



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:55 PM UTC

PDB ID : 2MLS / pdb_00002mls
BMRB ID : 7089
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Beta-face
Authors : Koppiseti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.
Deposited on : 2014-03-04

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

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

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

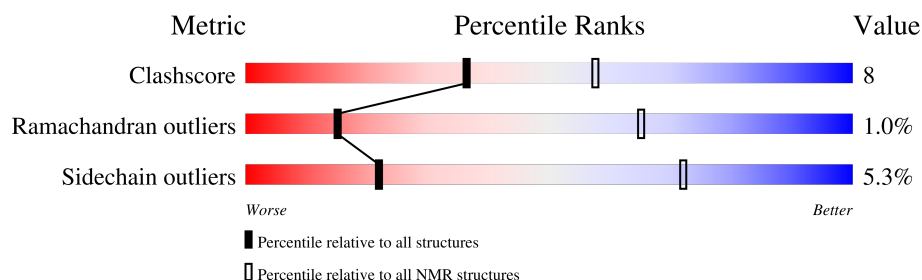
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	164	 69% 28% ..

2 Ensemble composition and analysis

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

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

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

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

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

The models can be grouped into 3 clusters and 5 single-model clusters were found.

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

3 Entry composition

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

- Molecule 1 is a protein called Macrophage metalloelastase.

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

There is a discrepancy between the modelled and reference sequences:

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

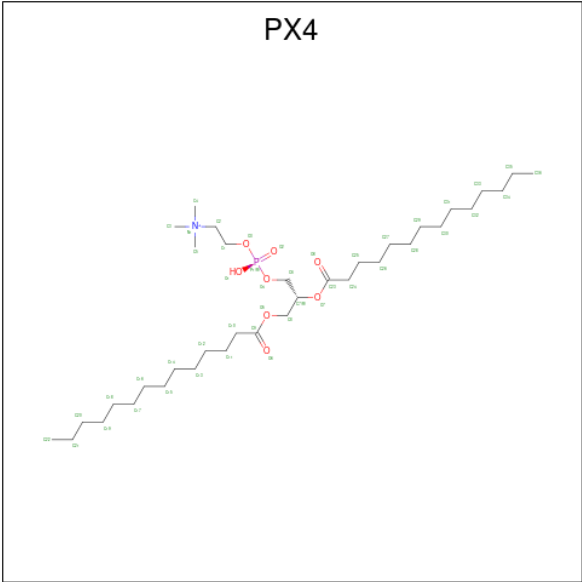
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

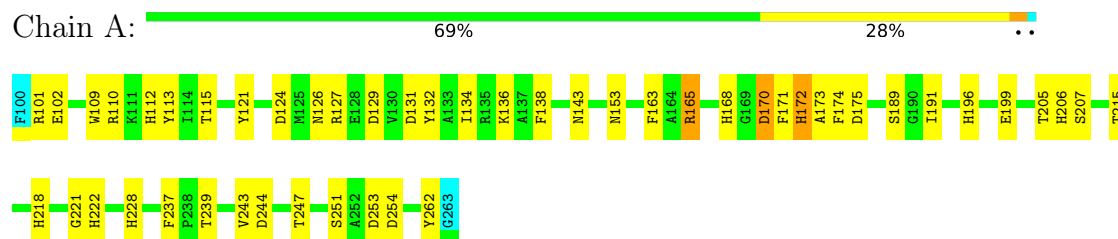
Mol	Chain	Residues	Atoms				
			Total	C	N	O	P
4	A	1	Total 46	36	1	8	1
4	A	1	Total 46	36	1	8	1
4	A	1	Total 46	36	1	8	1
4	A	1	Total 46	36	1	8	1
4	A	1	Total 46	36	1	8	1
4	A	1	Total 46	36	1	8	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Macrophage metalloelastase

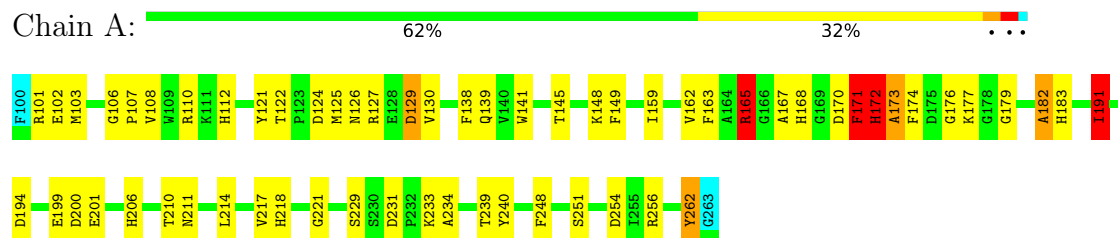


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

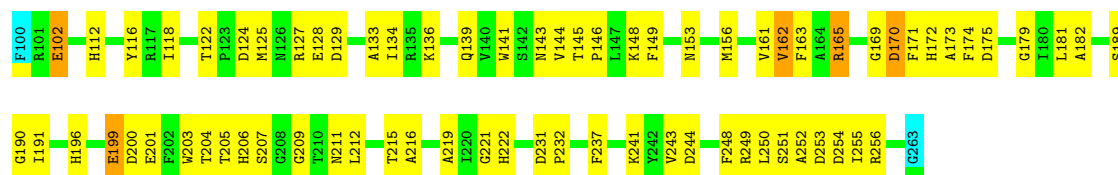
- Molecule 1: Macrophage metalloelastase



4.2.2 Score per residue for model 2

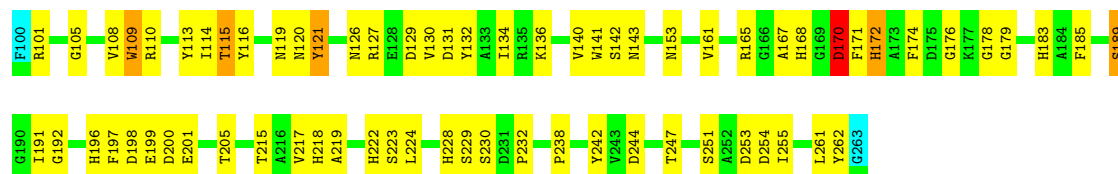
- Molecule 1: Macrophage metalloelastase





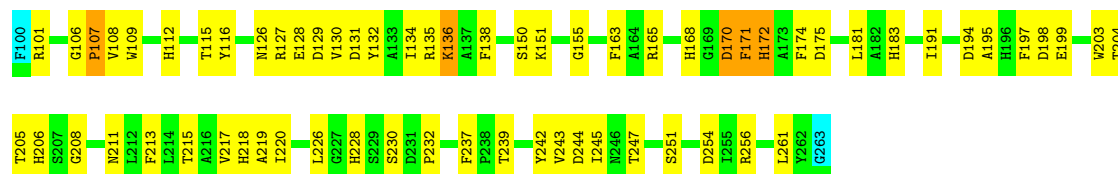
4.2.3 Score per residue for model 3

- Molecule 1: Macrophage metalloelastase



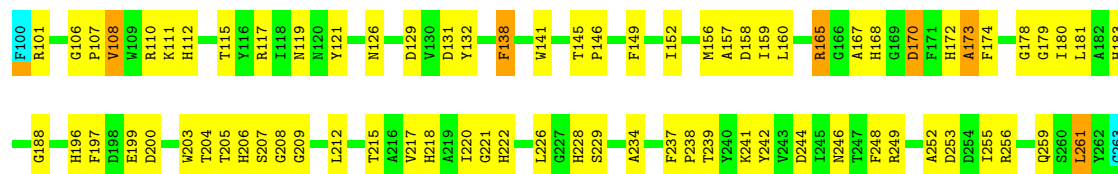
4.2.4 Score per residue for model 4

- Molecule 1: Macrophage metalloelastase



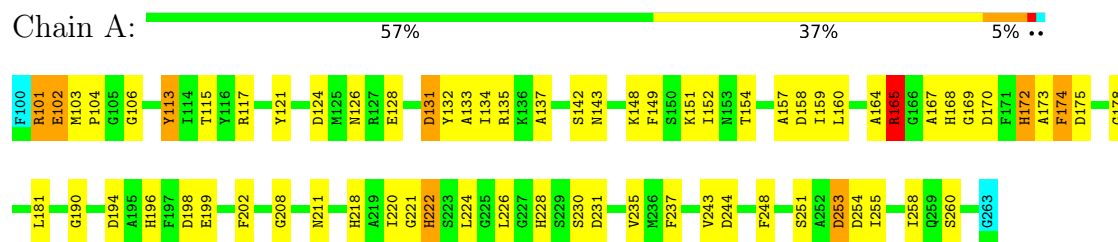
4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase



4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



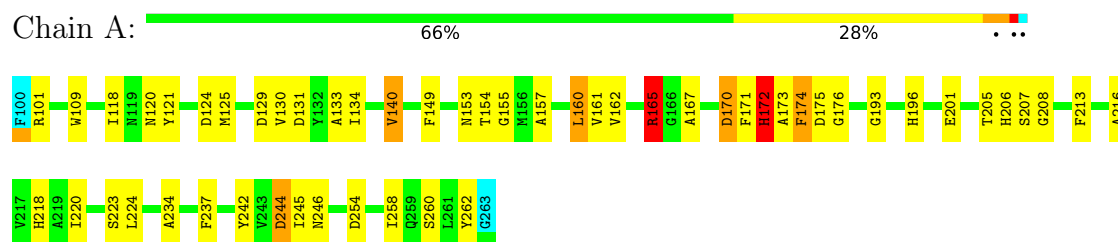
4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



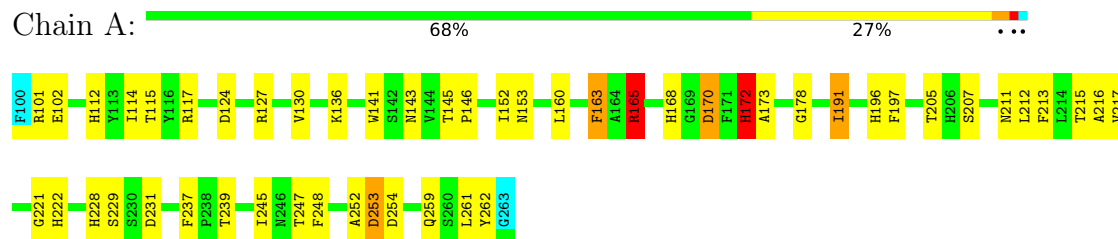
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Macrophage metalloelastase



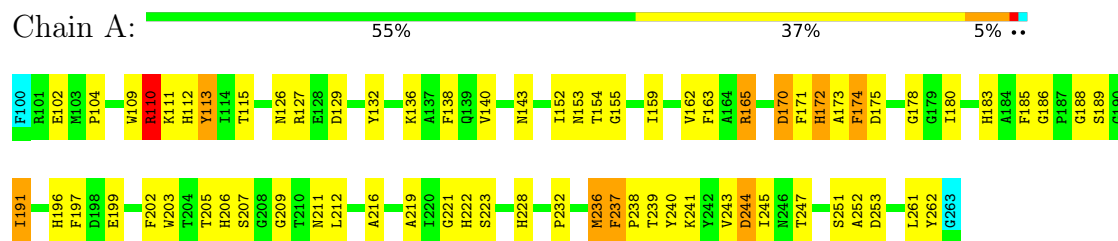
4.2.9 Score per residue for model 9

- Molecule 1: Macrophage metalloelastase



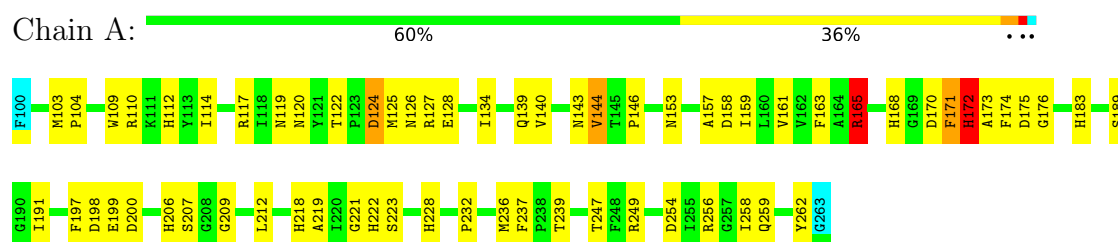
4.2.10 Score per residue for model 10

- Molecule 1: Macrophage metalloelastase



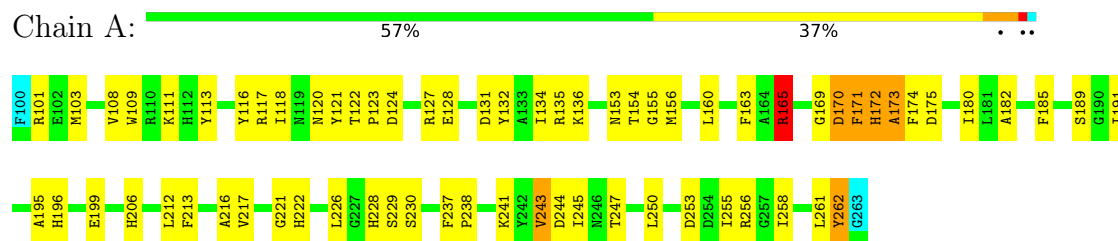
4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



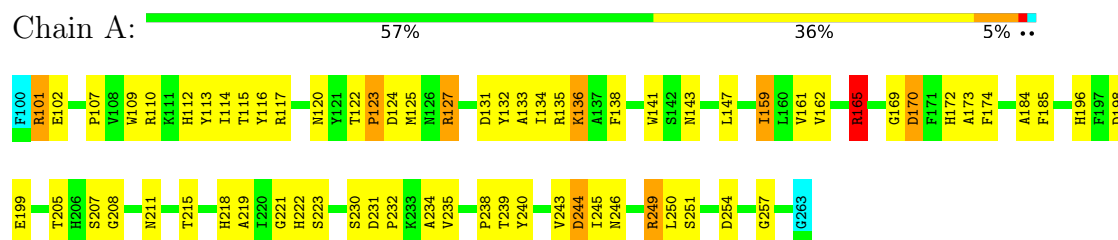
4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



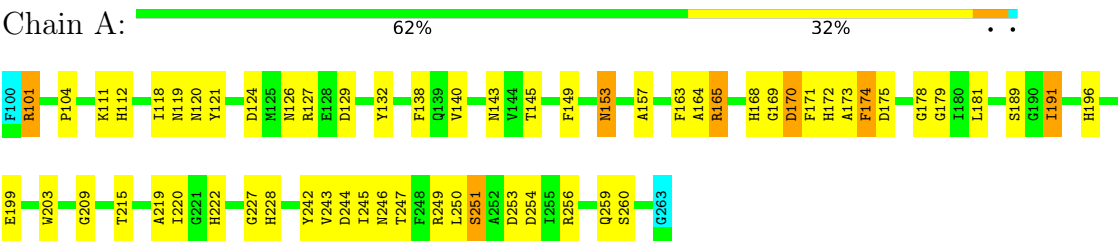
4.2.13 Score per residue for model 13

- 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)	82%

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.65±0.01	0±0/1311 (0.0± 0.0%)	2.52±0.07	94±11/1779 (5.3± 0.6%)
All	All	0.65	0/18354 (0.0%)	2.52	1318/24906 (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	4.9±2.3
All	All	0	68

