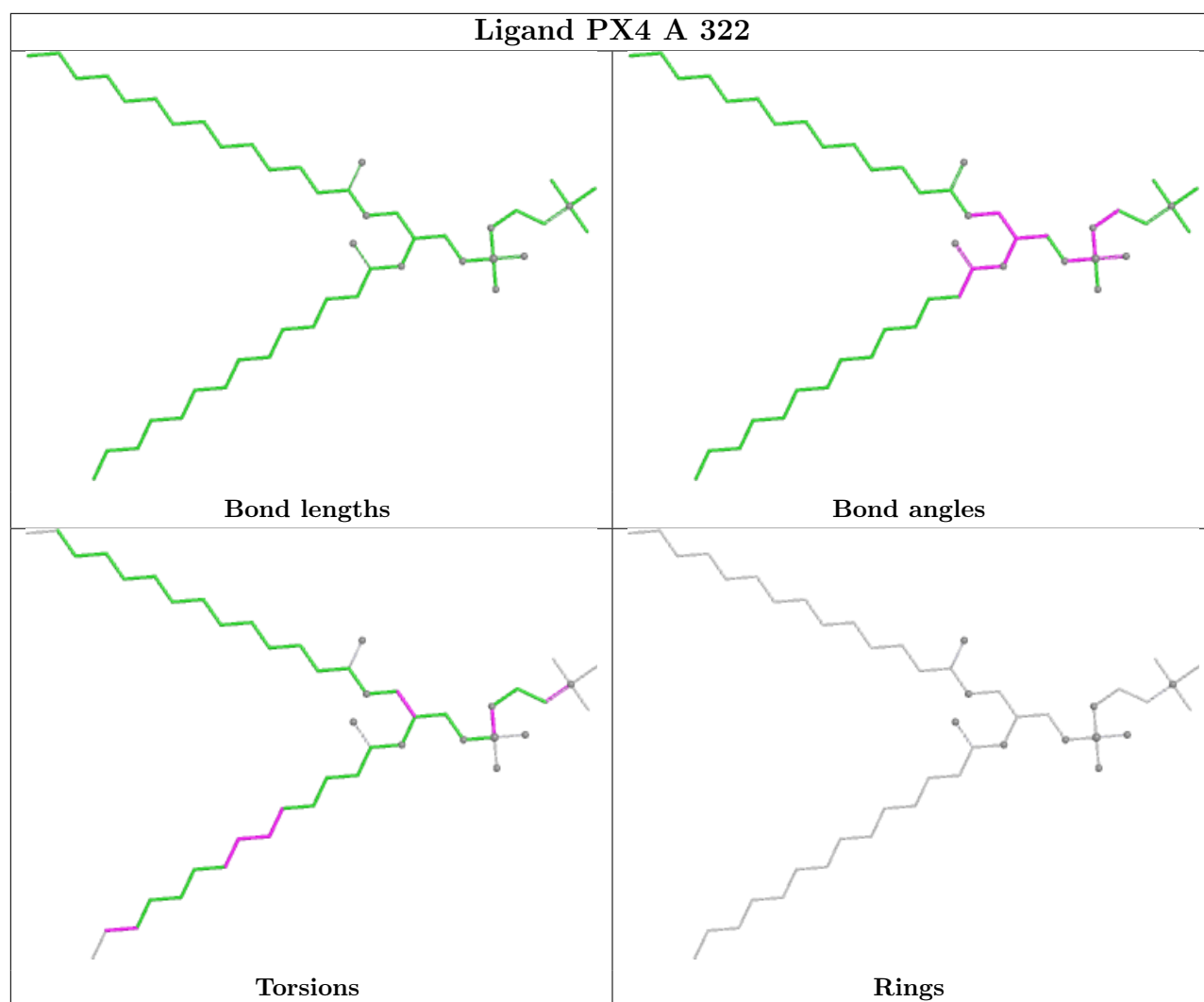


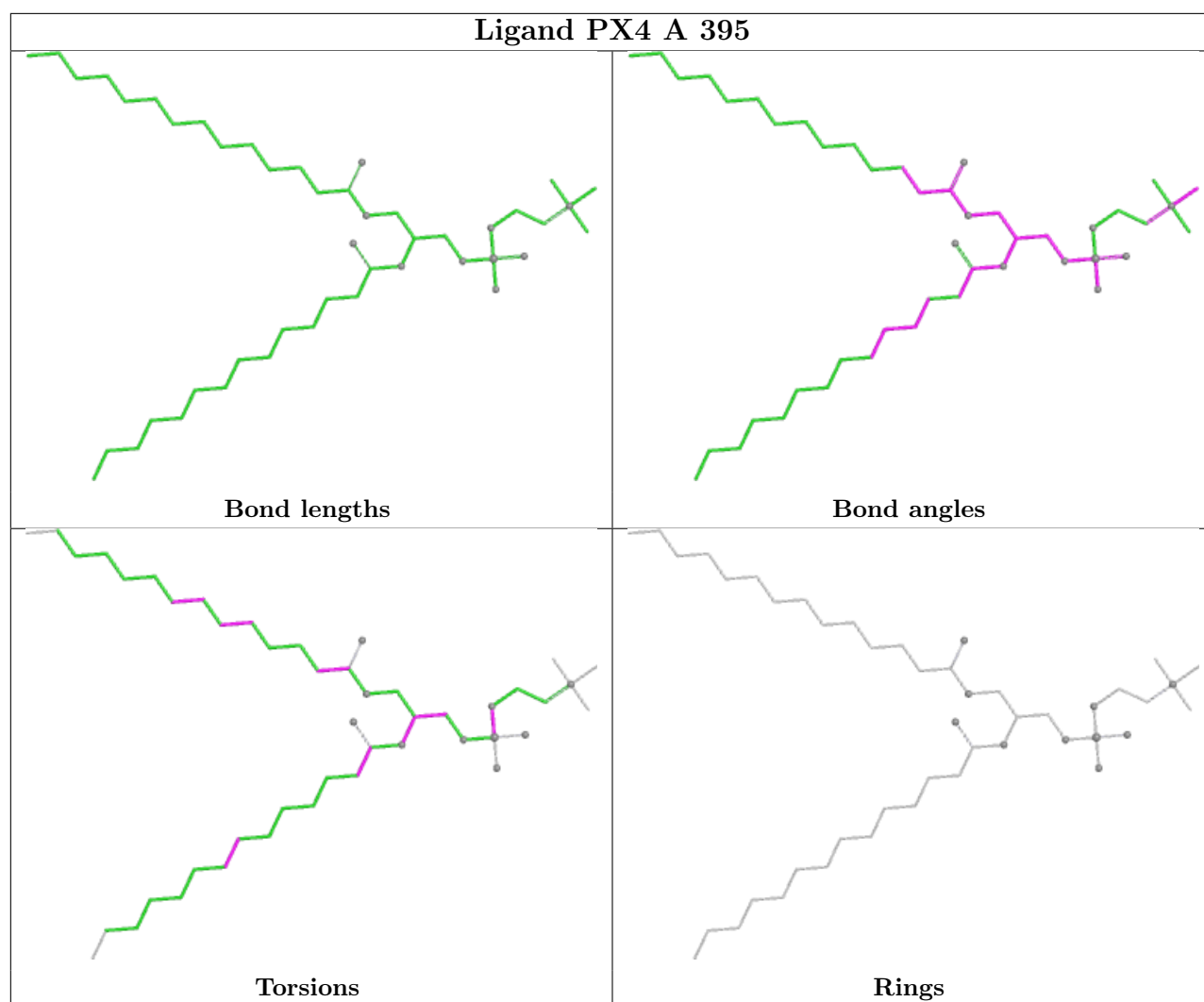


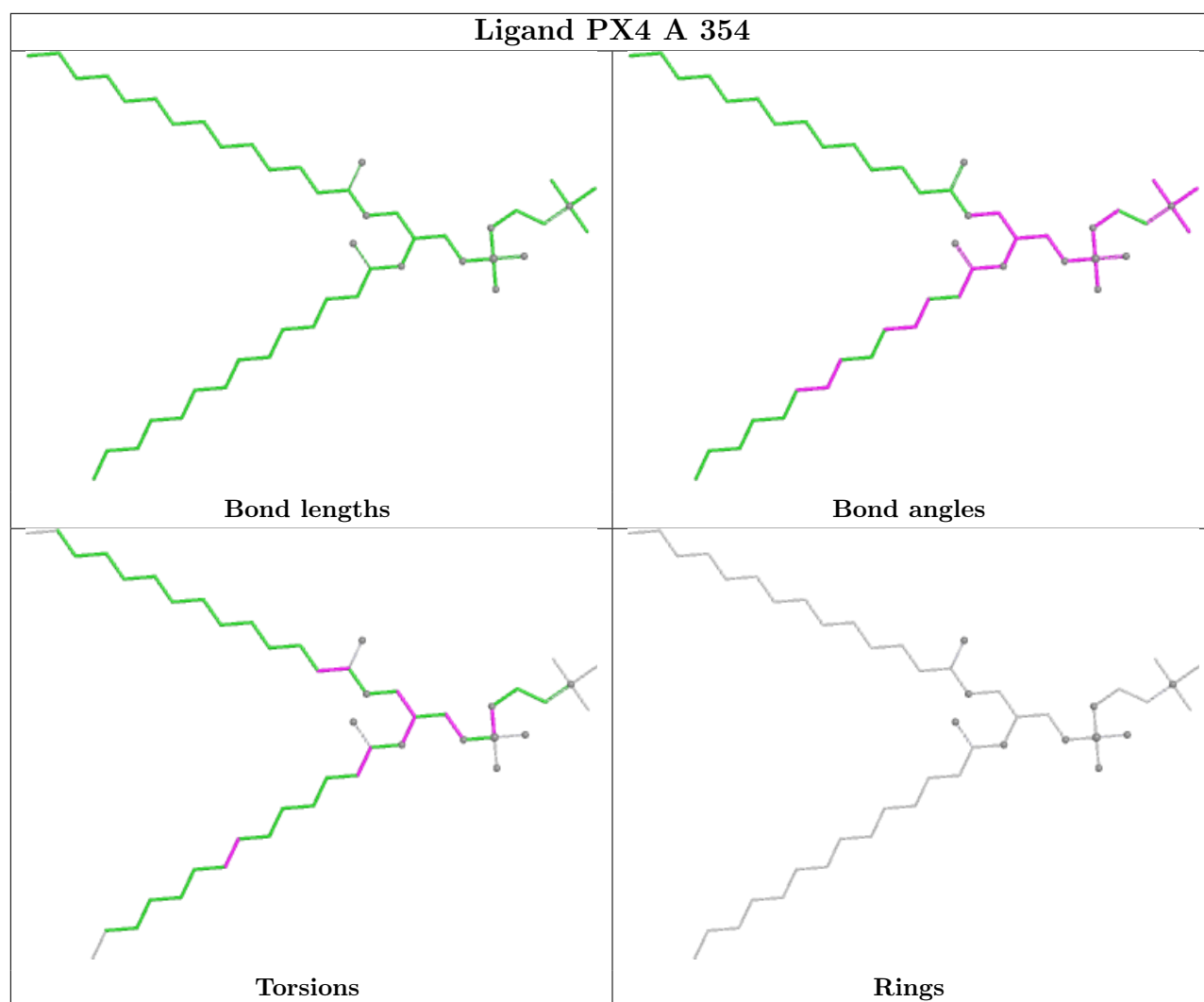


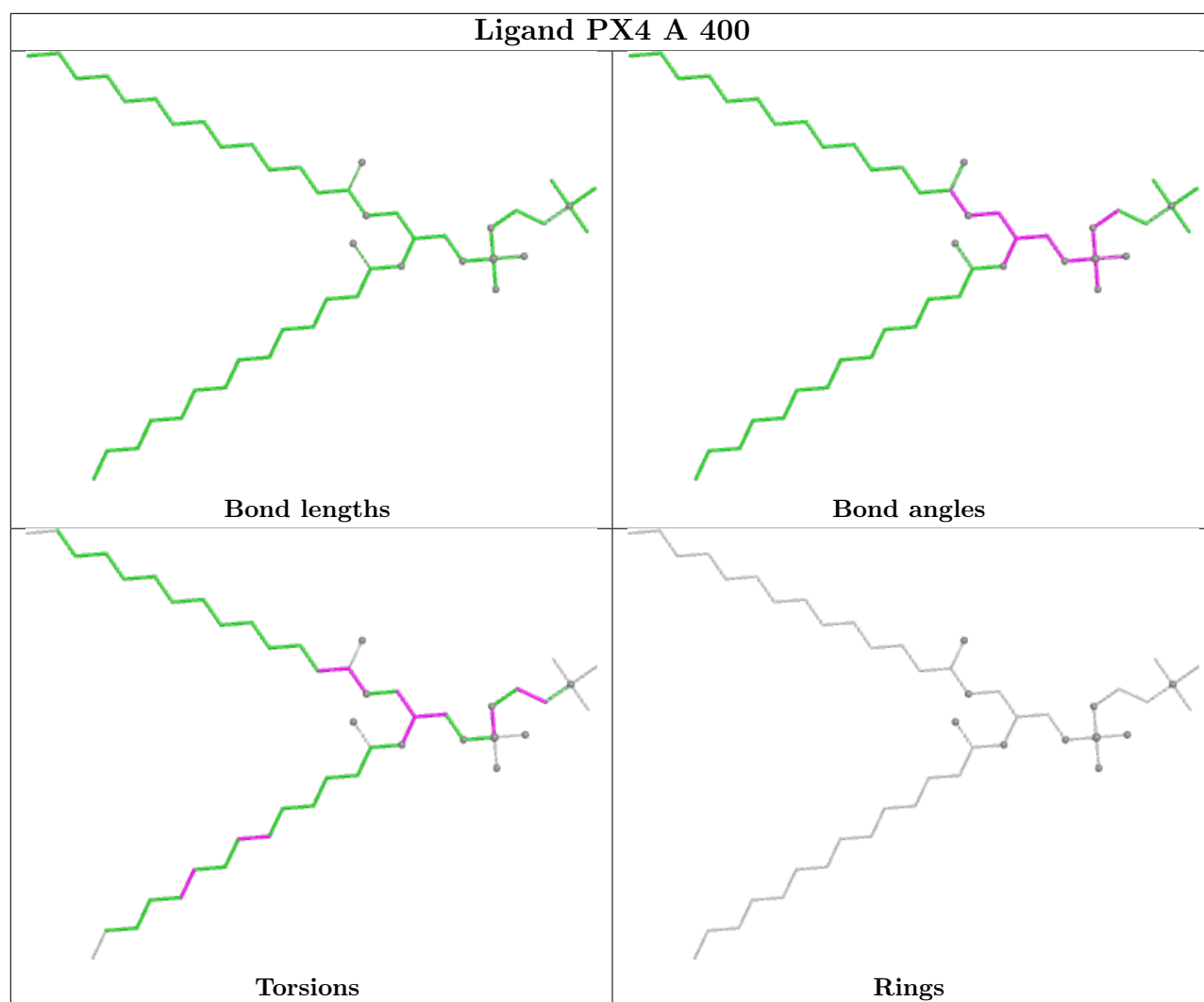


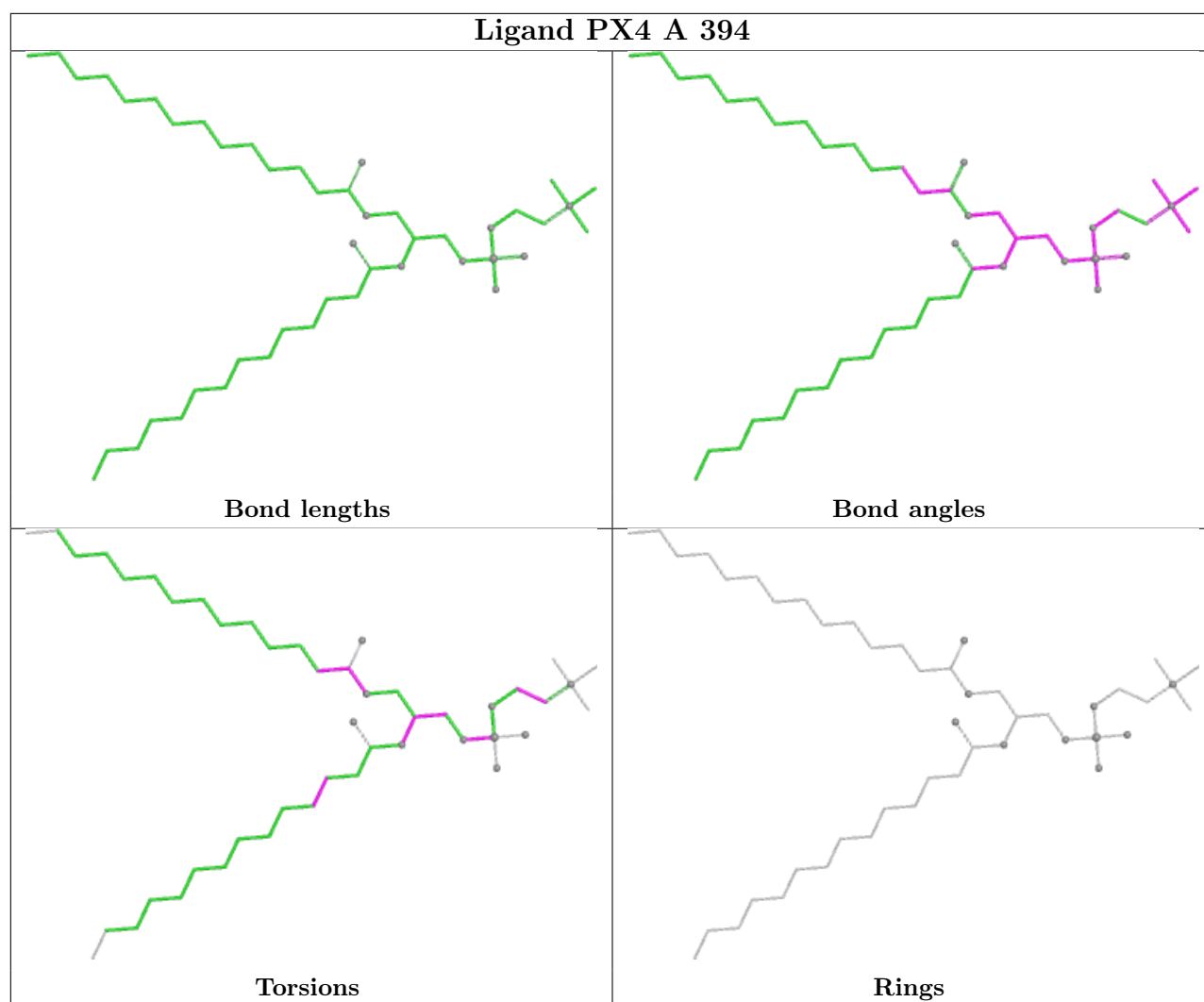