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	175	ASP	CA-CB-CG	12.97	125.57	112.60	14	6
1	A	145	THR	O-C-N	-12.62	113.63	121.71	14	1
1	A	222	HIS	CA-CB-CG	12.53	126.33	113.80	10	3
1	A	124	ASP	CA-CB-CG	12.02	124.62	112.60	11	7
1	A	170	ASP	CB-CA-C	11.22	120.94	109.83	14	4
1	A	120	ASN	CA-CB-CG	11.20	123.80	112.60	3	3
1	A	131	ASP	CA-CB-CG	10.95	123.55	112.60	5	3
1	A	174	PHE	CA-CB-CG	10.76	124.56	113.80	8	3
1	A	121	TYR	CA-C-N	10.69	135.18	120.65	7	3
1	A	121	TYR	C-N-CA	10.69	135.18	120.65	7	3
1	A	172	HIS	CA-CB-CG	10.57	124.37	113.80	11	7
1	A	113	TYR	CA-C-N	10.29	136.65	122.34	10	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	113	TYR	C-N-CA	10.29	136.65	122.34	10	3
1	A	170	ASP	CA-CB-CG	10.21	122.81	112.60	14	9
1	A	196	HIS	CA-CB-CG	10.12	123.92	113.80	5	6
1	A	220	ILE	CA-C-N	10.09	131.39	119.99	7	3
1	A	220	ILE	C-N-CA	10.09	131.39	119.99	7	3
1	A	205	THR	CA-C-N	9.55	134.43	120.87	5	4
1	A	205	THR	C-N-CA	9.55	134.43	120.87	5	4
1	A	208	GLY	CA-C-N	9.33	129.66	121.82	5	3
1	A	208	GLY	C-N-CA	9.33	129.66	121.82	5	3
1	A	188	GLY	CA-C-N	9.25	134.00	120.87	10	2
1	A	188	GLY	C-N-CA	9.25	134.00	120.87	10	2
1	A	101	ARG	NE-CZ-NH1	-9.14	112.36	121.50	6	1
1	A	254	ASP	CA-C-N	9.13	133.38	120.42	1	6
1	A	254	ASP	C-N-CA	9.13	133.38	120.42	1	6
1	A	155	GLY	N-CA-C	-9.10	100.92	111.85	4	2
1	A	218	HIS	ND1-CE1-NE2	9.04	117.44	108.40	4	4
1	A	248	PHE	CA-C-N	9.00	137.02	122.53	9	3
1	A	248	PHE	C-N-CA	9.00	137.02	122.53	9	3
1	A	244	ASP	CA-CB-CG	8.99	121.59	112.60	10	8
1	A	144	VAL	N-CA-C	-8.95	104.75	113.53	7	1
1	A	235	VAL	O-C-N	-8.95	112.62	121.83	6	1
1	A	254	ASP	CA-CB-CG	8.93	121.53	112.60	14	6
1	A	153	ASN	CA-CB-CG	8.85	121.45	112.60	12	3
1	A	128	GLU	N-CA-C	8.76	122.96	111.75	12	1
1	A	197	PHE	CA-CB-CG	8.74	122.54	113.80	5	4
1	A	237	PHE	CA-C-N	8.73	128.05	118.97	5	6
1	A	237	PHE	C-N-CA	8.73	128.05	118.97	5	6
1	A	158	ASP	CA-C-N	8.71	136.36	122.33	11	1
1	A	158	ASP	C-N-CA	8.71	136.36	122.33	11	1
1	A	110	ARG	NE-CZ-NH1	8.71	130.21	121.50	10	1
1	A	101	ARG	CA-C-N	8.69	133.87	120.75	3	7
1	A	101	ARG	C-N-CA	8.69	133.87	120.75	3	7
1	A	171	PHE	CA-CB-CG	8.65	122.45	113.80	7	5
1	A	220	ILE	CA-CB-CG2	8.58	125.09	110.50	5	1
1	A	119	ASN	OD1-CG-ND2	-8.53	114.07	122.60	7	2
1	A	234	ALA	CA-C-N	8.52	132.52	120.42	7	3
1	A	234	ALA	C-N-CA	8.52	132.52	120.42	7	3
1	A	110	ARG	CB-CA-C	8.51	118.25	109.83	13	1
1	A	127	ARG	CA-C-N	8.48	132.00	120.38	4	3
1	A	127	ARG	C-N-CA	8.48	132.00	120.38	4	3
1	A	252	ALA	N-CA-C	8.48	121.59	111.33	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	149	PHE	CA-CB-CG	8.42	122.22	113.80	7	3
1	A	126	ASN	CA-CB-CG	8.31	120.91	112.60	11	1
1	A	212	LEU	CA-C-N	8.29	131.21	120.44	7	5
1	A	212	LEU	C-N-CA	8.29	131.21	120.44	7	5
1	A	112	HIS	CA-CB-CG	8.28	122.08	113.80	4	6
1	A	138	PHE	CA-CB-CG	8.22	122.02	113.80	7	2
1	A	138	PHE	CA-C-N	8.19	131.59	120.38	5	1
1	A	138	PHE	C-N-CA	8.19	131.59	120.38	5	1
1	A	122	THR	CA-C-N	8.17	127.81	119.56	1	2
1	A	122	THR	C-N-CA	8.17	127.81	119.56	1	2
1	A	253	ASP	CA-CB-CG	-8.17	104.43	112.60	14	2
1	A	251	SER	CA-C-N	8.14	131.53	120.54	10	4
1	A	251	SER	C-N-CA	8.14	131.53	120.54	10	4
1	A	260	SER	CA-C-O	-8.13	108.47	119.12	6	1
1	A	206	HIS	CA-C-N	8.11	131.96	120.28	5	3
1	A	206	HIS	C-N-CA	8.11	131.96	120.28	5	3
1	A	178	GLY	CA-C-O	-8.08	114.17	122.01	7	5
1	A	129	ASP	CA-C-N	8.08	130.74	120.56	5	3
1	A	129	ASP	C-N-CA	8.08	130.74	120.56	5	3
1	A	240	TYR	CA-C-O	-8.04	112.19	120.96	13	2
1	A	129	ASP	CA-CB-CG	8.04	120.64	112.60	4	3
1	A	211	ASN	CA-CB-CG	-8.04	104.56	112.60	13	3
1	A	235	VAL	N-CA-C	-8.03	102.61	110.72	13	1
1	A	246	ASN	OD1-CG-ND2	-8.03	114.57	122.60	14	1
1	A	230	SER	CA-C-N	8.01	132.74	121.61	3	3
1	A	230	SER	C-N-CA	8.01	132.74	121.61	3	3
1	A	252	ALA	CA-C-N	7.99	130.99	120.28	9	1
1	A	252	ALA	C-N-CA	7.99	130.99	120.28	9	1
1	A	130	VAL	N-CA-C	7.99	118.04	110.53	1	2
1	A	143	ASN	CA-CB-CG	7.97	120.57	112.60	11	5
1	A	150	SER	CA-C-N	7.92	133.65	122.72	4	1
1	A	150	SER	C-N-CA	7.92	133.65	122.72	4	1
1	A	223	SER	N-CA-C	7.92	122.52	113.01	7	2
1	A	232	PRO	N-CA-CB	7.89	111.08	103.51	10	5
1	A	215	THR	CA-C-N	7.88	130.84	120.28	5	5
1	A	215	THR	C-N-CA	7.88	130.84	120.28	5	5
1	A	128	GLU	CA-C-N	7.88	131.15	120.44	2	2
1	A	128	GLU	C-N-CA	7.88	131.15	120.44	2	2
1	A	231	ASP	N-CA-C	-7.84	100.19	110.07	1	1
1	A	176	GLY	CA-C-O	-7.83	114.50	122.26	3	3
1	A	102	GLU	O-C-N	-7.83	114.29	123.06	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	169	GLY	N-CA-C	-7.82	102.46	111.85	13	1
1	A	189	SER	N-CA-CB	-7.79	98.45	110.29	12	3
1	A	126	ASN	CA-C-N	7.74	130.98	120.38	10	7
1	A	126	ASN	C-N-CA	7.74	130.98	120.38	10	7
1	A	200	ASP	CA-CB-CG	7.72	120.32	112.60	1	3
1	A	259	GLN	OE1-CD-NE2	-7.72	114.88	122.60	14	4
1	A	245	ILE	CA-C-N	7.71	131.24	120.29	4	2
1	A	245	ILE	C-N-CA	7.71	131.24	120.29	4	2
1	A	185	PHE	CA-CB-CG	7.68	121.48	113.80	3	3
1	A	246	ASN	CA-CB-CG	7.68	120.28	112.60	8	2
1	A	154	THR	CB-CA-C	7.66	123.06	109.65	8	2
1	A	185	PHE	CA-C-O	-7.60	112.67	121.49	12	1
1	A	213	PHE	CA-C-N	7.59	131.21	120.28	12	1
1	A	213	PHE	C-N-CA	7.59	131.21	120.28	12	1
1	A	178	GLY	O-C-N	-7.58	116.98	123.43	6	1
1	A	196	HIS	ND1-CE1-NE2	7.58	115.98	108.40	8	4
1	A	102	GLU	N-CA-C	7.57	120.08	110.24	2	2
1	A	186	GLY	CA-C-N	7.57	128.01	120.52	10	1
1	A	186	GLY	C-N-CA	7.57	128.01	120.52	10	1
1	A	255	ILE	CA-C-N	7.57	132.71	120.60	12	1
1	A	255	ILE	C-N-CA	7.57	132.71	120.60	12	1
1	A	165	ARG	NH1-CZ-NH2	-7.57	109.46	119.30	8	2
1	A	133	ALA	CA-C-N	7.51	130.02	120.56	2	3
1	A	133	ALA	C-N-CA	7.51	130.02	120.56	2	3
1	A	111	LYS	CA-C-N	7.47	133.76	122.56	14	3
1	A	111	LYS	C-N-CA	7.47	133.76	122.56	14	3
1	A	168	HIS	ND1-CE1-NE2	7.44	115.84	108.40	5	3
1	A	237	PHE	CA-C-O	-7.44	112.59	120.70	8	2
1	A	172	HIS	ND1-CG-CD2	7.43	113.53	106.10	14	3
1	A	195	ALA	CA-C-O	-7.41	112.25	120.70	4	1
1	A	138	PHE	N-CA-C	7.38	119.40	111.36	10	1
1	A	152	ILE	CA-C-N	7.36	134.03	121.14	10	2
1	A	152	ILE	C-N-CA	7.36	134.03	121.14	10	2
1	A	108	VAL	CA-CB-CG2	7.36	122.91	110.40	12	1
1	A	141	TRP	N-CA-C	-7.35	103.27	112.90	9	4
1	A	183	HIS	CA-CB-CG	7.33	121.13	113.80	4	3
1	A	115	THR	CA-CB-OG1	7.33	120.59	109.60	7	2
1	A	198	ASP	CA-CB-CG	7.32	119.92	112.60	11	2
1	A	243	VAL	CA-C-N	7.32	131.10	120.71	10	5
1	A	243	VAL	C-N-CA	7.32	131.10	120.71	10	5
1	A	113	TYR	CA-C-O	-7.32	112.75	120.58	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	249	ARG	CA-C-N	7.31	132.91	122.09	2	1
1	A	249	ARG	C-N-CA	7.31	132.91	122.09	2	1
1	A	172	HIS	CB-CG-CD2	-7.29	121.73	131.20	1	2
1	A	178	GLY	CA-C-N	7.29	135.69	121.41	5	2
1	A	178	GLY	C-N-CA	7.29	135.69	121.41	5	2
1	A	115	THR	CA-CB-CG2	7.27	122.86	110.50	3	2
1	A	253	ASP	CA-C-N	7.26	130.61	120.29	12	4
1	A	253	ASP	C-N-CA	7.26	130.61	120.29	12	4
1	A	140	VAL	CA-C-N	7.26	130.32	120.38	7	5
1	A	140	VAL	C-N-CA	7.26	130.32	120.38	7	5
1	A	239	THR	CA-C-N	7.25	131.43	121.05	13	3
1	A	239	THR	C-N-CA	7.25	131.43	121.05	13	3
1	A	221	GLY	CA-C-N	7.25	130.31	120.38	1	8
1	A	221	GLY	C-N-CA	7.25	130.31	120.38	1	8
1	A	109	TRP	CA-CB-CG	7.25	127.37	113.60	3	2
1	A	161	VAL	CA-CB-CG1	7.23	122.69	110.40	3	1
1	A	257	GLY	CA-C-N	7.21	132.12	120.30	13	1
1	A	257	GLY	C-N-CA	7.21	132.12	120.30	13	1
1	A	238	PRO	N-CA-CB	7.21	110.94	103.23	5	3
1	A	191	ILE	CA-CB-CG2	7.19	122.72	110.50	9	1
1	A	163	PHE	CA-CB-CG	7.18	120.98	113.80	10	4
1	A	122	THR	CA-CB-CG2	7.18	122.70	110.50	13	3
1	A	165	ARG	NE-CZ-NH2	7.17	125.65	119.20	5	3
1	A	170	ASP	O-C-N	-7.17	114.69	122.00	9	1
1	A	157	ALA	O-C-N	-7.15	115.07	123.22	11	2
1	A	168	HIS	CE1-NE2-CD2	-7.15	101.85	109.00	5	7
1	A	156	MET	CA-C-N	7.14	130.95	120.95	2	3
1	A	156	MET	C-N-CA	7.14	130.95	120.95	2	3
1	A	222	HIS	CA-C-N	7.14	129.85	120.28	3	4
1	A	222	HIS	C-N-CA	7.14	129.85	120.28	3	4
1	A	183	HIS	ND1-CE1-NE2	7.12	115.52	108.40	1	3
1	A	218	HIS	CA-CB-CG	7.08	120.88	113.80	13	3
1	A	108	VAL	CB-CA-C	7.08	122.27	110.30	3	1
1	A	155	GLY	CA-C-O	-7.08	117.20	122.37	10	1
1	A	244	ASP	CA-C-N	7.08	132.23	120.62	5	7
1	A	244	ASP	C-N-CA	7.08	132.23	120.62	5	7
1	A	196	HIS	ND1-CG-CD2	7.06	113.16	106.10	14	5
1	A	207	SER	CA-CB-OG	7.02	125.13	111.10	5	1
1	A	174	PHE	CA-C-N	7.00	132.70	121.98	10	3
1	A	174	PHE	C-N-CA	7.00	132.70	121.98	10	3
1	A	127	ARG	NE-CZ-NH2	6.98	125.48	119.20	10	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	148	LYS	CA-C-N	6.98	133.05	122.65	2	1
1	A	148	LYS	C-N-CA	6.98	133.05	122.65	2	1
1	A	207	SER	N-CA-C	6.97	121.41	112.34	11	5
1	A	190	GLY	CA-C-N	6.96	133.40	121.63	2	1
1	A	190	GLY	C-N-CA	6.96	133.40	121.63	2	1
1	A	245	ILE	CB-CA-C	6.92	122.16	112.05	13	1
1	A	163	PHE	O-C-N	-6.91	114.00	123.12	2	2
1	A	144	VAL	N-CA-CB	-6.91	102.79	112.12	7	1
1	A	170	ASP	CA-C-N	6.90	134.72	121.54	6	5
1	A	170	ASP	C-N-CA	6.90	134.72	121.54	6	5
1	A	179	GLY	O-C-N	6.89	128.99	123.41	14	1
1	A	109	TRP	N-CA-C	-6.88	103.89	112.90	8	2
1	A	194	ASP	CA-CB-CG	6.88	119.48	112.60	1	2
1	A	131	ASP	CA-C-N	6.87	129.72	120.65	6	7
1	A	131	ASP	C-N-CA	6.87	129.72	120.65	6	7
1	A	243	VAL	CA-C-O	-6.87	114.11	121.19	14	1
1	A	164	ALA	O-C-N	-6.86	114.87	123.17	14	1
1	A	150	SER	N-CA-C	6.85	120.14	109.52	7	1
1	A	244	ASP	CB-CA-C	6.84	118.21	109.80	7	1
1	A	152	ILE	CA-C-O	-6.83	114.04	121.28	5	2
1	A	256	ARG	NE-CZ-NH1	6.82	128.32	121.50	5	1
1	A	127	ARG	N-CA-C	6.80	119.56	111.33	2	3
1	A	158	ASP	O-C-N	6.80	129.08	122.07	6	2
1	A	115	THR	CA-C-O	-6.78	113.97	121.23	10	2
1	A	231	ASP	CA-C-N	6.77	127.04	119.32	2	3
1	A	231	ASP	C-N-CA	6.77	127.04	119.32	2	3
1	A	222	HIS	ND1-CG-CD2	6.76	112.86	106.10	14	5
1	A	216	ALA	CA-C-N	6.75	129.06	120.56	8	4
1	A	216	ALA	C-N-CA	6.75	129.06	120.56	8	4
1	A	251	SER	CA-CB-OG	6.74	124.58	111.10	3	1
1	A	124	ASP	CA-C-O	6.74	127.69	120.55	2	1
1	A	219	ALA	N-CA-CB	6.74	120.17	110.06	11	1
1	A	231	ASP	CA-CB-CG	6.71	119.31	112.60	9	3
1	A	206	HIS	CA-CB-CG	-6.71	107.09	113.80	8	3
1	A	212	LEU	CA-C-O	-6.71	113.76	120.80	12	2
1	A	170	ASP	OD1-CG-OD2	-6.70	106.81	122.90	6	7
1	A	127	ARG	CD-NE-CZ	6.70	133.77	124.40	3	2
1	A	244	ASP	N-CA-C	6.69	120.34	110.30	3	1
1	A	181	LEU	CA-C-O	6.69	127.43	119.60	2	2
1	A	232	PRO	N-CD-CG	6.68	113.23	103.20	2	1
1	A	135	ARG	CD-NE-CZ	6.66	133.72	124.40	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	116	TYR	CA-C-O	6.64	129.21	121.44	13	1
1	A	206	HIS	ND1-CE1-NE2	6.62	115.02	108.40	2	3
1	A	124	ASP	N-CA-C	-6.61	104.24	112.90	8	3
1	A	169	GLY	O-C-N	-6.61	116.00	122.87	6	4
1	A	207	SER	CA-C-N	6.61	134.36	121.41	9	1
1	A	207	SER	C-N-CA	6.61	134.36	121.41	9	1
1	A	181	LEU	N-CA-C	-6.61	105.85	114.04	14	3
1	A	222	HIS	ND1-CE1-NE2	6.60	115.00	108.40	3	3
1	A	114	ILE	CA-CB-CG1	6.60	121.62	110.40	11	1
1	A	140	VAL	CA-CB-CG1	6.59	121.61	110.40	3	1
1	A	112	HIS	ND1-CE1-NE2	6.59	114.99	108.40	5	4
1	A	154	THR	CA-C-N	6.56	133.28	122.65	12	1
1	A	154	THR	C-N-CA	6.56	133.28	122.65	12	1
1	A	218	HIS	CE1-NE2-CD2	-6.55	102.45	109.00	4	2
1	A	229	SER	N-CA-C	-6.54	102.09	110.53	3	1
1	A	228	HIS	ND1-CE1-NE2	6.54	114.94	108.40	6	5
1	A	222	HIS	O-C-N	6.52	128.79	122.07	3	1
1	A	129	ASP	CA-C-O	-6.52	113.01	120.24	3	1
1	A	158	ASP	CA-CB-CG	6.51	119.11	112.60	5	1
1	A	153	ASN	N-CA-C	-6.50	105.35	113.28	14	1
1	A	126	ASN	OD1-CG-ND2	-6.49	116.11	122.60	1	1
1	A	153	ASN	O-C-N	-6.49	113.20	122.41	14	1
1	A	170	ASP	N-CA-CB	6.48	121.45	110.49	3	1
1	A	206	HIS	CB-CG-CD2	-6.48	122.78	131.20	1	4
1	A	144	VAL	CB-CA-C	6.48	117.12	110.70	2	2
1	A	255	ILE	CA-C-O	-6.47	114.22	120.95	2	2
1	A	197	PHE	CB-CG-CD1	6.46	131.69	120.70	5	1
1	A	260	SER	O-C-N	-6.46	115.27	122.12	8	1
1	A	209	GLY	CA-C-N	6.45	130.57	121.02	5	4
1	A	209	GLY	C-N-CA	6.45	130.57	121.02	5	4
1	A	191	ILE	CB-CA-C	6.45	121.76	111.69	7	2
1	A	120	ASN	N-CA-C	6.44	119.76	108.75	8	1
1	A	171	PHE	O-C-N	-6.44	114.03	122.59	12	2
1	A	215	THR	N-CA-C	-6.43	103.78	111.69	2	3
1	A	232	PRO	N-CA-C	6.43	122.33	113.65	3	1
1	A	162	VAL	O-C-N	-6.43	115.64	123.09	13	1
1	A	223	SER	CA-C-N	6.41	132.37	121.14	8	4
1	A	223	SER	C-N-CA	6.41	132.37	121.14	8	4
1	A	219	ALA	N-CA-C	6.41	118.27	111.28	2	2
1	A	229	SER	O-C-N	6.41	130.27	122.84	12	1
1	A	118	ILE	CA-CB-CG2	6.41	121.39	110.50	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	247	THR	CB-CA-C	6.40	121.17	111.18	12	2
1	A	163	PHE	CB-CA-C	6.40	120.28	110.62	4	2
1	A	134	ILE	CA-CB-CG1	6.39	121.26	110.40	6	2
1	A	218	HIS	CA-C-N	6.39	129.36	120.29	5	2
1	A	218	HIS	C-N-CA	6.39	129.36	120.29	5	2
1	A	222	HIS	CB-CG-CD2	-6.38	122.91	131.20	2	3
1	A	185	PHE	CA-C-N	6.37	131.88	121.87	3	3
1	A	185	PHE	C-N-CA	6.37	131.88	121.87	3	3
1	A	130	VAL	CA-C-N	6.37	129.34	120.29	3	3
1	A	130	VAL	C-N-CA	6.37	129.34	120.29	3	3
1	A	132	TYR	N-CA-C	6.37	117.88	111.07	5	1
1	A	261	LEU	N-CA-C	-6.36	106.15	114.04	10	2
1	A	140	VAL	CA-C-O	-6.36	113.61	120.47	10	1
1	A	217	VAL	CA-C-O	-6.35	114.44	121.17	1	1
1	A	194	ASP	CA-C-O	-6.35	114.23	121.72	6	1
1	A	155	GLY	O-C-N	-6.35	117.32	123.35	7	2
1	A	250	LEU	CA-C-O	-6.34	114.89	121.87	12	3
1	A	215	THR	CA-CB-CG2	6.33	121.27	110.50	9	1
1	A	170	ASP	CB-CG-OD1	6.33	132.96	118.40	7	4
1	A	237	PHE	CA-CB-CG	6.33	120.13	113.80	9	2
1	A	157	ALA	N-CA-CB	-6.33	99.56	109.87	6	1
1	A	226	LEU	CA-C-N	6.32	133.80	121.41	6	3
1	A	226	LEU	C-N-CA	6.32	133.80	121.41	6	3
1	A	230	SER	CB-CA-C	6.31	121.03	110.44	12	1
1	A	176	GLY	CA-C-N	6.30	130.31	121.24	8	2
1	A	176	GLY	C-N-CA	6.30	130.31	121.24	8	2
1	A	197	PHE	CA-C-N	6.30	129.77	120.95	9	1
1	A	197	PHE	C-N-CA	6.30	129.77	120.95	9	1
1	A	104	PRO	N-CA-CB	6.30	109.19	103.33	6	2
1	A	104	PRO	N-CD-CG	6.30	112.65	103.20	14	2
1	A	247	THR	CA-CB-CG2	6.30	121.21	110.50	7	3
1	A	235	VAL	CA-C-O	6.30	127.53	120.85	6	1
1	A	110	ARG	CA-C-O	6.29	128.12	120.57	3	2
1	A	205	THR	CA-C-O	6.29	127.95	120.53	10	2
1	A	255	ILE	CB-CA-C	6.29	120.02	111.97	3	2
1	A	120	ASN	OD1-CG-ND2	-6.27	116.33	122.60	12	1
1	A	239	THR	O-C-N	-6.27	115.70	123.04	11	3
1	A	253	ASP	N-CA-C	6.27	118.11	111.28	6	1
1	A	154	THR	CA-C-O	-6.26	113.04	120.43	6	1
1	A	173	ALA	CA-C-O	6.25	129.46	120.51	8	1
1	A	248	PHE	CA-CB-CG	6.25	120.05	113.80	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	171	PHE	CA-C-N	6.25	128.90	120.65	7	2
1	A	171	PHE	C-N-CA	6.25	128.90	120.65	7	2
1	A	206	HIS	ND1-CG-CD2	6.24	112.33	106.10	11	1
1	A	106	GLY	CA-C-N	6.23	127.21	119.98	1	3
1	A	106	GLY	C-N-CA	6.23	127.21	119.98	1	3
1	A	120	ASN	CA-C-O	-6.23	114.01	120.99	13	1
1	A	137	ALA	CA-C-N	6.23	128.62	120.28	6	1
1	A	137	ALA	C-N-CA	6.23	128.62	120.28	6	1
1	A	132	TYR	CA-CB-CG	6.22	125.09	113.90	4	2
1	A	163	PHE	N-CA-CB	-6.21	100.96	110.65	11	1
1	A	227	GLY	CA-C-N	6.21	132.30	122.62	14	1
1	A	227	GLY	C-N-CA	6.21	132.30	122.62	14	1
1	A	160	LEU	CA-C-N	6.21	131.79	123.10	5	2
1	A	160	LEU	C-N-CA	6.21	131.79	123.10	5	2
1	A	200	ASP	CA-C-N	6.18	129.49	120.71	2	2
1	A	200	ASP	C-N-CA	6.18	129.49	120.71	2	2
1	A	241	LYS	CB-CA-C	6.18	120.31	109.80	12	1
1	A	203	TRP	CA-C-O	6.18	127.75	120.58	2	1
1	A	253	ASP	O-C-N	-6.18	114.67	122.27	5	1
1	A	196	HIS	CB-CG-ND1	-6.17	113.45	122.70	9	2
1	A	167	ALA	N-CA-CB	-6.16	101.71	110.46	7	2
1	A	103	MET	CB-CA-C	6.16	119.28	109.62	6	1
1	A	259	GLN	CB-CG-CD	6.15	123.06	112.60	11	1
1	A	245	ILE	N-CA-C	6.15	118.74	111.05	14	3
1	A	162	VAL	CB-CA-C	6.15	122.68	111.30	1	2
1	A	189	SER	CA-CB-OG	6.14	123.39	111.10	7	1
1	A	102	GLU	CA-C-N	6.14	128.93	120.39	10	4
1	A	102	GLU	C-N-CA	6.14	128.93	120.39	10	4
1	A	211	ASN	CA-C-N	6.13	131.06	120.58	2	1
1	A	211	ASN	C-N-CA	6.13	131.06	120.58	2	1
1	A	204	THR	CA-C-O	-6.13	114.65	121.51	2	1
1	A	197	PHE	CB-CG-CD2	-6.13	110.28	120.70	5	1
1	A	168	HIS	CB-CA-C	6.13	120.31	109.65	3	2
1	A	173	ALA	CA-C-N	6.12	130.18	121.42	5	1
1	A	173	ALA	C-N-CA	6.12	130.18	121.42	5	1
1	A	191	ILE	N-CA-CB	-6.12	104.03	110.82	3	2
1	A	239	THR	N-CA-CB	-6.12	100.06	110.16	10	1
1	A	182	ALA	CA-C-N	6.12	131.83	122.77	1	2
1	A	182	ALA	C-N-CA	6.12	131.83	122.77	1	2
1	A	213	PHE	CA-CB-CG	6.12	119.92	113.80	9	3
1	A	242	TYR	CA-C-N	6.12	131.63	122.58	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	242	TYR	C-N-CA	6.12	131.63	122.58	4	1
1	A	222	HIS	CG-CD2-NE2	-6.09	101.11	107.20	13	2
1	A	161	VAL	CB-CA-C	6.09	118.91	110.99	3	2
1	A	183	HIS	ND1-CG-CD2	6.09	112.19	106.10	10	1
1	A	128	GLU	CA-C-O	-6.08	114.39	120.90	11	2
1	A	173	ALA	N-CA-CB	6.08	120.77	110.49	5	1
1	A	248	PHE	O-C-N	6.08	130.31	122.89	5	1
1	A	250	LEU	N-CA-C	-6.08	99.75	109.96	14	1
1	A	108	VAL	CA-C-O	-6.07	114.02	120.39	4	2
1	A	153	ASN	CB-CA-C	6.06	120.79	110.85	3	1
1	A	172	HIS	CA-C-O	6.06	126.84	120.42	4	1
1	A	256	ARG	CD-NE-CZ	6.04	132.86	124.40	14	2
1	A	165	ARG	CA-C-O	-6.04	113.61	120.32	10	1
1	A	139	GLN	CA-C-O	6.04	126.92	120.10	11	1
1	A	101	ARG	NE-CZ-NH2	6.04	124.64	119.20	4	3
1	A	164	ALA	CB-CA-C	6.04	122.26	110.30	7	1
1	A	261	LEU	CA-C-N	6.03	131.96	122.49	5	2
1	A	261	LEU	C-N-CA	6.03	131.96	122.49	5	2
1	A	115	THR	N-CA-CB	-6.03	100.78	111.08	9	1
1	A	220	ILE	O-C-N	-6.02	116.03	121.87	4	1
1	A	217	VAL	N-CA-C	6.02	116.68	110.36	4	2
1	A	166	GLY	CA-C-N	6.01	132.90	122.32	7	1
1	A	166	GLY	C-N-CA	6.01	132.90	122.32	7	1
1	A	245	ILE	CA-CB-CG1	6.00	120.61	110.40	8	1
1	A	162	VAL	CA-CB-CG2	6.00	120.61	110.40	10	1
1	A	208	GLY	O-C-N	5.99	127.66	121.97	4	2
1	A	101	ARG	CD-NE-CZ	5.99	132.78	124.40	14	2
1	A	113	TYR	O-C-N	-5.98	115.08	122.68	13	2
1	A	228	HIS	CB-CG-CD2	-5.97	123.44	131.20	7	4
1	A	115	THR	O-C-N	5.97	129.81	123.42	10	1
1	A	210	THR	OG1-CB-CG2	-5.96	97.38	109.30	1	1
1	A	132	TYR	CA-C-O	-5.96	114.11	120.42	13	2
1	A	124	ASP	CB-CA-C	-5.96	98.79	110.11	14	2
1	A	134	ILE	CA-C-N	5.95	128.57	120.54	8	5
1	A	134	ILE	C-N-CA	5.95	128.57	120.54	8	5
1	A	222	HIS	CE1-NE2-CD2	-5.95	103.05	109.00	3	1
1	A	118	ILE	CA-C-N	5.95	128.73	120.29	2	3
1	A	118	ILE	C-N-CA	5.95	128.73	120.29	2	3
1	A	161	VAL	N-CA-CB	-5.95	104.49	111.39	2	2
1	A	211	ASN	CB-CG-ND2	5.94	125.31	116.40	6	1
1	A	174	PHE	N-CA-C	5.94	117.71	110.41	14	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	201	GLU	CA-C-O	-5.93	115.10	121.56	1	1
1	A	200	ASP	N-CA-C	-5.92	106.02	113.18	2	2
1	A	231	ASP	O-C-N	-5.92	114.79	121.36	6	1
1	A	247	THR	CA-C-N	5.92	129.88	121.42	11	2
1	A	247	THR	C-N-CA	5.92	129.88	121.42	11	2
1	A	237	PHE	O-C-N	-5.92	113.59	121.64	4	3
1	A	218	HIS	N-CA-C	-5.91	104.42	111.69	6	2
1	A	110	ARG	NH1-CZ-NH2	5.91	126.98	119.30	1	1
1	A	102	GLU	CA-C-O	-5.90	115.06	121.44	1	1
1	A	198	ASP	O-C-N	-5.90	116.31	123.16	13	2
1	A	216	ALA	CA-C-O	-5.89	113.71	120.24	12	1
1	A	141	TRP	CA-C-O	-5.88	113.72	120.24	3	1
1	A	172	HIS	CA-C-N	5.88	132.77	121.54	13	3
1	A	172	HIS	C-N-CA	5.88	132.77	121.54	13	3
1	A	189	SER	CA-C-N	5.88	127.06	120.42	7	2
1	A	189	SER	C-N-CA	5.88	127.06	120.42	7	2
1	A	159	ILE	N-CA-C	-5.87	98.51	106.85	10	1
1	A	202	PHE	CB-CA-C	5.87	121.39	111.41	10	1
1	A	112	HIS	N-CA-CB	-5.87	101.44	110.42	7	1
1	A	171	PHE	N-CA-CB	5.85	120.38	110.49	1	1
1	A	228	HIS	CA-C-O	5.85	128.80	121.66	10	2
1	A	197	PHE	CA-C-O	-5.84	114.39	120.70	11	1
1	A	151	LYS	O-C-N	-5.84	116.52	123.06	6	1
1	A	103	MET	CA-C-N	5.84	125.75	119.85	1	2
1	A	103	MET	C-N-CA	5.84	125.75	119.85	1	2
1	A	165	ARG	O-C-N	-5.83	115.56	123.15	1	1
1	A	153	ASN	OD1-CG-ND2	-5.83	116.77	122.60	2	3
1	A	136	LYS	CA-C-N	5.83	128.09	120.28	7	5
1	A	136	LYS	C-N-CA	5.83	128.09	120.28	7	5
1	A	112	HIS	CA-C-N	5.82	131.37	123.11	11	1
1	A	112	HIS	C-N-CA	5.82	131.37	123.11	11	1
1	A	221	GLY	N-CA-C	5.81	119.67	112.64	13	1
1	A	234	ALA	N-CA-C	5.81	118.25	110.35	13	1
1	A	246	ASN	CB-CG-ND2	5.81	125.11	116.40	14	1
1	A	160	LEU	CA-C-O	-5.80	113.76	120.49	9	1
1	A	221	GLY	CA-C-O	5.80	126.30	120.09	10	1
1	A	185	PHE	N-CA-CB	-5.80	102.06	111.22	12	1
1	A	165	ARG	CD-NE-CZ	5.79	132.51	124.40	9	1
1	A	196	HIS	CA-C-O	-5.79	114.57	120.71	5	2
1	A	135	ARG	CA-C-O	-5.79	112.96	119.79	4	1
1	A	254	ASP	CB-CA-C	-5.78	101.02	110.85	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	241	LYS	N-CA-C	-5.78	98.84	108.32	2	2
1	A	133	ALA	O-C-N	5.78	129.38	122.27	8	1
1	A	261	LEU	N-CA-CB	-5.78	102.90	110.59	12	1
1	A	231	ASP	CA-C-O	-5.77	114.63	119.76	13	1
1	A	159	ILE	CB-CA-C	-5.76	104.44	111.88	6	2
1	A	145	THR	CA-CB-CG2	5.76	120.30	110.50	9	1
1	A	163	PHE	CA-C-O	5.76	127.83	120.57	9	1
1	A	211	ASN	O-C-N	-5.75	116.77	123.27	4	1
1	A	216	ALA	O-C-N	5.75	128.21	122.12	2	1
1	A	137	ALA	N-CA-C	5.75	117.22	111.07	6	1
1	A	192	GLY	O-C-N	-5.75	117.02	122.65	3	1
1	A	220	ILE	CB-CA-C	5.75	121.07	112.16	6	1
1	A	249	ARG	NE-CZ-NH2	-5.74	114.03	119.20	11	1
1	A	139	GLN	N-CA-C	5.73	119.37	112.38	2	1
1	A	175	ASP	N-CA-C	5.72	119.98	112.89	2	1
1	A	138	PHE	O-C-N	5.72	128.18	122.12	1	1
1	A	160	LEU	N-CA-C	-5.72	99.87	108.96	8	2
1	A	224	LEU	CA-C-N	5.71	132.60	121.41	7	2
1	A	224	LEU	C-N-CA	5.71	132.60	121.41	7	2
1	A	106	GLY	CA-C-O	-5.71	113.36	121.52	6	1
1	A	241	LYS	CA-C-N	5.71	129.46	121.24	10	2
1	A	241	LYS	C-N-CA	5.71	129.46	121.24	10	2
1	A	180	ILE	CA-CB-CG1	5.71	120.10	110.40	10	2
1	A	177	LYS	CA-C-O	-5.70	114.42	120.92	1	1
1	A	147	LEU	CA-C-N	5.69	132.15	122.37	13	1
1	A	147	LEU	C-N-CA	5.69	132.15	122.37	13	1
1	A	136	LYS	N-CA-CB	-5.69	101.47	110.28	3	2
1	A	234	ALA	CA-C-O	-5.69	115.36	121.56	8	1
1	A	114	ILE	O-C-N	-5.68	117.21	123.18	13	1
1	A	229	SER	CA-C-N	5.67	131.65	121.15	3	4
1	A	229	SER	C-N-CA	5.67	131.65	121.15	3	4
1	A	101	ARG	CB-CA-C	-5.67	99.80	110.01	9	1
1	A	146	PRO	CA-C-N	5.67	129.15	120.82	2	1
1	A	146	PRO	C-N-CA	5.67	129.15	120.82	2	1
1	A	250	LEU	O-C-N	-5.66	116.18	122.86	7	1
1	A	148	LYS	CA-C-O	-5.65	114.26	120.36	2	1
1	A	141	TRP	CH2-CZ2-CE2	5.64	124.84	117.50	2	1
1	A	119	ASN	CA-CB-CG	5.64	118.24	112.60	7	2
1	A	261	LEU	CB-CA-C	5.64	118.08	109.34	3	1
1	A	262	TYR	CA-C-O	5.64	126.77	119.95	8	1
1	A	189	SER	O-C-N	-5.64	116.62	123.16	14	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	243	VAL	CA-CB-CG2	5.63	119.98	110.40	4	2
1	A	146	PRO	N-CA-CB	5.63	109.07	102.76	9	1
1	A	145	THR	CA-C-N	5.63	126.50	120.47	9	1
1	A	145	THR	C-N-CA	5.63	126.50	120.47	9	1
1	A	135	ARG	CA-C-N	5.63	130.12	120.72	12	2
1	A	135	ARG	C-N-CA	5.63	130.12	120.72	12	2
1	A	168	HIS	CB-CG-ND1	-5.63	114.26	122.70	5	1
1	A	172	HIS	N-CA-CB	-5.63	101.55	110.22	12	1
1	A	188	GLY	CA-C-O	-5.63	118.26	122.37	10	1
1	A	258	ILE	N-CA-C	-5.62	105.04	110.72	8	1
1	A	165	ARG	N-CA-CB	5.62	120.52	110.80	10	1
1	A	189	SER	CA-C-O	-5.62	114.35	120.81	11	3
1	A	256	ARG	CA-C-O	-5.62	112.47	119.38	2	1
1	A	120	ASN	CA-C-N	5.61	130.47	122.72	3	1
1	A	120	ASN	C-N-CA	5.61	130.47	122.72	3	1
1	A	218	HIS	ND1-CG-CD2	5.61	111.71	106.10	5	2
1	A	245	ILE	O-C-N	-5.60	116.40	121.89	9	1
1	A	219	ALA	CA-C-N	5.60	128.14	120.46	11	3
1	A	219	ALA	C-N-CA	5.60	128.14	120.46	11	3
1	A	115	THR	CB-CA-C	5.60	120.36	109.33	13	3
1	A	202	PHE	CA-CB-CG	-5.60	108.20	113.80	6	2
1	A	251	SER	N-CA-CB	-5.59	101.94	110.49	4	2
1	A	142	SER	CA-C-N	5.58	131.48	121.66	7	3
1	A	142	SER	C-N-CA	5.58	131.48	121.66	7	3
1	A	109	TRP	CA-C-N	5.58	130.77	122.74	3	2
1	A	109	TRP	C-N-CA	5.58	130.77	122.74	3	2
1	A	101	ARG	NH1-CZ-NH2	-5.57	112.06	119.30	4	1
1	A	117	ARG	NE-CZ-NH2	5.56	124.21	119.20	11	2
1	A	204	THR	CA-C-N	5.56	131.11	122.49	7	1
1	A	204	THR	C-N-CA	5.56	131.11	122.49	7	1
1	A	203	TRP	CE2-CD2-CE3	-5.56	113.24	118.80	5	2
1	A	259	GLN	N-CA-CB	-5.55	101.17	110.39	14	1
1	A	254	ASP	N-CA-CB	5.55	118.26	109.82	3	1
1	A	168	HIS	N-CA-CB	-5.55	103.22	110.88	1	1
1	A	123	PRO	CA-C-O	-5.55	112.21	118.98	13	1
1	A	247	THR	CA-C-O	5.54	126.02	119.48	14	1
1	A	183	HIS	CE1-NE2-CD2	-5.53	103.47	109.00	1	1
1	A	161	VAL	CA-C-N	5.53	130.93	122.25	13	1
1	A	161	VAL	C-N-CA	5.53	130.93	122.25	13	1
1	A	136	LYS	CB-CG-CD	5.53	124.01	111.30	2	1
1	A	125	MET	CA-C-N	5.53	128.72	120.87	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	125	MET	C-N-CA	5.53	128.72	120.87	8	1
1	A	127	ARG	NH1-CZ-NH2	-5.51	112.14	119.30	13	1
1	A	145	THR	CB-CA-C	5.50	118.73	109.32	1	1
1	A	206	HIS	CE1-NE2-CD2	-5.50	103.50	109.00	12	1
1	A	141	TRP	CD2-CE3-CZ3	5.50	125.75	118.60	13	1
1	A	180	ILE	CA-C-N	5.50	131.81	122.36	5	1
1	A	180	ILE	C-N-CA	5.50	131.81	122.36	5	1
1	A	219	ALA	CB-CA-C	-5.49	101.34	110.68	11	1
1	A	217	VAL	CA-CB-CG1	5.49	119.73	110.40	5	3
1	A	172	HIS	ND1-CE1-NE2	5.47	113.87	108.40	1	1
1	A	179	GLY	CA-C-N	5.47	128.51	120.91	1	1
1	A	179	GLY	C-N-CA	5.47	128.51	120.91	1	1
1	A	144	VAL	O-C-N	-5.47	116.15	121.78	2	1
1	A	212	LEU	N-CA-C	-5.47	104.19	111.24	11	1
1	A	224	LEU	N-CA-C	5.46	119.04	112.38	3	1
1	A	175	ASP	N-CA-CB	-5.46	103.78	110.98	10	1
1	A	242	TYR	O-C-N	5.44	129.41	123.04	5	1
1	A	249	ARG	CD-NE-CZ	5.44	132.02	124.40	13	1
1	A	146	PRO	O-C-N	-5.44	115.30	122.64	11	1
1	A	117	ARG	CA-C-O	-5.44	114.90	120.99	12	1
1	A	148	LYS	CB-CA-C	5.43	119.65	109.71	1	2
1	A	228	HIS	ND1-CG-CD2	5.43	111.53	106.10	4	1
1	A	211	ASN	OD1-CG-ND2	5.42	128.03	122.60	1	1
1	A	213	PHE	N-CA-C	5.42	117.62	111.11	9	1
1	A	173	ALA	N-CA-C	5.42	122.35	110.80	12	1
1	A	140	VAL	O-C-N	5.42	127.92	121.80	10	1
1	A	244	ASP	CA-C-O	-5.42	115.09	121.16	12	1
1	A	205	THR	CA-CB-CG2	5.41	119.70	110.50	7	1
1	A	182	ALA	O-C-N	-5.41	117.08	123.41	12	1
1	A	151	LYS	CA-C-N	5.41	130.37	122.69	4	1
1	A	151	LYS	C-N-CA	5.41	130.37	122.69	4	1
1	A	187	PRO	N-CA-CB	5.40	109.05	103.38	7	1
1	A	193	GLY	CA-C-N	5.40	131.82	122.64	8	1
1	A	193	GLY	C-N-CA	5.40	131.82	122.64	8	1
1	A	164	ALA	CA-C-O	-5.39	115.13	121.44	6	1
1	A	149	PHE	CA-C-N	5.39	131.49	121.62	14	1
1	A	149	PHE	C-N-CA	5.39	131.49	121.62	14	1
1	A	217	VAL	CA-CB-CG2	5.39	119.56	110.40	9	1
1	A	205	THR	CA-CB-OG1	5.39	117.68	109.60	3	1
1	A	256	ARG	O-C-N	-5.38	115.92	122.22	4	1
1	A	236	MET	CA-C-N	5.38	128.13	120.49	7	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	236	MET	C-N-CA	5.38	128.13	120.49	7	3
1	A	203	TRP	CA-C-N	5.38	131.19	122.53	14	1
1	A	203	TRP	C-N-CA	5.38	131.19	122.53	14	1
1	A	101	ARG	N-CA-CB	-5.38	103.44	110.59	4	1
1	A	161	VAL	CA-CB-CG2	5.37	119.53	110.40	11	1
1	A	201	GLU	O-C-N	5.37	128.91	122.79	8	1
1	A	112	HIS	CB-CA-C	5.37	118.70	109.15	4	1
1	A	109	TRP	CE2-CD2-CE3	-5.36	113.44	118.80	13	1
1	A	138	PHE	N-CA-CB	-5.36	102.23	110.16	10	1
1	A	142	SER	CA-CB-OG	5.35	121.81	111.10	3	1
1	A	125	MET	CB-CA-C	5.35	119.94	109.35	1	2
1	A	243	VAL	CB-CA-C	5.35	117.09	110.73	10	1
1	A	249	ARG	CA-C-O	-5.35	114.51	120.66	14	1
1	A	124	ASP	N-CA-CB	5.34	118.04	110.13	1	1
1	A	195	ALA	O-C-N	5.34	129.95	123.01	4	2
1	A	141	TRP	CZ3-CH2-CZ2	-5.34	114.56	121.50	2	1
1	A	155	GLY	CA-C-N	5.34	129.13	121.50	12	1
1	A	155	GLY	C-N-CA	5.34	129.13	121.50	12	1
1	A	169	GLY	CA-C-O	-5.34	118.55	122.23	14	2
1	A	134	ILE	N-CA-CB	-5.34	100.53	110.40	3	1
1	A	204	THR	CA-CB-CG2	5.34	119.57	110.50	5	1
1	A	214	LEU	O-C-N	-5.33	115.98	122.22	1	1
1	A	165	ARG	CB-CA-C	5.33	119.35	109.70	13	1
1	A	139	GLN	OE1-CD-NE2	-5.33	117.27	122.60	1	1
1	A	152	ILE	O-C-N	-5.33	117.45	123.20	10	1
1	A	128	GLU	O-C-N	5.33	128.27	122.20	12	1
1	A	143	ASN	CA-C-N	5.32	128.53	122.36	2	2
1	A	143	ASN	C-N-CA	5.32	128.53	122.36	2	2
1	A	216	ALA	CB-CA-C	-5.32	101.95	110.79	2	1
1	A	174	PHE	O-C-N	-5.32	116.46	122.68	10	1
1	A	110	ARG	CD-NE-CZ	5.32	131.84	124.40	1	1
1	A	167	ALA	CA-C-N	5.32	130.71	122.26	6	2
1	A	167	ALA	C-N-CA	5.32	130.71	122.26	6	2
1	A	127	ARG	NE-CZ-NH1	5.32	126.81	121.50	13	1
1	A	191	ILE	CA-CB-CG1	5.31	119.43	110.40	1	1
1	A	198	ASP	CA-C-O	5.31	126.37	120.43	6	1
1	A	112	HIS	N-CA-C	-5.30	106.13	113.18	9	1
1	A	234	ALA	N-CA-CB	-5.30	101.98	110.46	1	1
1	A	111	LYS	N-CA-C	-5.30	101.24	109.72	5	1
1	A	114	ILE	CA-CB-CG2	5.29	119.50	110.50	3	1
1	A	213	PHE	N-CA-CB	-5.29	102.31	110.20	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	203	TRP	CD2-CE3-CZ3	5.29	125.47	118.60	4	1
1	A	167	ALA	CB-CA-C	5.29	120.14	111.41	7	1
1	A	159	ILE	CA-CB-CG1	5.29	119.39	110.40	13	1
1	A	121	TYR	N-CA-C	5.28	117.84	109.24	3	1
1	A	168	HIS	CA-C-O	5.28	124.86	119.05	6	1
1	A	122	THR	OG1-CB-CG2	-5.27	98.75	109.30	11	1
1	A	204	THR	N-CA-C	5.27	116.29	108.86	4	1
1	A	165	ARG	NE-CZ-NH1	-5.26	116.24	121.50	5	1
1	A	226	LEU	O-C-N	5.25	129.05	122.43	12	1
1	A	124	ASP	OD1-CG-OD2	-5.24	110.32	122.90	14	1
1	A	104	PRO	CA-C-O	5.24	127.76	121.48	10	1
1	A	172	HIS	N-CA-C	5.24	116.67	111.07	14	1
1	A	118	ILE	O-C-N	-5.23	116.98	123.10	7	1
1	A	239	THR	CA-CB-OG1	-5.23	101.75	109.60	13	1
1	A	258	ILE	CA-CB-CG2	5.23	119.39	110.50	6	2
1	A	228	HIS	CA-CB-CG	5.23	119.03	113.80	5	2
1	A	240	TYR	O-C-N	5.23	129.33	123.06	13	1
1	A	146	PRO	N-CA-C	5.22	120.88	114.35	5	1
1	A	149	PHE	CA-C-O	5.22	126.07	120.38	6	1
1	A	157	ALA	CA-C-O	-5.22	114.91	120.92	8	1
1	A	103	MET	CA-C-O	-5.22	114.74	120.17	12	1
1	A	109	TRP	NE1-CE2-CD2	-5.21	100.63	107.40	4	1
1	A	219	ALA	O-C-N	5.21	128.09	122.15	3	1
1	A	205	THR	N-CA-CB	-5.21	101.69	110.49	3	1
1	A	238	PRO	N-CA-C	5.20	121.49	113.75	13	1
1	A	205	THR	N-CA-C	5.19	119.72	113.17	2	1
1	A	113	TYR	CB-CG-CD1	-5.19	113.01	120.80	12	1
1	A	239	THR	CA-CB-CG2	5.19	119.32	110.50	13	2
1	A	116	TYR	CA-C-N	5.19	130.72	122.94	2	1
1	A	116	TYR	C-N-CA	5.19	130.72	122.94	2	1
1	A	238	PRO	N-CD-CG	5.19	110.98	103.20	5	1
1	A	207	SER	O-C-N	-5.18	115.65	122.39	10	1
1	A	209	GLY	O-C-N	-5.17	118.79	123.29	10	1
1	A	159	ILE	O-C-N	-5.17	116.92	122.45	11	1
1	A	145	THR	N-CA-C	5.17	118.00	109.58	2	1
1	A	153	ASN	CB-CG-ND2	5.17	124.15	116.40	9	1
1	A	168	HIS	CB-CG-CD2	5.17	137.91	131.20	5	1
1	A	101	ARG	N-CA-C	-5.16	107.15	113.50	6	1
1	A	105	GLY	CA-C-N	5.16	129.97	121.87	3	1
1	A	105	GLY	C-N-CA	5.16	129.97	121.87	3	1
1	A	140	VAL	CB-CA-C	-5.16	104.37	111.65	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	143	ASN	OD1-CG-ND2	-5.16	117.44	122.60	10	1
1	A	262	TYR	CA-C-N	5.15	130.96	121.70	12	2
1	A	262	TYR	C-N-CA	5.15	130.96	121.70	12	2
1	A	194	ASP	OD1-CG-OD2	-5.14	110.56	122.90	4	1
1	A	206	HIS	CB-CG-ND1	5.14	130.41	122.70	12	1
1	A	181	LEU	CA-C-N	5.13	131.20	122.37	5	1
1	A	181	LEU	C-N-CA	5.13	131.20	122.37	5	1
1	A	236	MET	O-C-N	-5.13	115.76	122.59	11	1
1	A	196	HIS	CE1-NE2-CD2	-5.13	103.87	109.00	8	1
1	A	107	PRO	CA-C-N	5.13	129.86	123.14	4	1
1	A	107	PRO	C-N-CA	5.13	129.86	123.14	4	1
1	A	109	TRP	CA-C-O	5.13	125.00	118.54	12	1
1	A	190	GLY	O-C-N	5.13	126.41	123.08	6	1
1	A	116	TYR	CB-CA-C	5.12	121.34	110.07	12	1
1	A	107	PRO	CB-CA-C	-5.12	106.74	111.40	13	2
1	A	145	THR	CA-CB-OG1	5.12	117.28	109.60	5	1
1	A	173	ALA	O-C-N	-5.12	115.78	122.59	5	1
1	A	199	GLU	N-CA-C	-5.12	107.21	113.50	2	1
1	A	117	ARG	NE-CZ-NH1	-5.11	116.39	121.50	13	1
1	A	157	ALA	CA-C-N	5.11	127.58	120.63	14	1
1	A	157	ALA	C-N-CA	5.11	127.58	120.63	14	1
1	A	162	VAL	CA-C-O	5.11	126.36	120.90	13	1
1	A	165	ARG	CA-CB-CG	5.09	124.29	114.10	2	1
1	A	262	TYR	CB-CG-CD1	-5.09	113.16	120.80	1	1
1	A	158	ASP	N-CA-C	-5.09	105.43	111.69	5	1
1	A	161	VAL	N-CA-C	-5.08	101.26	108.58	13	1
1	A	141	TRP	CE2-CD2-CE3	-5.08	113.72	118.80	13	1
1	A	110	ARG	CA-C-N	5.08	130.56	122.94	1	1
1	A	110	ARG	C-N-CA	5.08	130.56	122.94	1	1
1	A	247	THR	CA-CB-OG1	5.08	117.22	109.60	4	1
1	A	134	ILE	CB-CA-C	5.08	118.38	111.88	7	1
1	A	246	ASN	CA-C-O	-5.07	115.12	120.55	5	1
1	A	140	VAL	CA-CB-CG2	5.07	119.02	110.40	14	1
1	A	129	ASP	O-C-N	5.07	129.12	122.33	14	1
1	A	125	MET	CA-CB-CG	5.06	124.22	114.10	11	1
1	A	173	ALA	CB-CA-C	5.06	120.48	110.42	1	1
1	A	133	ALA	CA-C-O	-5.05	114.16	119.97	8	1
1	A	134	ILE	N-CA-C	5.05	115.66	110.36	7	1
1	A	103	MET	O-C-N	-5.05	116.23	121.28	11	1
1	A	184	ALA	N-CA-C	5.04	116.63	108.41	13	1
1	A	219	ALA	CA-C-O	-5.04	114.18	119.97	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	233	LYS	CB-CA-C	5.04	118.41	109.75	1	1
1	A	118	ILE	N-CA-C	-5.04	99.45	107.15	14	1
1	A	108	VAL	O-C-N	5.03	128.74	123.00	5	1
1	A	189	SER	N-CA-C	5.03	117.51	109.96	11	1
1	A	161	VAL	O-C-N	-5.03	117.20	122.83	11	1
1	A	123	PRO	N-CA-CB	5.03	108.85	103.52	12	1
1	A	172	HIS	CB-CA-C	5.02	118.69	110.96	7	1
1	A	206	HIS	CG-CD2-NE2	-5.02	102.18	107.20	11	1
1	A	175	ASP	CA-C-O	-5.01	113.21	118.77	4	1
1	A	165	ARG	N-CA-C	5.01	116.58	108.26	14	1
1	A	112	HIS	CA-C-O	5.01	125.84	119.78	7	1
1	A	107	PRO	N-CA-CB	5.00	107.62	103.17	1	1
1	A	115	THR	OG1-CB-CG2	-5.00	99.30	109.30	13	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	174	PHE	Peptide,Sidechain	11
1	A	121	TYR	Sidechain	6
1	A	262	TYR	Sidechain	5
1	A	171	PHE	Sidechain	4
1	A	132	TYR	Sidechain,Mainchain	4
1	A	242	TYR	Sidechain	3
1	A	113	TYR	Sidechain	3
1	A	117	ARG	Sidechain	2
1	A	249	ARG	Peptide,Sidechain	2
1	A	101	ARG	Sidechain	2
1	A	110	ARG	Sidechain	2
1	A	135	ARG	Sidechain	2
1	A	172	HIS	Sidechain	2
1	A	127	ARG	Sidechain,Mainchain	2
1	A	256	ARG	Sidechain	2
1	A	182	ALA	Peptide	1
1	A	240	TYR	Sidechain	1
1	A	191	ILE	Peptide	1
1	A	116	TYR	Sidechain	1
1	A	167	ALA	Peptide	1
1	A	165	ARG	Sidechain	1
1	A	175	ASP	Sidechain	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	213	PHE	Sidechain	1
1	A	237	PHE	Sidechain	1
1	A	248	PHE	Sidechain	1
1	A	149	PHE	Sidechain	1
1	A	219	ALA	Mainchain	1
1	A	196	HIS	Sidechain	1
1	A	185	PHE	Sidechain	1
1	A	138	PHE	Sidechain	1
1	A	251	SER	Mainchain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1271	1207	1207	2±1
4	A	5750	0	9000	132±12
All	All	98364	16898	142898	1850

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:423:PX4:H16	4:A:424:PX4:H24	1.02	1.23	7	1
4:A:347:PX4:H56	4:A:355:PX4:H25	0.99	1.33	11	1
4:A:321:PX4:H51	4:A:354:PX4:H34	0.93	1.41	10	1
4:A:306:PX4:H23	4:A:360:PX4:H44	0.91	1.42	1	1
4:A:408:PX4:H15	4:A:409:PX4:H2	0.90	1.44	10	2
4:A:361:PX4:H68	4:A:369:PX4:H36	0.84	1.49	12	1
4:A:404:PX4:H34	4:A:412:PX4:H37	0.84	1.49	11	1
4:A:347:PX4:H37	4:A:348:PX4:H64	0.84	1.49	8	1
4:A:313:PX4:H26	4:A:366:PX4:H22	0.84	1.47	13	1
4:A:308:PX4:H30	4:A:308:PX4:H67	0.83	1.50	3	1
4:A:422:PX4:H17	4:A:425:PX4:H56	0.83	1.48	13	1
4:A:415:PX4:H53	4:A:422:PX4:H28	0.83	1.50	4	1
4:A:350:PX4:H30	4:A:350:PX4:H59	0.83	1.49	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H15	4:A:398:PX4:H15	0.83	1.49	12	2
4:A:399:PX4:H62	4:A:407:PX4:H36	0.82	1.49	2	1
4:A:314:PX4:H39	4:A:362:PX4:H16	0.82	1.48	4	4
4:A:396:PX4:H57	4:A:398:PX4:H28	0.82	1.49	4	1
4:A:313:PX4:H47	4:A:328:PX4:H16	0.81	1.50	12	4
4:A:312:PX4:H51	4:A:359:PX4:H46	0.81	1.51	2	1
4:A:396:PX4:H19	4:A:397:PX4:H22	0.81	1.50	12	1
4:A:345:PX4:H22	4:A:353:PX4:H17	0.80	1.54	11	1
4:A:315:PX4:H52	4:A:323:PX4:H49	0.80	1.54	7	1
4:A:313:PX4:H27	4:A:359:PX4:H25	0.80	1.53	6	1
4:A:353:PX4:H50	4:A:354:PX4:H61	0.79	1.52	4	1
4:A:388:PX4:H49	4:A:397:PX4:H60	0.79	1.52	7	1
4:A:317:PX4:H55	4:A:342:PX4:H19	0.79	1.55	4	1
4:A:345:PX4:H20	4:A:345:PX4:H54	0.78	1.54	10	1
4:A:368:PX4:H37	4:A:418:PX4:H29	0.78	1.56	2	1
4:A:375:PX4:H49	4:A:429:PX4:H19	0.77	1.54	8	1
4:A:338:PX4:H35	4:A:343:PX4:H58	0.77	1.55	11	1
4:A:338:PX4:H49	4:A:355:PX4:H16	0.77	1.54	10	1
4:A:323:PX4:H60	4:A:368:PX4:H42	0.76	1.57	11	1
4:A:325:PX4:H22	4:A:341:PX4:H56	0.76	1.55	4	1
4:A:405:PX4:H25	4:A:423:PX4:H70	0.76	1.58	12	1
4:A:310:PX4:H50	4:A:311:PX4:H46	0.76	1.57	2	1
4:A:387:PX4:H65	4:A:402:PX4:H25	0.76	1.58	3	1
4:A:406:PX4:H37	4:A:422:PX4:H30	0.76	1.58	3	1
4:A:383:PX4:H35	4:A:390:PX4:H39	0.76	1.58	6	1
4:A:400:PX4:H30	4:A:417:PX4:H28	0.75	1.56	8	1
4:A:307:PX4:H48	4:A:314:PX4:H22	0.75	1.57	2	1
4:A:381:PX4:H51	4:A:397:PX4:H47	0.75	1.57	8	1
4:A:340:PX4:H60	4:A:341:PX4:H24	0.75	1.57	12	1
4:A:345:PX4:H61	4:A:345:PX4:H28	0.75	1.55	7	1
4:A:321:PX4:H62	4:A:425:PX4:H41	0.75	1.59	14	1
4:A:389:PX4:H37	4:A:397:PX4:H41	0.75	1.59	14	1
4:A:378:PX4:H49	4:A:410:PX4:H17	0.75	1.59	12	1
4:A:323:PX4:H42	4:A:333:PX4:H68	0.74	1.58	13	1
4:A:374:PX4:H24	4:A:427:PX4:H19	0.74	1.58	6	1
4:A:310:PX4:H57	4:A:364:PX4:H27	0.74	1.57	1	1
4:A:388:PX4:H24	4:A:396:PX4:H47	0.74	1.58	14	1
4:A:385:PX4:H45	4:A:394:PX4:H65	0.74	1.59	9	1
4:A:307:PX4:H46	4:A:314:PX4:H19	0.74	1.58	5	1
4:A:338:PX4:H16	4:A:345:PX4:H52	0.74	1.59	10	1
4:A:373:PX4:H32	4:A:381:PX4:H47	0.74	1.58	14	1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H52	4:A:324:PX4:H54	0.70	1.64	11	1
4:A:317:PX4:H17	4:A:324:PX4:H53	0.70	1.64	2	1
4:A:338:PX4:O8	4:A:348:PX4:H4	0.69	1.87	9	2
4:A:311:PX4:H58	4:A:363:PX4:H44	0.69	1.61	14	1
4:A:372:PX4:H51	4:A:384:PX4:H51	0.69	1.63	12	1
4:A:353:PX4:H72	4:A:354:PX4:H29	0.69	1.62	7	1
4:A:410:PX4:H49	4:A:426:PX4:H19	0.69	1.63	8	1
4:A:307:PX4:H4	4:A:361:PX4:H17	0.69	1.64	7	2
4:A:368:PX4:H34	4:A:429:PX4:H67	0.69	1.65	5	1
4:A:326:PX4:H25	4:A:341:PX4:H62	0.69	1.64	6	1
4:A:350:PX4:H45	4:A:363:PX4:H56	0.69	1.62	1	1
4:A:398:PX4:H30	4:A:407:PX4:H54	0.69	1.63	10	1
4:A:418:PX4:H26	4:A:425:PX4:H24	0.69	1.65	4	1
4:A:360:PX4:H50	4:A:366:PX4:H18	0.69	1.65	8	1
4:A:353:PX4:H70	4:A:413:PX4:H43	0.69	1.63	4	1
4:A:322:PX4:H28	4:A:323:PX4:H25	0.69	1.65	14	1
4:A:350:PX4:H72	4:A:365:PX4:H35	0.68	1.65	1	1
4:A:343:PX4:H64	4:A:347:PX4:H27	0.68	1.62	2	1
4:A:391:PX4:H24	4:A:393:PX4:H58	0.68	1.65	13	1
4:A:392:PX4:H52	4:A:393:PX4:H54	0.68	1.64	4	1
4:A:367:PX4:H55	4:A:430:PX4:H22	0.68	1.63	6	2
4:A:377:PX4:H13	4:A:377:PX4:H15	0.68	1.65	8	1
4:A:335:PX4:H16	4:A:344:PX4:H20	0.68	1.64	14	1
4:A:340:PX4:H30	4:A:347:PX4:H72	0.68	1.64	5	1
4:A:360:PX4:H68	4:A:419:PX4:H67	0.68	1.65	2	1
4:A:323:PX4:H14	4:A:333:PX4:H47	0.68	1.64	10	1
4:A:405:PX4:H41	4:A:414:PX4:H42	0.68	1.64	14	1
4:A:332:PX4:H28	4:A:340:PX4:H31	0.68	1.66	2	1
4:A:314:PX4:H38	4:A:355:PX4:H8	0.68	1.64	8	1
4:A:385:PX4:H23	4:A:393:PX4:H22	0.68	1.64	3	1
4:A:346:PX4:H40	4:A:355:PX4:H68	0.68	1.64	6	1
4:A:345:PX4:H34	4:A:353:PX4:H46	0.68	1.64	14	1
4:A:370:PX4:H42	4:A:403:PX4:H33	0.67	1.64	5	1
4:A:316:PX4:H47	4:A:319:PX4:H46	0.67	1.67	6	1
4:A:313:PX4:H26	4:A:366:PX4:H21	0.67	1.64	7	1
4:A:308:PX4:H47	4:A:310:PX4:H60	0.67	1.65	14	1
4:A:315:PX4:H52	4:A:316:PX4:H23	0.67	1.65	14	1
4:A:306:PX4:H57	4:A:423:PX4:H42	0.67	1.65	4	1
4:A:405:PX4:H17	4:A:414:PX4:H19	0.67	1.67	9	1
4:A:409:PX4:H55	4:A:415:PX4:H27	0.66	1.67	1	1
4:A:353:PX4:H69	4:A:362:PX4:H72	0.66	1.65	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:416:PX4:H48	4:A:422:PX4:H59	0.66	1.67	14	1
4:A:340:PX4:H43	4:A:407:PX4:H66	0.66	1.67	1	1
4:A:388:PX4:H16	4:A:395:PX4:H15	0.66	1.66	5	1
4:A:314:PX4:H58	4:A:364:PX4:H54	0.66	1.66	8	1
4:A:387:PX4:H15	4:A:411:PX4:H49	0.66	1.66	8	1
4:A:314:PX4:H64	4:A:422:PX4:H68	0.66	1.65	2	1
4:A:347:PX4:H16	4:A:348:PX4:H46	0.66	1.67	4	1
4:A:386:PX4:H17	4:A:387:PX4:H24	0.66	1.68	10	1
4:A:403:PX4:H56	4:A:404:PX4:H39	0.66	1.67	12	1
4:A:340:PX4:H58	4:A:341:PX4:H16	0.66	1.68	14	1
4:A:339:PX4:H30	4:A:355:PX4:H40	0.66	1.67	10	1
4:A:306:PX4:H16	4:A:322:PX4:H9	0.66	1.68	13	1
4:A:356:PX4:H32	4:A:362:PX4:H24	0.66	1.66	2	2
4:A:336:PX4:H27	4:A:344:PX4:H62	0.66	1.67	6	1
4:A:331:PX4:H21	4:A:340:PX4:H17	0.66	1.66	5	1
4:A:385:PX4:H71	4:A:399:PX4:H61	0.66	1.67	14	1
4:A:357:PX4:H58	4:A:357:PX4:H31	0.66	1.66	8	1
4:A:336:PX4:H65	4:A:344:PX4:H71	0.66	1.68	9	1
4:A:335:PX4:H42	4:A:337:PX4:H38	0.66	1.65	10	1
4:A:400:PX4:H17	4:A:401:PX4:H3	0.66	1.65	10	1
4:A:408:PX4:H50	4:A:409:PX4:H17	0.66	1.66	10	1
4:A:349:PX4:H36	4:A:350:PX4:H40	0.65	1.68	2	1
4:A:391:PX4:H19	4:A:414:PX4:H17	0.65	1.67	8	1
4:A:389:PX4:H42	4:A:389:PX4:H71	0.65	1.66	1	1
4:A:413:PX4:H41	4:A:421:PX4:H67	0.65	1.69	3	1
4:A:420:PX4:H51	4:A:427:PX4:H49	0.65	1.68	7	1
4:A:308:PX4:H66	4:A:410:PX4:H68	0.65	1.68	10	1
4:A:373:PX4:H21	4:A:381:PX4:H32	0.65	1.68	11	1
4:A:332:PX4:H37	4:A:340:PX4:H35	0.65	1.68	7	1
4:A:359:PX4:H37	4:A:412:PX4:H64	0.65	1.67	8	1
4:A:358:PX4:H71	4:A:358:PX4:H39	0.65	1.69	11	1
4:A:393:PX4:H18	4:A:394:PX4:H18	0.65	1.67	9	1
4:A:403:PX4:H16	4:A:404:PX4:H24	0.65	1.69	12	1
4:A:373:PX4:H46	4:A:382:PX4:H46	0.65	1.67	5	1
4:A:306:PX4:H54	4:A:321:PX4:H48	0.65	1.68	7	2
4:A:391:PX4:H53	4:A:408:PX4:H20	0.65	1.68	9	1
4:A:419:PX4:H46	4:A:427:PX4:H50	0.65	1.68	1	1
4:A:322:PX4:H62	4:A:361:PX4:H71	0.65	1.69	3	1
4:A:405:PX4:H21	4:A:415:PX4:H50	0.65	1.68	4	1
4:A:368:PX4:H25	4:A:429:PX4:H66	0.65	1.69	9	1
4:A:312:PX4:H38	4:A:366:PX4:H48	0.65	1.69	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PX4:H37	4:A:423:PX4:H28	0.65	1.69	4	1
4:A:335:PX4:H16	4:A:344:PX4:H19	0.65	1.67	10	2
4:A:390:PX4:H44	4:A:407:PX4:H17	0.65	1.67	14	1
4:A:402:PX4:H52	4:A:403:PX4:H27	0.65	1.69	1	1
4:A:400:PX4:H20	4:A:401:PX4:H17	0.65	1.68	6	1
4:A:335:PX4:H34	4:A:343:PX4:H65	0.65	1.69	11	1
4:A:391:PX4:H47	4:A:394:PX4:H28	0.65	1.67	2	1
4:A:406:PX4:H46	4:A:421:PX4:H50	0.65	1.68	7	1
4:A:348:PX4:H26	4:A:355:PX4:H25	0.65	1.69	12	1
4:A:400:PX4:H28	4:A:401:PX4:H46	0.64	1.67	2	1
4:A:308:PX4:H19	4:A:364:PX4:H22	0.64	1.68	9	1
4:A:391:PX4:H50	4:A:393:PX4:H60	0.64	1.69	10	1
4:A:397:PX4:H53	4:A:402:PX4:H21	0.64	1.68	6	1
4:A:376:PX4:H20	4:A:377:PX4:H16	0.64	1.67	14	2
4:A:404:PX4:O1	4:A:419:PX4:H13	0.64	1.93	2	1
4:A:317:PX4:H40	4:A:342:PX4:H38	0.64	1.68	1	1
4:A:339:PX4:H23	4:A:347:PX4:H29	0.64	1.69	1	1
4:A:379:PX4:H19	4:A:384:PX4:H20	0.64	1.70	4	1
4:A:359:PX4:H36	4:A:366:PX4:H40	0.64	1.69	6	1
4:A:353:PX4:H46	4:A:354:PX4:H64	0.64	1.68	7	1
4:A:376:PX4:H35	4:A:383:PX4:H60	0.64	1.67	7	1
4:A:312:PX4:H55	4:A:359:PX4:H56	0.64	1.70	9	1
4:A:316:PX4:H56	4:A:316:PX4:H25	0.64	1.69	9	1
4:A:350:PX4:H51	4:A:363:PX4:H59	0.64	1.69	1	1
4:A:397:PX4:H28	4:A:398:PX4:H58	0.64	1.68	1	1
4:A:405:PX4:H4	4:A:414:PX4:H22	0.64	1.67	1	1
4:A:313:PX4:H53	4:A:359:PX4:H23	0.64	1.68	10	1
4:A:371:PX4:H31	4:A:376:PX4:H23	0.64	1.70	14	1
4:A:378:PX4:H63	4:A:418:PX4:H66	0.64	1.69	4	1
4:A:403:PX4:H24	4:A:404:PX4:H53	0.64	1.68	5	1
4:A:357:PX4:H45	4:A:365:PX4:H72	0.64	1.70	10	1
4:A:368:PX4:H4	4:A:418:PX4:H2	0.63	1.70	1	1
4:A:369:PX4:H25	4:A:429:PX4:H64	0.63	1.68	2	2
4:A:317:PX4:H55	4:A:342:PX4:H53	0.63	1.68	2	1
4:A:370:PX4:H46	4:A:411:PX4:H53	0.63	1.70	13	1
4:A:417:PX4:H50	4:A:426:PX4:H47	0.63	1.70	8	1
4:A:320:PX4:H36	4:A:418:PX4:H66	0.63	1.70	9	1
4:A:332:PX4:H41	4:A:407:PX4:H66	0.63	1.68	6	1
4:A:386:PX4:H17	4:A:387:PX4:H21	0.63	1.69	9	1
4:A:405:PX4:H3	4:A:414:PX4:O6	0.63	1.94	13	1
4:A:416:PX4:H23	4:A:422:PX4:H52	0.63	1.70	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:428:PX4:H19	4:A:429:PX4:H37	0.63	1.69	7	2
4:A:355:PX4:H46	4:A:355:PX4:H10	0.63	1.70	8	1
4:A:375:PX4:H67	4:A:375:PX4:H36	0.63	1.71	14	1
4:A:312:PX4:H21	4:A:366:PX4:H17	0.63	1.70	2	2
4:A:370:PX4:H46	4:A:411:PX4:H49	0.63	1.69	14	1
4:A:386:PX4:H64	4:A:387:PX4:H34	0.63	1.69	2	1
4:A:367:PX4:H45	4:A:429:PX4:H31	0.63	1.70	3	1
4:A:376:PX4:H21	4:A:377:PX4:H20	0.63	1.71	5	1
4:A:406:PX4:H35	4:A:425:PX4:H68	0.63	1.70	10	1
4:A:314:PX4:H34	4:A:362:PX4:H14	0.63	1.70	9	1
4:A:314:PX4:H57	4:A:361:PX4:H27	0.63	1.70	9	1
4:A:355:PX4:H10	4:A:355:PX4:H49	0.63	1.68	12	1
4:A:355:PX4:H68	4:A:415:PX4:H64	0.63	1.71	13	1
4:A:398:PX4:H30	4:A:407:PX4:H53	0.63	1.71	14	1
4:A:407:PX4:H22	4:A:414:PX4:H50	0.63	1.69	12	1
4:A:332:PX4:H72	4:A:391:PX4:H25	0.63	1.70	14	1
4:A:378:PX4:H15	4:A:410:PX4:H47	0.62	1.69	3	1
4:A:406:PX4:H34	4:A:424:PX4:H35	0.62	1.71	5	1
4:A:378:PX4:H46	4:A:410:PX4:H17	0.62	1.70	10	1
4:A:329:PX4:H12	4:A:333:PX4:H41	0.62	1.71	12	1
4:A:307:PX4:H65	4:A:349:PX4:H22	0.62	1.71	14	1
4:A:393:PX4:H21	4:A:394:PX4:H29	0.62	1.69	11	1
4:A:309:PX4:H56	4:A:319:PX4:H48	0.62	1.70	13	1
4:A:313:PX4:H70	4:A:375:PX4:H69	0.62	1.71	6	1
4:A:338:PX4:H16	4:A:345:PX4:H49	0.62	1.71	7	1
4:A:308:PX4:H22	4:A:310:PX4:H65	0.62	1.70	3	1
4:A:313:PX4:H60	4:A:327:PX4:H32	0.62	1.70	9	1
4:A:419:PX4:H36	4:A:430:PX4:H27	0.62	1.71	1	1
4:A:375:PX4:H54	4:A:389:PX4:H60	0.61	1.70	3	1
4:A:334:PX4:H54	4:A:356:PX4:H8	0.61	1.69	9	1
4:A:339:PX4:H26	4:A:347:PX4:H54	0.61	1.71	12	1
4:A:310:PX4:H53	4:A:364:PX4:H31	0.61	1.70	13	1
4:A:345:PX4:H59	4:A:345:PX4:H22	0.61	1.72	3	1
4:A:353:PX4:H19	4:A:357:PX4:H46	0.61	1.72	5	1
4:A:315:PX4:H43	4:A:369:PX4:H28	0.61	1.70	7	1
4:A:347:PX4:H54	4:A:355:PX4:H22	0.61	1.71	10	1
4:A:326:PX4:H42	4:A:332:PX4:H51	0.61	1.70	4	1
4:A:355:PX4:H66	4:A:362:PX4:H64	0.61	1.73	4	1
4:A:375:PX4:H18	4:A:429:PX4:H24	0.61	1.71	7	1
4:A:317:PX4:H26	4:A:342:PX4:H19	0.61	1.73	8	1
4:A:373:PX4:H39	4:A:402:PX4:H38	0.61	1.72	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:392:PX4:H7	4:A:392:PX4:H15	0.61	1.71	13	1
4:A:387:PX4:H47	4:A:411:PX4:H48	0.61	1.71	14	1
4:A:397:PX4:H31	4:A:398:PX4:H63	0.61	1.73	2	1
4:A:338:PX4:H25	4:A:347:PX4:H23	0.61	1.72	7	1
4:A:335:PX4:H31	4:A:337:PX4:H33	0.61	1.71	8	1
4:A:410:PX4:H59	4:A:417:PX4:H54	0.61	1.72	12	1
4:A:423:PX4:H16	4:A:424:PX4:H19	0.61	1.70	13	1
4:A:350:PX4:H37	4:A:408:PX4:H39	0.61	1.73	4	1
4:A:331:PX4:H14	4:A:347:PX4:H50	0.61	1.71	10	2
1:A:191:ILE:HD13	4:A:314:PX4:H21	0.61	1.72	14	3
4:A:315:PX4:H43	4:A:424:PX4:H71	0.61	1.72	10	1
4:A:380:PX4:H39	4:A:386:PX4:H38	0.61	1.73	12	1
4:A:325:PX4:H61	4:A:341:PX4:H60	0.61	1.72	10	1
4:A:396:PX4:H37	4:A:397:PX4:H42	0.61	1.72	12	1
4:A:395:PX4:H52	4:A:421:PX4:H50	0.61	1.73	2	1
4:A:306:PX4:H58	4:A:321:PX4:H21	0.61	1.72	10	1
4:A:337:PX4:H58	4:A:348:PX4:H32	0.61	1.73	12	1
4:A:330:PX4:H64	4:A:338:PX4:H39	0.61	1.72	1	1
4:A:407:PX4:H32	4:A:414:PX4:H55	0.61	1.72	4	1
4:A:319:PX4:H29	4:A:320:PX4:H28	0.61	1.72	6	1
4:A:360:PX4:H57	4:A:366:PX4:H56	0.61	1.73	12	1
4:A:368:PX4:H17	4:A:390:PX4:H50	0.61	1.73	1	1
4:A:407:PX4:H34	4:A:414:PX4:H65	0.61	1.73	1	1
4:A:349:PX4:H36	4:A:350:PX4:H37	0.61	1.71	11	1
4:A:421:PX4:H47	4:A:423:PX4:H66	0.61	1.73	11	1
4:A:331:PX4:H22	4:A:340:PX4:H17	0.61	1.73	13	1
4:A:355:PX4:H43	4:A:398:PX4:H70	0.60	1.71	3	1
4:A:316:PX4:H37	4:A:316:PX4:H72	0.60	1.72	6	1
4:A:407:PX4:H16	4:A:414:PX4:H49	0.60	1.73	10	3
4:A:334:PX4:H48	4:A:349:PX4:H20	0.60	1.71	11	1
4:A:335:PX4:H34	4:A:337:PX4:H34	0.60	1.74	2	1
4:A:345:PX4:H19	4:A:353:PX4:H47	0.60	1.71	12	1
4:A:387:PX4:H47	4:A:411:PX4:H52	0.60	1.73	13	1
4:A:331:PX4:H40	4:A:331:PX4:H69	0.60	1.73	1	1
4:A:357:PX4:H24	4:A:358:PX4:H22	0.60	1.73	6	1
4:A:387:PX4:H53	4:A:411:PX4:H50	0.60	1.72	9	1
4:A:338:PX4:H28	4:A:348:PX4:H57	0.60	1.72	11	1
4:A:428:PX4:H62	4:A:429:PX4:H50	0.60	1.73	1	1
4:A:314:PX4:H36	4:A:362:PX4:H16	0.60	1.72	8	1
4:A:360:PX4:H70	4:A:404:PX4:H42	0.60	1.74	14	1
4:A:307:PX4:H19	4:A:361:PX4:H15	0.60	1.73	14	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:376:PX4:H52	4:A:377:PX4:H19	0.60	1.72	8	1
4:A:331:PX4:H54	4:A:339:PX4:H35	0.60	1.72	13	1
4:A:392:PX4:H20	4:A:399:PX4:H48	0.60	1.74	1	1
4:A:368:PX4:H67	4:A:424:PX4:H17	0.60	1.72	8	1
4:A:327:PX4:H37	4:A:328:PX4:H53	0.60	1.72	12	1
4:A:335:PX4:H16	4:A:344:PX4:H22	0.60	1.72	7	1
4:A:410:PX4:H46	4:A:426:PX4:H15	0.60	1.72	13	2
4:A:332:PX4:H55	4:A:334:PX4:H36	0.60	1.74	11	1
4:A:350:PX4:H34	4:A:394:PX4:H43	0.59	1.73	2	1
1:A:191:ILE:HD12	4:A:314:PX4:H21	0.59	1.73	11	1
4:A:396:PX4:H20	4:A:396:PX4:H55	0.59	1.73	2	1
4:A:307:PX4:H43	4:A:410:PX4:H29	0.59	1.74	5	1
4:A:406:PX4:H21	4:A:423:PX4:H65	0.59	1.74	7	1
4:A:370:PX4:H70	4:A:402:PX4:H34	0.59	1.74	9	1
4:A:369:PX4:H61	4:A:425:PX4:H47	0.59	1.73	1	1
4:A:313:PX4:H63	4:A:328:PX4:H66	0.59	1.73	2	1
4:A:391:PX4:H25	4:A:392:PX4:H62	0.59	1.73	4	1
4:A:396:PX4:H53	4:A:398:PX4:H24	0.59	1.75	4	1
4:A:400:PX4:H11	4:A:401:PX4:O6	0.59	1.97	10	1
4:A:389:PX4:H53	4:A:398:PX4:H55	0.59	1.73	11	1
4:A:330:PX4:C9	4:A:344:PX4:H49	0.59	2.28	2	1
4:A:308:PX4:H23	4:A:364:PX4:H26	0.59	1.73	6	2
4:A:317:PX4:H53	4:A:342:PX4:H17	0.59	1.75	10	1
4:A:368:PX4:H62	4:A:424:PX4:H23	0.59	1.73	13	1
4:A:408:PX4:H40	4:A:422:PX4:H40	0.59	1.75	14	1
4:A:338:PX4:H53	4:A:346:PX4:H53	0.59	1.73	11	1
4:A:374:PX4:H30	4:A:427:PX4:H26	0.59	1.73	11	1
4:A:322:PX4:H64	4:A:361:PX4:H64	0.59	1.74	4	1
4:A:428:PX4:H56	4:A:429:PX4:H46	0.59	1.74	6	1
4:A:428:PX4:H23	4:A:429:PX4:H42	0.59	1.73	8	1
4:A:330:PX4:H52	4:A:338:PX4:H36	0.59	1.73	11	1
4:A:391:PX4:H20	4:A:392:PX4:H61	0.59	1.75	11	1
4:A:338:PX4:H60	4:A:355:PX4:H63	0.59	1.75	9	1
4:A:334:PX4:H69	4:A:349:PX4:H66	0.58	1.73	5	1
4:A:396:PX4:H69	4:A:398:PX4:H43	0.58	1.75	8	1
4:A:306:PX4:O8	4:A:322:PX4:H13	0.58	1.98	14	1
4:A:331:PX4:H10	4:A:347:PX4:H49	0.58	1.75	14	1
4:A:329:PX4:H42	4:A:336:PX4:H62	0.58	1.74	2	1
4:A:330:PX4:H50	4:A:337:PX4:H48	0.58	1.74	7	1
4:A:342:PX4:H16	4:A:351:PX4:H20	0.58	1.75	8	1
4:A:400:PX4:H47	4:A:409:PX4:H20	0.58	1.74	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:395:PX4:H33	4:A:405:PX4:H34	0.58	1.74	10	1
4:A:381:PX4:H50	4:A:397:PX4:H47	0.58	1.74	4	2
4:A:356:PX4:H12	4:A:356:PX4:H16	0.58	1.75	8	1
4:A:331:PX4:H65	4:A:339:PX4:H69	0.58	1.74	11	1
4:A:403:PX4:H29	4:A:404:PX4:H35	0.58	1.76	13	1
4:A:400:PX4:H22	4:A:408:PX4:H67	0.58	1.75	14	1
4:A:405:PX4:H4	4:A:414:PX4:H23	0.58	1.74	2	1
4:A:314:PX4:H45	4:A:346:PX4:H38	0.58	1.76	7	1
4:A:315:PX4:H35	4:A:322:PX4:H49	0.58	1.74	10	1
4:A:348:PX4:H27	4:A:348:PX4:H60	0.58	1.74	11	1
4:A:393:PX4:H23	4:A:394:PX4:H29	0.58	1.74	12	1
4:A:339:PX4:H21	4:A:347:PX4:H50	0.58	1.74	13	1
4:A:410:PX4:H48	4:A:426:PX4:H22	0.58	1.74	13	1
4:A:324:PX4:H61	4:A:341:PX4:H24	0.58	1.74	2	1
4:A:370:PX4:H35	4:A:427:PX4:H71	0.58	1.74	2	1
4:A:330:PX4:H41	4:A:336:PX4:H35	0.58	1.75	6	1
4:A:366:PX4:H27	4:A:427:PX4:H68	0.58	1.74	8	1
4:A:349:PX4:H15	4:A:356:PX4:H28	0.58	1.75	12	2
4:A:366:PX4:H38	4:A:412:PX4:H41	0.58	1.76	1	1
4:A:392:PX4:H48	4:A:393:PX4:H57	0.58	1.73	1	1
4:A:343:PX4:H9	4:A:344:PX4:H16	0.58	1.75	3	1
4:A:318:PX4:H47	4:A:327:PX4:H15	0.58	1.74	10	1
4:A:318:PX4:H18	4:A:327:PX4:H47	0.58	1.76	3	1
4:A:391:PX4:H16	4:A:393:PX4:H65	0.58	1.76	3	1
4:A:341:PX4:H40	4:A:385:PX4:H64	0.58	1.75	6	1
4:A:346:PX4:H43	4:A:356:PX4:H31	0.58	1.74	7	1
4:A:373:PX4:H29	4:A:384:PX4:H59	0.58	1.73	13	1
4:A:326:PX4:H50	4:A:351:PX4:H49	0.58	1.75	1	1
4:A:332:PX4:H10	4:A:356:PX4:O1	0.58	1.98	2	1
4:A:338:PX4:H46	4:A:355:PX4:H16	0.58	1.75	5	4
4:A:400:PX4:H22	4:A:408:PX4:H63	0.58	1.74	1	1
4:A:421:PX4:H4	4:A:423:PX4:H51	0.58	1.76	2	1
4:A:420:PX4:H47	4:A:427:PX4:H16	0.58	1.75	3	1
4:A:389:PX4:H25	4:A:398:PX4:H58	0.58	1.75	5	1
4:A:316:PX4:C24	4:A:319:PX4:H46	0.58	2.29	6	1
4:A:332:PX4:H70	4:A:425:PX4:H62	0.58	1.74	7	1
4:A:330:PX4:H63	4:A:337:PX4:H61	0.58	1.74	8	1
4:A:383:PX4:H35	4:A:407:PX4:H26	0.58	1.74	3	1
4:A:378:PX4:H69	4:A:410:PX4:H42	0.58	1.74	4	1
4:A:413:PX4:H64	4:A:421:PX4:H62	0.58	1.76	4	1
4:A:326:PX4:H60	4:A:350:PX4:H71	0.58	1.74	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:310:PX4:H43	4:A:351:PX4:H66	0.58	1.74	12	1
4:A:310:PX4:H53	4:A:364:PX4:H25	0.58	1.76	12	1
4:A:404:PX4:H50	4:A:413:PX4:H26	0.58	1.75	12	1
4:A:383:PX4:H17	4:A:392:PX4:H26	0.58	1.75	14	1
4:A:390:PX4:H47	4:A:399:PX4:H24	0.58	1.76	14	1
4:A:310:PX4:H35	4:A:417:PX4:H31	0.57	1.75	2	1
4:A:372:PX4:H72	4:A:384:PX4:H38	0.57	1.75	11	1
4:A:378:PX4:H48	4:A:417:PX4:H72	0.57	1.74	7	1
4:A:380:PX4:H51	4:A:402:PX4:H24	0.57	1.74	7	1
4:A:383:PX4:H40	4:A:390:PX4:H41	0.57	1.76	8	1
4:A:332:PX4:H32	4:A:339:PX4:H44	0.57	1.76	13	1
4:A:310:PX4:H61	4:A:426:PX4:H44	0.57	1.76	1	1
4:A:338:PX4:H14	4:A:348:PX4:H4	0.57	1.75	2	1
4:A:345:PX4:H20	4:A:353:PX4:H52	0.57	1.75	3	1
4:A:368:PX4:H51	4:A:424:PX4:C30	0.57	2.29	3	1
4:A:330:PX4:H7	4:A:344:PX4:H49	0.57	1.75	5	1
4:A:326:PX4:H49	4:A:363:PX4:H55	0.57	1.75	7	1
4:A:389:PX4:H60	4:A:407:PX4:H55	0.57	1.75	12	1
4:A:355:PX4:H18	4:A:356:PX4:H15	0.57	1.75	13	1
4:A:331:PX4:H27	4:A:340:PX4:H53	0.57	1.76	14	1
4:A:393:PX4:H29	4:A:394:PX4:H56	0.57	1.75	5	1
4:A:368:PX4:H46	4:A:369:PX4:H22	0.57	1.74	8	1
4:A:331:PX4:H4	4:A:347:PX4:H50	0.57	1.74	9	1
4:A:316:PX4:H20	4:A:316:PX4:H49	0.57	1.74	10	1
4:A:395:PX4:H21	4:A:406:PX4:H51	0.57	1.77	10	1
4:A:423:PX4:H67	4:A:424:PX4:H37	0.57	1.75	14	1
4:A:370:PX4:H23	4:A:403:PX4:H17	0.57	1.75	10	1
4:A:378:PX4:H23	4:A:417:PX4:H64	0.57	1.75	10	1
4:A:404:PX4:H8	4:A:430:PX4:O6	0.57	2.00	6	2
4:A:337:PX4:H58	4:A:357:PX4:H56	0.57	1.75	8	1
4:A:396:PX4:H61	4:A:396:PX4:H29	0.57	1.77	11	1
4:A:412:PX4:H56	4:A:419:PX4:H35	0.57	1.76	13	1
4:A:376:PX4:H30	4:A:383:PX4:H64	0.57	1.76	2	1
4:A:403:PX4:H2	4:A:411:PX4:O3	0.57	1.99	2	1
4:A:423:PX4:H16	4:A:424:PX4:H26	0.57	1.74	2	1
4:A:307:PX4:H37	4:A:410:PX4:H44	0.57	1.75	12	1
4:A:378:PX4:H48	4:A:417:PX4:H67	0.57	1.77	13	1
4:A:317:PX4:H58	4:A:342:PX4:H24	0.57	1.76	3	1
4:A:335:PX4:H51	4:A:344:PX4:H24	0.57	1.77	6	1
4:A:332:PX4:H5	4:A:347:PX4:H61	0.57	1.75	10	1
1:A:165:ARG:NH1	4:A:362:PX4:H7	0.57	2.14	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:346:PX4:H35	4:A:354:PX4:H34	0.57	1.75	9	1
4:A:330:PX4:H22	4:A:344:PX4:H48	0.57	1.77	4	1
4:A:337:PX4:H61	4:A:345:PX4:H36	0.57	1.76	9	1
4:A:316:PX4:H45	4:A:418:PX4:H57	0.57	1.77	14	1
4:A:378:PX4:H51	4:A:418:PX4:H49	0.56	1.77	2	1
4:A:307:PX4:H67	4:A:314:PX4:H67	0.56	1.77	4	1
4:A:391:PX4:H22	4:A:414:PX4:H17	0.56	1.77	12	3
4:A:320:PX4:H34	4:A:378:PX4:H42	0.56	1.75	8	1
4:A:346:PX4:O6	4:A:346:PX4:H16	0.56	1.99	1	1
4:A:367:PX4:H17	4:A:430:PX4:H49	0.56	1.76	1	1
4:A:371:PX4:H8	4:A:377:PX4:O6	0.56	1.99	1	1
4:A:329:PX4:O6	4:A:336:PX4:H3	0.56	2.00	2	1
4:A:349:PX4:H70	4:A:422:PX4:H32	0.56	1.77	4	1
4:A:400:PX4:H1	4:A:409:PX4:H18	0.56	1.75	6	1
4:A:331:PX4:O1	4:A:332:PX4:H3	0.56	2.00	8	1
4:A:338:PX4:H57	4:A:346:PX4:H57	0.56	1.77	11	1
4:A:345:PX4:H65	4:A:348:PX4:H19	0.56	1.76	13	1
4:A:361:PX4:H64	4:A:425:PX4:H24	0.56	1.75	13	1
4:A:325:PX4:H47	4:A:341:PX4:H49	0.56	1.77	4	1
4:A:311:PX4:H22	4:A:311:PX4:H52	0.56	1.77	6	1
4:A:316:PX4:H68	4:A:368:PX4:H38	0.56	1.77	6	1
4:A:367:PX4:H23	4:A:368:PX4:H66	0.56	1.76	6	1
4:A:357:PX4:H29	4:A:357:PX4:H53	0.56	1.75	7	1
4:A:371:PX4:H52	4:A:377:PX4:H54	0.56	1.77	8	1
4:A:380:PX4:H21	4:A:381:PX4:H53	0.56	1.76	11	1
4:A:395:PX4:H50	4:A:402:PX4:H62	0.56	1.77	11	1
4:A:423:PX4:H49	4:A:424:PX4:H21	0.56	1.76	13	1
1:A:171:PHE:CZ	4:A:307:PX4:H17	0.56	2.36	1	2
4:A:400:PX4:H33	4:A:401:PX4:H60	0.56	1.77	4	1
4:A:376:PX4:H64	4:A:393:PX4:H50	0.56	1.77	2	1
4:A:403:PX4:H55	4:A:419:PX4:H59	0.56	1.77	4	1
4:A:368:PX4:H50	4:A:369:PX4:H25	0.56	1.76	9	1
4:A:393:PX4:H68	4:A:399:PX4:H68	0.56	1.78	14	1
4:A:312:PX4:H30	4:A:360:PX4:H53	0.56	1.76	1	1
4:A:321:PX4:H48	4:A:354:PX4:H23	0.56	1.77	3	1
4:A:329:PX4:H58	4:A:333:PX4:H43	0.56	1.78	3	1
4:A:306:PX4:H27	4:A:328:PX4:H41	0.56	1.78	8	1
4:A:306:PX4:H19	4:A:321:PX4:H23	0.56	1.76	12	2
4:A:370:PX4:H28	4:A:403:PX4:H17	0.56	1.77	12	1
4:A:396:PX4:H11	4:A:405:PX4:O8	0.56	2.00	13	1
4:A:345:PX4:H71	4:A:357:PX4:H57	0.56	1.78	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:C35	4:A:364:PX4:H29	0.56	2.30	6	1
4:A:339:PX4:H70	4:A:355:PX4:H43	0.56	1.78	8	1
4:A:370:PX4:H37	4:A:404:PX4:H29	0.56	1.76	11	1
4:A:354:PX4:H44	4:A:423:PX4:H36	0.56	1.78	14	1
4:A:332:PX4:H12	4:A:332:PX4:H16	0.56	1.77	1	1
4:A:371:PX4:H19	4:A:377:PX4:H17	0.56	1.77	1	1
4:A:380:PX4:H56	4:A:387:PX4:H64	0.56	1.78	2	1
4:A:316:PX4:H25	4:A:320:PX4:H30	0.56	1.78	3	1
4:A:314:PX4:H69	4:A:364:PX4:H29	0.56	1.77	6	1
4:A:342:PX4:H38	4:A:394:PX4:H70	0.56	1.78	9	1
4:A:325:PX4:H20	4:A:326:PX4:H22	0.56	1.75	10	1
4:A:355:PX4:H68	4:A:422:PX4:H37	0.56	1.77	1	1
4:A:330:PX4:H53	4:A:338:PX4:H21	0.56	1.76	4	1
4:A:406:PX4:H48	4:A:421:PX4:H53	0.56	1.78	11	1
4:A:412:PX4:H29	4:A:419:PX4:H49	0.56	1.78	12	1
4:A:322:PX4:H67	4:A:367:PX4:H30	0.56	1.77	13	1
4:A:359:PX4:H41	4:A:366:PX4:H44	0.56	1.78	1	1
4:A:343:PX4:H31	4:A:344:PX4:H32	0.56	1.78	3	1
4:A:374:PX4:H15	4:A:420:PX4:H19	0.56	1.76	12	2
4:A:306:PX4:H64	4:A:354:PX4:H19	0.56	1.76	10	1
4:A:311:PX4:H56	4:A:311:PX4:H25	0.56	1.75	14	1
4:A:348:PX4:H57	4:A:355:PX4:H32	0.55	1.77	3	1
4:A:329:PX4:H70	4:A:369:PX4:H41	0.55	1.78	6	1
4:A:421:PX4:H17	4:A:423:PX4:H52	0.55	1.77	7	2
4:A:374:PX4:H44	4:A:427:PX4:H17	0.55	1.76	7	1
4:A:412:PX4:H44	4:A:419:PX4:H39	0.55	1.79	12	1
4:A:388:PX4:H63	4:A:406:PX4:H62	0.55	1.78	13	1
4:A:313:PX4:H10	4:A:359:PX4:O2	0.55	2.01	14	1
4:A:391:PX4:H17	4:A:408:PX4:H20	0.55	1.78	6	1
4:A:331:PX4:H24	4:A:340:PX4:H17	0.55	1.78	7	1
4:A:309:PX4:H54	4:A:319:PX4:H53	0.55	1.78	12	1
4:A:308:PX4:H68	4:A:426:PX4:H51	0.55	1.78	7	1
4:A:349:PX4:H47	4:A:356:PX4:H38	0.55	1.79	11	1
4:A:422:PX4:H17	4:A:425:PX4:C29	0.55	2.30	13	1
4:A:308:PX4:H18	4:A:426:PX4:H43	0.55	1.79	2	1
4:A:406:PX4:H53	4:A:423:PX4:H61	0.55	1.77	2	1
4:A:349:PX4:O6	4:A:349:PX4:H6	0.55	2.02	5	2
4:A:423:PX4:H16	4:A:424:PX4:H23	0.55	1.79	4	1
4:A:421:PX4:H36	4:A:424:PX4:H37	0.55	1.77	7	1
4:A:336:PX4:H21	4:A:344:PX4:H56	0.55	1.77	9	1
4:A:420:PX4:H25	4:A:427:PX4:H31	0.55	1.77	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:341:PX4:H72	4:A:407:PX4:H40	0.55	1.78	1	1
4:A:371:PX4:H25	4:A:377:PX4:H21	0.55	1.79	8	1
4:A:342:PX4:H67	4:A:385:PX4:H43	0.55	1.77	10	1
4:A:405:PX4:H71	4:A:407:PX4:H54	0.55	1.78	12	1
4:A:309:PX4:H30	4:A:377:PX4:H70	0.55	1.78	1	1
4:A:400:PX4:H61	4:A:417:PX4:H25	0.55	1.78	4	1
4:A:388:PX4:H62	4:A:395:PX4:H55	0.55	1.79	6	1
4:A:417:PX4:H47	4:A:426:PX4:H51	0.55	1.77	6	1
4:A:363:PX4:H30	4:A:364:PX4:H32	0.55	1.79	10	1
4:A:404:PX4:H57	4:A:430:PX4:H27	0.55	1.78	12	1
4:A:310:PX4:H71	4:A:316:PX4:H22	0.55	1.78	13	1
4:A:348:PX4:H34	4:A:407:PX4:H70	0.55	1.79	1	1
4:A:404:PX4:H33	4:A:412:PX4:H35	0.55	1.77	7	1
4:A:342:PX4:H57	4:A:351:PX4:H36	0.55	1.78	8	1
4:A:338:PX4:H26	4:A:348:PX4:H22	0.55	1.78	12	1
4:A:312:PX4:H56	4:A:359:PX4:H50	0.55	1.79	1	1
4:A:349:PX4:H34	4:A:415:PX4:H45	0.55	1.79	2	1
4:A:412:PX4:H31	4:A:419:PX4:H47	0.55	1.77	4	1
4:A:327:PX4:H24	4:A:329:PX4:H31	0.55	1.79	5	1
4:A:371:PX4:H16	4:A:377:PX4:H47	0.55	1.79	5	2
4:A:391:PX4:H17	4:A:408:PX4:H19	0.55	1.78	8	1
4:A:339:PX4:H25	4:A:347:PX4:H53	0.55	1.79	1	1
4:A:308:PX4:O6	4:A:315:PX4:H11	0.55	2.02	3	1
4:A:372:PX4:H71	4:A:386:PX4:H37	0.55	1.78	4	1
4:A:374:PX4:H68	4:A:420:PX4:H41	0.55	1.77	4	1
4:A:391:PX4:H18	4:A:414:PX4:O2	0.55	2.02	7	1
4:A:400:PX4:H30	4:A:400:PX4:H59	0.55	1.77	7	1
4:A:325:PX4:H37	4:A:325:PX4:H67	0.55	1.79	10	1
4:A:306:PX4:H54	4:A:321:PX4:H49	0.55	1.78	5	1
4:A:313:PX4:H23	4:A:359:PX4:H21	0.55	1.78	6	1
4:A:423:PX4:H14	4:A:424:PX4:H19	0.55	1.78	7	1
4:A:386:PX4:H50	4:A:387:PX4:H58	0.55	1.77	9	1
4:A:321:PX4:H5	4:A:362:PX4:O1	0.54	2.02	4	2
4:A:317:PX4:H39	4:A:317:PX4:H68	0.54	1.79	3	1
4:A:380:PX4:H62	4:A:387:PX4:H30	0.54	1.79	7	1
4:A:335:PX4:H66	4:A:343:PX4:H45	0.54	1.80	8	1
4:A:359:PX4:H44	4:A:366:PX4:H30	0.54	1.78	8	1
4:A:366:PX4:H29	4:A:427:PX4:H67	0.54	1.77	9	1
4:A:343:PX4:H34	4:A:344:PX4:H37	0.54	1.76	10	1
4:A:392:PX4:H62	4:A:407:PX4:H33	0.54	1.79	2	1
4:A:338:PX4:H32	4:A:347:PX4:H28	0.54	1.79	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H27	4:A:412:PX4:H46	0.54	1.78	9	1
4:A:357:PX4:H15	4:A:358:PX4:O1	0.54	2.02	11	1
4:A:392:PX4:H63	4:A:393:PX4:H57	0.54	1.78	11	1
4:A:309:PX4:H33	4:A:319:PX4:H37	0.54	1.78	13	1
4:A:357:PX4:H70	4:A:411:PX4:H42	0.54	1.78	4	1
4:A:405:PX4:H25	4:A:415:PX4:H54	0.54	1.80	4	1
4:A:421:PX4:H69	4:A:430:PX4:H44	0.54	1.78	4	1
4:A:327:PX4:H56	4:A:327:PX4:H19	0.54	1.80	5	1
4:A:404:PX4:H28	4:A:413:PX4:H32	0.54	1.79	5	1
4:A:342:PX4:H30	4:A:351:PX4:H33	0.54	1.78	7	1
4:A:369:PX4:H31	4:A:424:PX4:H71	0.54	1.77	11	1
4:A:306:PX4:H71	4:A:360:PX4:H30	0.54	1.79	13	1
4:A:338:PX4:H27	4:A:345:PX4:H63	0.54	1.80	13	1
4:A:348:PX4:H53	4:A:355:PX4:H28	0.54	1.79	3	1
4:A:332:PX4:H48	4:A:334:PX4:H38	0.54	1.80	5	1
4:A:370:PX4:H63	4:A:403:PX4:H33	0.54	1.80	7	1
4:A:395:PX4:H38	4:A:415:PX4:H62	0.54	1.77	9	1
4:A:381:PX4:H59	4:A:402:PX4:H27	0.54	1.79	10	1
4:A:367:PX4:H11	4:A:424:PX4:H18	0.54	1.78	2	1
4:A:383:PX4:H57	4:A:392:PX4:H31	0.54	1.80	2	1
1:A:119:ASN:OD1	4:A:355:PX4:H7	0.54	2.01	5	2
4:A:324:PX4:H67	4:A:341:PX4:H36	0.54	1.79	11	1
4:A:382:PX4:H57	4:A:427:PX4:H42	0.54	1.79	1	1
4:A:397:PX4:H39	4:A:398:PX4:H66	0.54	1.78	1	1
4:A:376:PX4:H17	4:A:383:PX4:H51	0.54	1.80	2	1
4:A:327:PX4:H21	4:A:329:PX4:H41	0.54	1.80	4	1
4:A:409:PX4:H50	4:A:422:PX4:H47	0.54	1.79	6	1
4:A:336:PX4:H28	4:A:339:PX4:H29	0.54	1.80	8	1
4:A:424:PX4:H60	4:A:429:PX4:H55	0.54	1.79	9	1
4:A:330:PX4:H30	4:A:336:PX4:H56	0.54	1.80	6	1
4:A:333:PX4:H53	4:A:341:PX4:H16	0.54	1.78	7	1
4:A:416:PX4:H47	4:A:422:PX4:H51	0.54	1.79	7	1
4:A:306:PX4:H14	4:A:321:PX4:C10	0.54	2.33	8	1
4:A:317:PX4:H52	4:A:324:PX4:H24	0.54	1.79	8	1
4:A:388:PX4:H18	4:A:396:PX4:H2	0.54	1.79	14	1
1:A:162:VAL:HG11	4:A:314:PX4:H34	0.54	1.80	2	1
4:A:400:PX4:H34	4:A:417:PX4:H32	0.54	1.79	8	1
4:A:380:PX4:H25	4:A:381:PX4:H56	0.54	1.80	11	1
4:A:337:PX4:H46	4:A:345:PX4:H56	0.54	1.79	3	1
4:A:420:PX4:H58	4:A:427:PX4:H52	0.54	1.78	3	1
4:A:391:PX4:H24	4:A:392:PX4:H61	0.54	1.79	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H64	4:A:417:PX4:H27	0.54	1.78	8	1
4:A:326:PX4:H37	4:A:334:PX4:H24	0.54	1.79	12	1
4:A:332:PX4:H39	4:A:339:PX4:H39	0.54	1.78	1	1
4:A:320:PX4:H69	4:A:378:PX4:H33	0.54	1.79	3	1
4:A:328:PX4:H62	4:A:329:PX4:H25	0.54	1.80	4	1
4:A:326:PX4:H8	4:A:351:PX4:H22	0.54	1.80	5	1
4:A:393:PX4:H16	4:A:394:PX4:H24	0.54	1.79	6	1
4:A:313:PX4:H42	4:A:430:PX4:H41	0.54	1.79	7	1
4:A:358:PX4:H20	4:A:365:PX4:H17	0.54	1.78	11	1
4:A:389:PX4:H25	4:A:389:PX4:H59	0.53	1.81	3	1
4:A:388:PX4:H63	4:A:402:PX4:H72	0.53	1.79	5	1
4:A:349:PX4:H50	4:A:356:PX4:H5	0.53	1.79	2	1
4:A:367:PX4:H66	4:A:428:PX4:H27	0.53	1.80	5	1
4:A:415:PX4:H53	4:A:422:PX4:H25	0.53	1.79	9	1
4:A:391:PX4:H58	4:A:401:PX4:H26	0.53	1.80	4	1
4:A:339:PX4:H31	4:A:347:PX4:H56	0.53	1.81	9	1
4:A:388:PX4:H7	4:A:397:PX4:H49	0.53	1.80	9	1
4:A:374:PX4:H43	4:A:412:PX4:H32	0.53	1.79	11	1
4:A:363:PX4:H44	4:A:426:PX4:H70	0.53	1.78	12	1
4:A:373:PX4:H52	4:A:381:PX4:H33	0.53	1.79	12	1
4:A:377:PX4:H54	4:A:378:PX4:H25	0.53	1.80	13	1
1:A:165:ARG:CZ	4:A:362:PX4:H7	0.53	2.33	13	4
4:A:388:PX4:H59	4:A:402:PX4:H27	0.53	1.79	5	1
4:A:361:PX4:H26	4:A:362:PX4:H31	0.53	1.80	8	1
4:A:420:PX4:H30	4:A:427:PX4:H33	0.53	1.80	8	1
4:A:383:PX4:H27	4:A:399:PX4:H21	0.53	1.81	10	1
4:A:348:PX4:H16	4:A:355:PX4:H20	0.53	1.79	12	1
4:A:389:PX4:H53	4:A:398:PX4:H52	0.53	1.81	13	1
4:A:392:PX4:H24	4:A:399:PX4:H49	0.53	1.81	2	1
4:A:388:PX4:O1	4:A:396:PX4:H4	0.53	2.03	9	1
4:A:389:PX4:O2	4:A:398:PX4:H15	0.53	2.02	9	1
4:A:345:PX4:H16	4:A:346:PX4:O8	0.53	2.04	12	1
4:A:343:PX4:H69	4:A:344:PX4:H65	0.53	1.79	1	1
4:A:342:PX4:H49	4:A:351:PX4:H25	0.53	1.80	2	1
4:A:337:PX4:H54	4:A:345:PX4:H63	0.53	1.79	5	1
4:A:369:PX4:H44	4:A:430:PX4:H72	0.53	1.80	6	1
4:A:312:PX4:H17	4:A:359:PX4:H8	0.53	1.80	7	1
4:A:380:PX4:O2	4:A:381:PX4:H15	0.53	2.03	9	1
4:A:395:PX4:H42	4:A:415:PX4:H69	0.53	1.81	9	1
4:A:394:PX4:H53	4:A:401:PX4:H25	0.53	1.79	13	1
4:A:326:PX4:O2	4:A:350:PX4:H6	0.53	2.03	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:316:PX4:H64	4:A:368:PX4:H42	0.53	1.81	6	1
4:A:367:PX4:H26	4:A:430:PX4:H69	0.53	1.78	6	1
4:A:368:PX4:O1	4:A:418:PX4:H7	0.53	2.04	10	1
4:A:328:PX4:H54	4:A:329:PX4:H22	0.53	1.80	13	1
4:A:395:PX4:H39	4:A:415:PX4:H59	0.53	1.80	5	1
4:A:393:PX4:H68	4:A:394:PX4:H41	0.53	1.80	6	1
4:A:313:PX4:H45	4:A:354:PX4:H58	0.53	1.79	9	1
4:A:412:PX4:H63	4:A:421:PX4:H45	0.53	1.79	9	1
4:A:389:PX4:H34	4:A:397:PX4:H34	0.53	1.79	10	1
4:A:366:PX4:H32	4:A:427:PX4:H64	0.53	1.81	11	1
4:A:350:PX4:H66	4:A:350:PX4:H33	0.53	1.81	13	1
4:A:339:PX4:H19	4:A:347:PX4:H22	0.53	1.80	14	1
4:A:326:PX4:H44	4:A:350:PX4:H28	0.53	1.79	1	1
4:A:340:PX4:H49	4:A:341:PX4:H46	0.53	1.81	7	1
4:A:317:PX4:H20	4:A:342:PX4:H22	0.53	1.80	5	1
4:A:397:PX4:H23	4:A:398:PX4:H53	0.53	1.81	5	1
4:A:421:PX4:H33	4:A:430:PX4:H63	0.53	1.81	12	1
4:A:306:PX4:H24	4:A:360:PX4:H43	0.52	1.80	4	1
4:A:325:PX4:H29	4:A:325:PX4:H58	0.52	1.80	9	1
4:A:351:PX4:H66	4:A:409:PX4:H42	0.52	1.80	4	1
4:A:385:PX4:H60	4:A:399:PX4:H62	0.52	1.82	5	1
4:A:346:PX4:H44	4:A:362:PX4:H67	0.52	1.81	8	1
4:A:308:PX4:H51	4:A:311:PX4:H14	0.52	1.82	9	1
4:A:332:PX4:H47	4:A:347:PX4:H66	0.52	1.80	14	1
4:A:337:PX4:H18	4:A:337:PX4:O3	0.52	2.03	6	1
4:A:406:PX4:H34	4:A:424:PX4:H38	0.52	1.81	6	1
4:A:388:PX4:H19	4:A:396:PX4:H48	0.52	1.80	8	1
4:A:355:PX4:H5	4:A:362:PX4:H46	0.52	1.81	9	1
4:A:311:PX4:H71	4:A:426:PX4:H59	0.52	1.82	12	1
4:A:358:PX4:H9	4:A:358:PX4:H16	0.52	1.81	2	1
4:A:380:PX4:H31	4:A:381:PX4:H65	0.52	1.81	2	1
4:A:367:PX4:H24	4:A:424:PX4:H50	0.52	1.82	3	1
4:A:319:PX4:H19	4:A:319:PX4:H58	0.52	1.82	7	1
4:A:310:PX4:H35	4:A:409:PX4:H38	0.52	1.80	9	1
4:A:307:PX4:H53	4:A:361:PX4:H24	0.52	1.80	8	1
4:A:315:PX4:H58	4:A:322:PX4:H24	0.52	1.80	9	1
4:A:390:PX4:H24	4:A:428:PX4:H53	0.52	1.82	9	1
4:A:337:PX4:H50	4:A:345:PX4:H34	0.52	1.81	12	1
4:A:404:PX4:H9	4:A:419:PX4:O1	0.52	2.05	4	2
4:A:330:PX4:H26	4:A:344:PX4:H52	0.52	1.81	4	1
4:A:309:PX4:H16	4:A:320:PX4:H23	0.52	1.82	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H26	4:A:333:PX4:H38	0.52	1.80	5	1
4:A:400:PX4:O1	4:A:401:PX4:H2	0.52	2.05	5	1
4:A:310:PX4:H25	4:A:363:PX4:H42	0.52	1.82	7	1
4:A:424:PX4:H50	4:A:429:PX4:H51	0.52	1.80	8	1
4:A:307:PX4:H52	4:A:356:PX4:H42	0.52	1.81	10	1
4:A:396:PX4:O2	4:A:396:PX4:H16	0.52	2.05	12	1
4:A:368:PX4:H58	4:A:424:PX4:H48	0.52	1.82	7	1
4:A:408:PX4:H67	4:A:409:PX4:H32	0.52	1.81	7	1
4:A:404:PX4:H53	4:A:413:PX4:H26	0.52	1.81	13	1
4:A:350:PX4:H45	4:A:363:PX4:C29	0.52	2.33	1	1
4:A:400:PX4:C14	4:A:401:PX4:H46	0.52	2.34	2	1
4:A:418:PX4:H26	4:A:425:PX4:C12	0.52	2.33	4	1
4:A:361:PX4:H44	4:A:415:PX4:H42	0.52	1.81	6	1
4:A:331:PX4:H56	4:A:339:PX4:H59	0.52	1.82	9	1
4:A:369:PX4:H56	4:A:425:PX4:H29	0.52	1.81	13	1
4:A:383:PX4:O6	4:A:399:PX4:H16	0.52	2.05	1	1
4:A:405:PX4:H10	4:A:414:PX4:H27	0.52	1.80	2	1
4:A:337:PX4:O1	4:A:357:PX4:H15	0.52	2.04	3	1
4:A:350:PX4:H22	4:A:363:PX4:H57	0.52	1.82	9	1
4:A:325:PX4:H41	4:A:394:PX4:H41	0.51	1.80	1	1
4:A:428:PX4:H52	4:A:429:PX4:H46	0.51	1.81	12	1
4:A:348:PX4:H32	4:A:355:PX4:H35	0.51	1.83	14	1
4:A:400:PX4:H20	4:A:409:PX4:H23	0.51	1.81	3	1
4:A:388:PX4:H57	4:A:411:PX4:H41	0.51	1.80	8	1
4:A:380:PX4:H39	4:A:402:PX4:H35	0.51	1.82	9	1
4:A:380:PX4:H20	4:A:381:PX4:H48	0.51	1.82	3	1
4:A:306:PX4:H41	4:A:329:PX4:H70	0.51	1.81	5	1
4:A:362:PX4:H44	4:A:409:PX4:H70	0.51	1.81	5	1
4:A:364:PX4:H60	4:A:426:PX4:H37	0.51	1.82	5	1
4:A:330:PX4:H41	4:A:344:PX4:H64	0.51	1.82	8	1
4:A:340:PX4:H37	4:A:350:PX4:H42	0.51	1.80	10	1
4:A:367:PX4:H48	4:A:430:PX4:H49	0.51	1.81	10	1
4:A:338:PX4:C6	4:A:348:PX4:H15	0.51	2.35	13	1
4:A:388:PX4:H35	4:A:405:PX4:H61	0.51	1.81	14	1
4:A:408:PX4:H51	4:A:409:PX4:H48	0.51	1.81	4	1
4:A:331:PX4:O1	4:A:332:PX4:H7	0.51	2.05	5	2
4:A:375:PX4:H51	4:A:389:PX4:H49	0.51	1.83	5	1
4:A:313:PX4:H49	4:A:327:PX4:H25	0.51	1.81	6	1
4:A:314:PX4:H54	4:A:361:PX4:H30	0.51	1.82	6	1
4:A:316:PX4:H27	4:A:368:PX4:H42	0.51	1.82	10	1
4:A:315:PX4:H36	4:A:361:PX4:H61	0.51	1.82	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:367:PX4:H41	4:A:375:PX4:H64	0.51	1.81	11	1
4:A:356:PX4:H35	4:A:362:PX4:H28	0.51	1.81	14	1
4:A:419:PX4:H31	4:A:430:PX4:H29	0.51	1.82	14	1
4:A:326:PX4:H47	4:A:363:PX4:H67	0.51	1.82	1	1
4:A:369:PX4:H50	4:A:424:PX4:H20	0.51	1.83	4	2
4:A:355:PX4:H17	4:A:356:PX4:H15	0.51	1.82	5	1
4:A:387:PX4:H47	4:A:411:PX4:H47	0.51	1.82	8	1
4:A:349:PX4:H43	4:A:415:PX4:H32	0.51	1.82	11	1
4:A:330:PX4:H35	4:A:336:PX4:H52	0.51	1.83	11	1
4:A:317:PX4:H45	4:A:326:PX4:H52	0.51	1.81	12	1
4:A:406:PX4:H27	4:A:423:PX4:H62	0.51	1.83	1	1
4:A:326:PX4:H17	4:A:363:PX4:H61	0.51	1.82	4	1
4:A:321:PX4:H42	4:A:367:PX4:H68	0.51	1.81	6	1
4:A:326:PX4:H21	4:A:363:PX4:H63	0.51	1.83	8	1
4:A:348:PX4:H16	4:A:355:PX4:H19	0.51	1.82	8	1
4:A:385:PX4:H62	4:A:392:PX4:H34	0.51	1.82	9	1
4:A:313:PX4:H50	4:A:327:PX4:H34	0.51	1.81	12	1
4:A:403:PX4:H10	4:A:411:PX4:O2	0.51	2.05	4	1
4:A:317:PX4:H29	4:A:363:PX4:H71	0.51	1.82	5	1
4:A:308:PX4:H53	4:A:311:PX4:H19	0.51	1.83	6	1
4:A:392:PX4:H58	4:A:414:PX4:H51	0.51	1.83	12	1
4:A:388:PX4:H35	4:A:395:PX4:H34	0.51	1.82	1	1
4:A:405:PX4:H6	4:A:414:PX4:H26	0.51	1.82	1	1
4:A:324:PX4:H59	4:A:342:PX4:H26	0.51	1.82	3	1
4:A:402:PX4:H55	4:A:404:PX4:H49	0.51	1.82	10	1
4:A:348:PX4:H71	4:A:348:PX4:H44	0.51	1.83	12	1
4:A:306:PX4:H14	4:A:321:PX4:H19	0.51	1.82	8	1
4:A:307:PX4:H64	4:A:314:PX4:H67	0.51	1.83	8	1
4:A:330:PX4:H60	4:A:337:PX4:H29	0.51	1.82	9	1
4:A:344:PX4:H62	4:A:347:PX4:H36	0.51	1.82	12	1
4:A:413:PX4:H60	4:A:421:PX4:H57	0.50	1.83	4	1
4:A:334:PX4:H47	4:A:350:PX4:H16	0.50	1.83	6	1
4:A:390:PX4:H63	4:A:429:PX4:H68	0.50	1.81	7	1
4:A:346:PX4:H7	4:A:353:PX4:H48	0.50	1.84	8	1
4:A:309:PX4:H39	4:A:319:PX4:H35	0.50	1.83	9	1
4:A:342:PX4:H39	4:A:394:PX4:H39	0.50	1.81	10	1
4:A:391:PX4:H34	4:A:407:PX4:H46	0.50	1.82	10	1
4:A:314:PX4:H51	4:A:364:PX4:H46	0.50	1.82	14	1
4:A:313:PX4:H68	4:A:328:PX4:H44	0.50	1.82	2	1
4:A:428:PX4:H14	4:A:429:PX4:H22	0.50	1.83	4	1
4:A:317:PX4:H20	4:A:324:PX4:H56	0.50	1.83	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:H26	4:A:357:PX4:H35	0.50	1.83	12	1
4:A:310:PX4:H30	4:A:364:PX4:H39	0.50	1.83	2	1
4:A:332:PX4:H30	4:A:339:PX4:H39	0.50	1.82	5	1
4:A:317:PX4:O8	4:A:342:PX4:H17	0.50	2.06	6	1
4:A:367:PX4:H21	4:A:424:PX4:H55	0.50	1.82	7	1
4:A:331:PX4:H61	4:A:333:PX4:H21	0.50	1.81	8	1
4:A:408:PX4:H15	4:A:409:PX4:C1	0.50	2.28	10	1
4:A:307:PX4:H36	4:A:361:PX4:H54	0.50	1.83	11	1
4:A:368:PX4:H4	4:A:418:PX4:O1	0.50	2.06	12	1
4:A:331:PX4:H47	4:A:347:PX4:H54	0.50	1.83	13	1
4:A:331:PX4:H59	4:A:339:PX4:H38	0.50	1.84	14	1
4:A:374:PX4:H36	4:A:427:PX4:H21	0.50	1.84	1	1
4:A:380:PX4:H16	4:A:381:PX4:H47	0.50	1.83	1	2
4:A:412:PX4:H26	4:A:419:PX4:H26	0.50	1.81	1	1
4:A:330:PX4:H12	4:A:344:PX4:H46	0.50	1.84	3	1
4:A:400:PX4:C10	4:A:401:PX4:H17	0.50	2.35	6	1
4:A:306:PX4:H52	4:A:322:PX4:H61	0.50	1.84	8	1
4:A:411:PX4:H45	4:A:421:PX4:H53	0.50	1.84	9	1
4:A:387:PX4:H72	4:A:402:PX4:H38	0.50	1.82	12	1
4:A:400:PX4:O4	4:A:401:PX4:H3	0.50	2.07	12	1
4:A:410:PX4:H62	4:A:417:PX4:H58	0.50	1.82	12	1
4:A:373:PX4:H28	4:A:381:PX4:H46	0.50	1.82	13	1
4:A:420:PX4:H17	4:A:427:PX4:H19	0.50	1.83	1	1
4:A:309:PX4:H16	4:A:320:PX4:H22	0.50	1.83	2	1
4:A:386:PX4:O1	4:A:387:PX4:H13	0.50	2.07	2	1
4:A:379:PX4:H26	4:A:379:PX4:H56	0.50	1.82	3	1
4:A:389:PX4:H67	4:A:398:PX4:H37	0.50	1.84	5	1
4:A:338:PX4:H55	4:A:356:PX4:H55	0.50	1.82	6	1
4:A:359:PX4:H63	4:A:420:PX4:H64	0.50	1.83	7	1
4:A:365:PX4:C23	4:A:366:PX4:H51	0.50	2.36	8	1
4:A:318:PX4:H17	4:A:327:PX4:H49	0.50	1.82	13	2
4:A:350:PX4:H19	4:A:363:PX4:H64	0.50	1.84	1	1
4:A:355:PX4:O4	4:A:356:PX4:H15	0.50	2.06	14	2
4:A:367:PX4:H68	4:A:421:PX4:H29	0.50	1.83	1	1
4:A:408:PX4:O3	4:A:409:PX4:H1	0.50	2.05	1	1
4:A:370:PX4:H13	4:A:411:PX4:O8	0.50	2.07	2	1
4:A:383:PX4:H24	4:A:390:PX4:H56	0.50	1.84	8	1
4:A:380:PX4:H35	4:A:380:PX4:H64	0.50	1.84	12	1
4:A:368:PX4:H11	4:A:369:PX4:O6	0.50	2.07	3	1
4:A:378:PX4:H39	4:A:418:PX4:H67	0.50	1.83	4	1
4:A:317:PX4:H40	4:A:326:PX4:H61	0.50	1.83	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:321:PX4:H11	4:A:362:PX4:O1	0.50	2.07	8	1
4:A:337:PX4:H16	4:A:357:PX4:H47	0.50	1.84	9	2
4:A:379:PX4:H47	4:A:384:PX4:H16	0.50	1.83	9	1
4:A:378:PX4:H28	4:A:417:PX4:H63	0.50	1.83	12	1
4:A:348:PX4:H36	4:A:396:PX4:H43	0.50	1.82	13	1
4:A:336:PX4:H33	4:A:339:PX4:H67	0.50	1.84	1	1
4:A:339:PX4:H57	4:A:339:PX4:H41	0.50	1.84	2	1
4:A:383:PX4:H40	4:A:390:PX4:H39	0.50	1.82	13	2
4:A:384:PX4:H21	4:A:385:PX4:H20	0.50	1.82	5	1
4:A:393:PX4:H3	4:A:394:PX4:O4	0.50	2.07	5	1
4:A:395:PX4:H57	4:A:421:PX4:H67	0.50	1.82	5	1
4:A:348:PX4:H40	4:A:395:PX4:H64	0.50	1.83	7	1
4:A:309:PX4:H48	4:A:319:PX4:H26	0.50	1.83	9	1
4:A:398:PX4:H20	4:A:407:PX4:H15	0.50	1.84	13	1
4:A:404:PX4:H26	4:A:413:PX4:H24	0.50	1.82	13	1
4:A:410:PX4:H46	4:A:426:PX4:C6	0.50	2.37	13	1
4:A:346:PX4:O8	4:A:362:PX4:H13	0.50	2.07	11	2
4:A:307:PX4:H45	4:A:425:PX4:H23	0.50	1.84	10	1
4:A:342:PX4:H14	4:A:351:PX4:H20	0.50	1.83	12	1
4:A:387:PX4:H67	4:A:402:PX4:H34	0.50	1.83	12	1
4:A:388:PX4:H32	4:A:397:PX4:H64	0.49	1.83	1	1
4:A:395:PX4:H40	4:A:405:PX4:H36	0.49	1.83	2	1
4:A:374:PX4:H30	4:A:412:PX4:H52	0.49	1.83	5	1
4:A:380:PX4:H34	4:A:387:PX4:H70	0.49	1.84	7	1
4:A:370:PX4:H19	4:A:403:PX4:O7	0.49	2.07	13	1
4:A:306:PX4:H34	4:A:328:PX4:H36	0.49	1.84	1	1
4:A:335:PX4:H17	4:A:343:PX4:O1	0.49	2.07	1	1
4:A:338:PX4:H16	4:A:345:PX4:H53	0.49	1.82	2	1
4:A:402:PX4:H62	4:A:404:PX4:H58	0.49	1.83	3	1
4:A:405:PX4:H40	4:A:422:PX4:H38	0.49	1.82	8	1
4:A:317:PX4:H46	4:A:342:PX4:H12	0.49	1.84	10	1
4:A:313:PX4:O2	4:A:360:PX4:H12	0.49	2.07	12	1
4:A:340:PX4:H16	4:A:341:PX4:H50	0.49	1.82	12	1
4:A:371:PX4:H34	4:A:377:PX4:H30	0.49	1.83	12	1
4:A:404:PX4:H6	4:A:430:PX4:O6	0.49	2.07	12	1
4:A:326:PX4:H36	4:A:332:PX4:H46	0.49	1.83	13	1
4:A:349:PX4:H33	4:A:363:PX4:H17	0.49	1.84	14	1
4:A:399:PX4:H58	4:A:407:PX4:H32	0.49	1.84	1	1
4:A:378:PX4:H46	4:A:418:PX4:H47	0.49	1.83	4	1
4:A:400:PX4:H54	4:A:416:PX4:H39	0.49	1.84	8	1
4:A:376:PX4:H35	4:A:418:PX4:H72	0.49	1.84	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:323:PX4:H26	4:A:333:PX4:H30	0.49	1.84	14	1
4:A:369:PX4:H56	4:A:423:PX4:H25	0.49	1.84	2	1
4:A:367:PX4:H54	4:A:412:PX4:H19	0.49	1.83	6	1
4:A:413:PX4:H21	4:A:430:PX4:H23	0.49	1.84	14	1
4:A:374:PX4:H45	4:A:419:PX4:H24	0.49	1.85	4	1
4:A:376:PX4:H44	4:A:377:PX4:H61	0.49	1.83	4	1
4:A:317:PX4:O7	4:A:324:PX4:H14	0.49	2.07	5	1
4:A:408:PX4:H32	4:A:425:PX4:H68	0.49	1.82	5	1
4:A:377:PX4:H55	4:A:378:PX4:H26	0.49	1.84	7	1
4:A:353:PX4:H20	4:A:366:PX4:H53	0.49	1.83	11	1
4:A:361:PX4:H59	4:A:425:PX4:H31	0.49	1.83	11	1
4:A:328:PX4:H24	4:A:360:PX4:H41	0.49	1.84	3	1
4:A:391:PX4:H42	4:A:414:PX4:H19	0.49	1.84	3	1
4:A:316:PX4:H58	4:A:316:PX4:H21	0.49	1.85	4	1
4:A:331:PX4:H15	4:A:332:PX4:H19	0.49	1.83	5	1
4:A:331:PX4:H29	4:A:340:PX4:H17	0.49	1.83	7	1
4:A:409:PX4:H13	4:A:409:PX4:H15	0.49	1.84	9	1
4:A:307:PX4:H48	4:A:361:PX4:H24	0.49	1.83	12	1
4:A:334:PX4:H48	4:A:349:PX4:O5	0.49	2.06	12	1
4:A:388:PX4:O2	4:A:395:PX4:H4	0.49	2.08	3	2
4:A:319:PX4:H39	4:A:377:PX4:H70	0.49	1.84	6	1
4:A:307:PX4:H46	4:A:314:PX4:H22	0.49	1.85	10	1
4:A:373:PX4:H15	4:A:373:PX4:H13	0.49	1.84	1	1
4:A:309:PX4:H15	4:A:319:PX4:O5	0.49	2.08	6	1
4:A:313:PX4:H54	4:A:327:PX4:H27	0.49	1.85	10	1
4:A:327:PX4:H32	4:A:329:PX4:H27	0.49	1.83	11	1
4:A:348:PX4:H26	4:A:355:PX4:C13	0.49	2.37	12	1
4:A:410:PX4:H54	4:A:417:PX4:H54	0.49	1.83	13	1
4:A:317:PX4:H55	4:A:342:PX4:H48	0.49	1.84	1	1
4:A:353:PX4:H28	4:A:366:PX4:H55	0.49	1.85	2	1
4:A:400:PX4:H1	4:A:401:PX4:O1	0.49	2.08	2	1
4:A:332:PX4:H62	4:A:415:PX4:H60	0.49	1.84	4	1
4:A:306:PX4:H72	4:A:354:PX4:H51	0.49	1.84	6	1
4:A:318:PX4:H63	4:A:329:PX4:H44	0.49	1.85	6	1
4:A:385:PX4:H55	4:A:393:PX4:H54	0.49	1.84	8	1
4:A:367:PX4:H28	4:A:424:PX4:H56	0.49	1.85	10	1
1:A:191:ILE:HG22	4:A:349:PX4:H3	0.49	1.85	12	1
4:A:370:PX4:H30	4:A:403:PX4:H26	0.49	1.85	14	1
4:A:325:PX4:H51	4:A:341:PX4:H49	0.49	1.83	1	1
4:A:348:PX4:H9	4:A:355:PX4:O2	0.49	2.08	3	2
4:A:371:PX4:H37	4:A:376:PX4:H42	0.49	1.84	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:354:PX4:H27	4:A:362:PX4:H60	0.49	1.85	11	1
4:A:355:PX4:H54	4:A:362:PX4:H53	0.49	1.84	11	1
4:A:376:PX4:H40	4:A:377:PX4:H57	0.49	1.83	11	1
4:A:405:PX4:H17	4:A:414:PX4:H22	0.49	1.85	14	1
4:A:315:PX4:H56	4:A:323:PX4:H16	0.48	1.85	4	1
4:A:346:PX4:H66	4:A:353:PX4:H66	0.48	1.83	6	1
4:A:403:PX4:O6	4:A:403:PX4:H1	0.48	2.08	10	1
4:A:418:PX4:H31	4:A:425:PX4:H22	0.48	1.85	13	1
4:A:391:PX4:H48	4:A:408:PX4:H20	0.48	1.83	14	1
4:A:306:PX4:H27	4:A:328:PX4:H53	0.48	1.84	3	1
4:A:388:PX4:H14	4:A:395:PX4:O3	0.48	2.08	13	3
4:A:310:PX4:H59	4:A:364:PX4:H30	0.48	1.83	7	1
4:A:306:PX4:H67	4:A:360:PX4:H30	0.48	1.86	8	1
4:A:315:PX4:H32	4:A:322:PX4:H48	0.48	1.83	9	1
4:A:306:PX4:H65	4:A:321:PX4:H17	0.48	1.84	10	1
4:A:321:PX4:H27	4:A:322:PX4:H59	0.48	1.84	13	1
4:A:331:PX4:H57	4:A:332:PX4:H29	0.48	1.85	5	1
4:A:353:PX4:H48	4:A:354:PX4:H62	0.48	1.84	12	1
4:A:346:PX4:H48	4:A:362:PX4:H50	0.48	1.85	4	1
4:A:380:PX4:H63	4:A:386:PX4:H20	0.48	1.85	7	1
4:A:313:PX4:H63	4:A:328:PX4:H38	0.48	1.84	10	1
4:A:328:PX4:H23	4:A:360:PX4:H33	0.48	1.85	14	1
1:A:163:PHE:CZ	1:A:212:LEU:HD11	0.48	2.43	9	1
4:A:370:PX4:H72	4:A:387:PX4:H71	0.48	1.84	9	1
4:A:318:PX4:H57	4:A:327:PX4:H54	0.48	1.84	10	1
4:A:322:PX4:H32	4:A:333:PX4:H55	0.48	1.86	14	1
4:A:306:PX4:H37	4:A:360:PX4:H38	0.48	1.83	2	1
4:A:322:PX4:H45	4:A:323:PX4:H65	0.48	1.84	4	1
4:A:358:PX4:H60	4:A:358:PX4:H36	0.48	1.86	4	1
4:A:417:PX4:H51	4:A:426:PX4:H46	0.48	1.85	4	1
4:A:316:PX4:H20	4:A:316:PX4:C25	0.48	2.38	10	1
4:A:328:PX4:H27	4:A:360:PX4:H36	0.48	1.85	13	1
4:A:343:PX4:H35	4:A:344:PX4:H28	0.48	1.84	13	1
4:A:332:PX4:O1	4:A:332:PX4:H7	0.48	2.09	2	1
4:A:393:PX4:H72	4:A:394:PX4:H32	0.48	1.84	2	1
4:A:405:PX4:H5	4:A:415:PX4:H17	0.48	1.85	7	1
4:A:368:PX4:H21	4:A:429:PX4:H62	0.48	1.84	9	1
4:A:323:PX4:H22	4:A:333:PX4:H49	0.48	1.86	12	1
4:A:351:PX4:H47	4:A:352:PX4:H19	0.48	1.86	3	1
4:A:309:PX4:H56	4:A:316:PX4:H50	0.48	1.84	8	1
4:A:333:PX4:H49	4:A:341:PX4:H14	0.48	1.85	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:336:PX4:H23	4:A:339:PX4:H57	0.48	1.86	9	1
4:A:350:PX4:H44	4:A:414:PX4:H42	0.48	1.84	9	1
4:A:343:PX4:H47	4:A:352:PX4:H53	0.48	1.84	11	1
4:A:345:PX4:H60	4:A:348:PX4:H22	0.48	1.85	11	1
4:A:358:PX4:H38	4:A:417:PX4:H45	0.48	1.84	12	1
4:A:400:PX4:H8	4:A:401:PX4:O6	0.48	2.09	13	1
4:A:349:PX4:H46	4:A:356:PX4:H11	0.48	1.86	4	1
4:A:392:PX4:H51	4:A:407:PX4:H23	0.48	1.86	4	1
4:A:336:PX4:H14	4:A:344:PX4:H51	0.48	1.86	5	1
4:A:377:PX4:H54	4:A:378:PX4:H30	0.48	1.85	6	1
4:A:400:PX4:H1	4:A:409:PX4:O1	0.48	2.09	9	1
4:A:396:PX4:H50	4:A:398:PX4:H28	0.48	1.85	1	1
4:A:388:PX4:H21	4:A:406:PX4:H70	0.48	1.85	5	1
4:A:388:PX4:H51	4:A:402:PX4:H19	0.48	1.85	5	1
4:A:393:PX4:H19	4:A:394:PX4:H48	0.48	1.85	8	1
4:A:382:PX4:H54	4:A:428:PX4:H27	0.48	1.84	12	1
4:A:381:PX4:H27	4:A:384:PX4:H54	0.48	1.84	13	1
4:A:318:PX4:H47	4:A:327:PX4:H46	0.48	1.85	14	1
4:A:393:PX4:H67	4:A:394:PX4:H33	0.47	1.84	1	1
4:A:392:PX4:H58	4:A:414:PX4:H50	0.47	1.86	4	1
4:A:387:PX4:H68	4:A:403:PX4:H36	0.47	1.86	10	1
4:A:330:PX4:H67	4:A:337:PX4:H36	0.47	1.86	12	1
4:A:308:PX4:H49	4:A:311:PX4:H4	0.47	1.85	13	1
4:A:319:PX4:H33	4:A:320:PX4:H29	0.47	1.85	14	1
4:A:317:PX4:H25	4:A:342:PX4:H28	0.47	1.83	1	1
4:A:314:PX4:H68	4:A:422:PX4:H64	0.47	1.85	2	1
1:A:138:PHE:CD1	1:A:149:PHE:CG	0.47	3.01	5	1
4:A:309:PX4:H17	4:A:319:PX4:H25	0.47	1.87	8	1
4:A:336:PX4:H52	4:A:344:PX4:H57	0.47	1.86	8	1
4:A:422:PX4:H47	4:A:425:PX4:H50	0.47	1.86	9	1
4:A:368:PX4:H8	4:A:369:PX4:O6	0.47	2.09	12	1
4:A:403:PX4:H8	4:A:411:PX4:O6	0.47	2.09	13	1
4:A:312:PX4:H48	4:A:359:PX4:H50	0.47	1.85	14	1
4:A:336:PX4:H38	4:A:344:PX4:H69	0.47	1.85	14	1
4:A:391:PX4:H44	4:A:395:PX4:H28	0.47	1.86	2	1
4:A:331:PX4:H5	4:A:348:PX4:O4	0.47	2.08	3	1
4:A:420:PX4:H27	4:A:427:PX4:H30	0.47	1.85	3	1
4:A:391:PX4:H62	4:A:415:PX4:H23	0.47	1.86	7	1
4:A:315:PX4:H65	4:A:323:PX4:H23	0.47	1.85	10	1
4:A:366:PX4:H44	4:A:374:PX4:H42	0.47	1.87	10	1
4:A:396:PX4:H65	4:A:396:PX4:H34	0.47	1.87	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:386:PX4:H46	4:A:387:PX4:H49	0.47	1.87	12	1
4:A:373:PX4:H28	4:A:381:PX4:C24	0.47	2.39	13	1
4:A:408:PX4:H17	4:A:415:PX4:O6	0.47	2.09	13	3
4:A:370:PX4:H23	4:A:403:PX4:H47	0.47	1.85	3	1
4:A:317:PX4:H32	4:A:363:PX4:H65	0.47	1.86	4	1
4:A:364:PX4:H68	4:A:422:PX4:H63	0.47	1.86	6	1
4:A:377:PX4:H46	4:A:378:PX4:H21	0.47	1.85	11	1
4:A:373:PX4:O2	4:A:381:PX4:H8	0.47	2.08	12	1
4:A:331:PX4:H63	4:A:331:PX4:H27	0.47	1.85	13	1
4:A:409:PX4:H55	4:A:416:PX4:H56	0.47	1.87	13	1
4:A:348:PX4:H44	4:A:405:PX4:H72	0.47	1.86	14	1
4:A:413:PX4:H56	4:A:430:PX4:H31	0.47	1.86	4	1
4:A:370:PX4:H20	4:A:403:PX4:H51	0.47	1.86	5	1
4:A:391:PX4:H39	4:A:414:PX4:H32	0.47	1.85	12	1
4:A:332:PX4:H60	4:A:393:PX4:H72	0.47	1.86	13	1
4:A:378:PX4:H47	4:A:410:PX4:H19	0.47	1.85	13	1
4:A:332:PX4:O1	4:A:356:PX4:H4	0.47	2.09	1	1
4:A:409:PX4:H52	4:A:415:PX4:H23	0.47	1.85	1	1
4:A:354:PX4:H65	4:A:366:PX4:H48	0.47	1.85	2	1
4:A:380:PX4:H51	4:A:381:PX4:H55	0.47	1.86	2	1
4:A:306:PX4:H23	4:A:360:PX4:H39	0.47	1.87	3	1
4:A:357:PX4:H40	4:A:357:PX4:H69	0.47	1.86	4	1
4:A:308:PX4:H57	4:A:310:PX4:H64	0.47	1.87	5	1
4:A:421:PX4:P1	4:A:423:PX4:H4	0.47	2.50	7	1
4:A:308:PX4:H13	4:A:310:PX4:H51	0.47	1.86	9	1
4:A:314:PX4:H68	4:A:361:PX4:H39	0.47	1.86	9	1
4:A:325:PX4:H57	4:A:341:PX4:H60	0.47	1.87	9	1
4:A:338:PX4:O7	4:A:348:PX4:H18	0.47	2.09	9	3
4:A:338:PX4:H30	4:A:348:PX4:H28	0.47	1.87	11	1
4:A:391:PX4:H71	4:A:408:PX4:H37	0.47	1.86	13	1
4:A:306:PX4:H58	4:A:321:PX4:H22	0.47	1.86	1	1
4:A:398:PX4:H19	4:A:407:PX4:H15	0.47	1.87	1	1
4:A:373:PX4:H54	4:A:375:PX4:H33	0.47	1.85	2	1
4:A:389:PX4:H63	4:A:389:PX4:H27	0.47	1.86	3	1
4:A:413:PX4:H54	4:A:423:PX4:H54	0.47	1.87	3	1
4:A:326:PX4:H40	4:A:350:PX4:H28	0.47	1.86	6	1
4:A:316:PX4:H36	4:A:378:PX4:H64	0.47	1.85	7	1
4:A:331:PX4:O1	4:A:332:PX4:H10	0.47	2.10	10	3
4:A:314:PX4:H70	4:A:349:PX4:H34	0.47	1.86	8	1
4:A:346:PX4:H60	4:A:362:PX4:H58	0.47	1.87	11	1
4:A:375:PX4:H48	4:A:382:PX4:H68	0.47	1.87	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:O2	4:A:414:PX4:H2	0.47	2.10	12	1
4:A:422:PX4:H67	4:A:426:PX4:H31	0.47	1.86	12	1
4:A:306:PX4:H38	4:A:329:PX4:H51	0.47	1.87	13	1
4:A:325:PX4:H22	4:A:326:PX4:H21	0.47	1.86	14	1
4:A:400:PX4:C11	4:A:408:PX4:H67	0.47	2.39	14	1
4:A:367:PX4:H65	4:A:421:PX4:H25	0.47	1.86	1	1
4:A:373:PX4:H36	4:A:397:PX4:H67	0.47	1.87	5	1
4:A:322:PX4:H17	4:A:333:PX4:H41	0.47	1.87	6	1
4:A:338:PX4:H62	4:A:356:PX4:H59	0.47	1.87	6	1
4:A:393:PX4:H13	4:A:394:PX4:O2	0.47	2.10	6	1
4:A:337:PX4:H31	4:A:343:PX4:H50	0.47	1.86	7	1
4:A:307:PX4:H50	4:A:314:PX4:H19	0.47	1.86	10	1
4:A:314:PX4:H71	4:A:409:PX4:H63	0.47	1.87	10	1
4:A:396:PX4:H30	4:A:397:PX4:H67	0.47	1.86	13	1
4:A:364:PX4:H45	4:A:426:PX4:H69	0.47	1.86	1	1
4:A:306:PX4:H3	4:A:329:PX4:O2	0.47	2.10	3	1
4:A:315:PX4:H2	4:A:316:PX4:H2	0.47	1.87	6	1
4:A:423:PX4:C7	4:A:424:PX4:H24	0.47	2.17	7	1
4:A:369:PX4:O1	4:A:425:PX4:H18	0.47	2.10	5	1
4:A:374:PX4:O2	4:A:420:PX4:H4	0.47	2.10	6	1
4:A:416:PX4:H5	4:A:426:PX4:O3	0.47	2.10	6	1
4:A:331:PX4:H57	4:A:332:PX4:H26	0.47	1.87	9	1
4:A:344:PX4:H50	4:A:347:PX4:H21	0.47	1.86	13	1
4:A:315:PX4:H7	4:A:316:PX4:O6	0.46	2.10	1	1
4:A:399:PX4:H54	4:A:407:PX4:H28	0.46	1.86	1	1
4:A:380:PX4:H68	4:A:386:PX4:H59	0.46	1.85	3	1
4:A:391:PX4:H33	4:A:407:PX4:H61	0.46	1.86	3	1
4:A:316:PX4:H44	4:A:316:PX4:H72	0.46	1.85	5	1
4:A:328:PX4:H11	4:A:360:PX4:H29	0.46	1.86	6	1
4:A:398:PX4:H21	4:A:407:PX4:H47	0.46	1.88	10	1
4:A:403:PX4:H29	4:A:413:PX4:H32	0.46	1.87	12	1
4:A:370:PX4:H22	4:A:403:PX4:H17	0.46	1.87	14	1
4:A:320:PX4:H40	4:A:418:PX4:H63	0.46	1.87	2	1
4:A:420:PX4:H40	4:A:427:PX4:H34	0.46	1.87	5	1
4:A:340:PX4:H44	4:A:399:PX4:H69	0.46	1.87	11	1
4:A:391:PX4:H17	4:A:408:PX4:H22	0.46	1.87	11	1
4:A:306:PX4:H70	4:A:328:PX4:H5	0.46	1.86	12	1
4:A:388:PX4:H51	4:A:406:PX4:H66	0.46	1.87	1	1
4:A:374:PX4:H39	4:A:427:PX4:H17	0.46	1.86	5	1
4:A:389:PX4:H21	4:A:398:PX4:H54	0.46	1.87	5	1
4:A:406:PX4:O2	4:A:415:PX4:H2	0.46	2.10	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:325:PX4:H7	4:A:325:PX4:H15	0.46	1.86	13	2
4:A:345:PX4:O6	4:A:353:PX4:H15	0.46	2.10	13	2
4:A:348:PX4:H50	4:A:355:PX4:H27	0.46	1.87	8	1
4:A:416:PX4:H63	4:A:416:PX4:H44	0.46	1.87	9	1
4:A:388:PX4:H39	4:A:405:PX4:H65	0.46	1.86	14	1
4:A:335:PX4:H59	4:A:344:PX4:H37	0.46	1.86	2	1
4:A:399:PX4:O7	4:A:407:PX4:H19	0.46	2.11	3	1
4:A:401:PX4:H22	4:A:408:PX4:H66	0.46	1.87	3	1
4:A:315:PX4:H46	4:A:316:PX4:H59	0.46	1.88	4	1
4:A:335:PX4:O1	4:A:343:PX4:H4	0.46	2.10	7	1
4:A:353:PX4:H23	4:A:357:PX4:H27	0.46	1.86	7	1
4:A:353:PX4:H43	4:A:413:PX4:H37	0.46	1.86	7	1
4:A:329:PX4:H5	4:A:333:PX4:H30	0.46	1.86	10	1
4:A:372:PX4:H59	4:A:384:PX4:H25	0.46	1.86	12	1
4:A:317:PX4:H35	4:A:342:PX4:H33	0.46	1.86	1	1
4:A:307:PX4:H27	4:A:361:PX4:H23	0.46	1.87	2	1
4:A:378:PX4:C6	4:A:410:PX4:H47	0.46	2.39	3	1
4:A:400:PX4:H22	4:A:401:PX4:O7	0.46	2.11	3	1
4:A:330:PX4:H21	4:A:343:PX4:H61	0.46	1.86	4	1
4:A:397:PX4:H40	4:A:398:PX4:H71	0.46	1.86	4	1
4:A:311:PX4:O6	4:A:311:PX4:H48	0.46	2.11	2	1
4:A:388:PX4:H44	4:A:405:PX4:H72	0.46	1.87	7	1
4:A:331:PX4:H14	4:A:347:PX4:H51	0.46	1.87	8	1
4:A:355:PX4:H68	