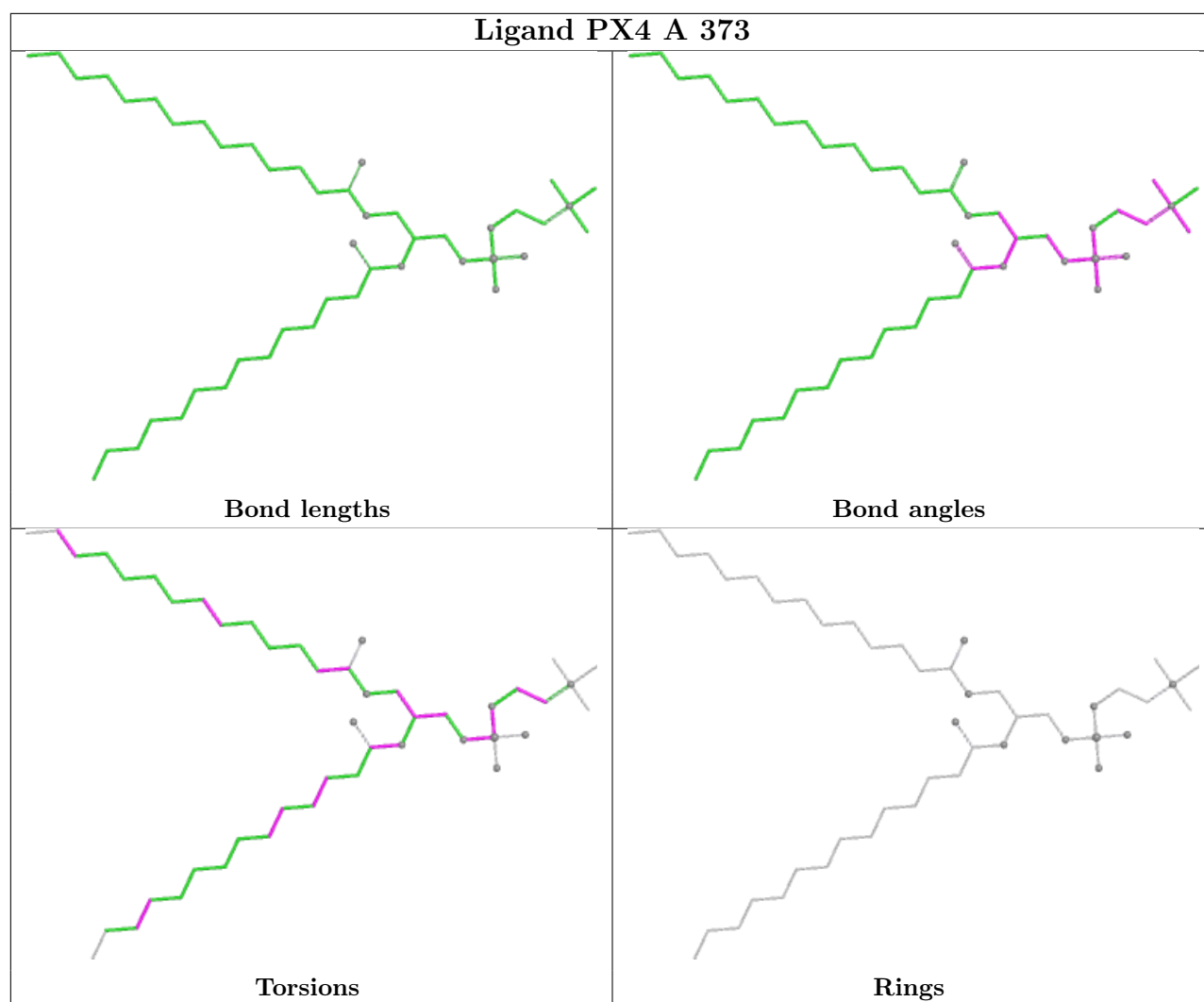












6.7 Other polymers [i](#)

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 81% 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 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	138	0.12 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	129	-0.18 ± 0.14	None needed (< 0.5 ppm)
^{15}N	154	-0.69 ± 0.29	Should be applied

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 81%, i.e. 1729 atoms were assigned a chemical shift out of a possible 2139. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	757/804 (94%)	323/331 (98%)	284/320 (89%)	150/153 (98%)
Sidechain	814/1053 (77%)	537/687 (78%)	268/326 (82%)	9/40 (22%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	158/282 (56%)	79/142 (56%)	76/128 (59%)	3/12 (25%)
Overall	1729/2139 (81%)	939/1160 (81%)	628/774 (81%)	162/205 (79%)

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.

	Total	¹ H	¹³ C	¹⁵ N
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 ⓘ

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 ⓘ

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:

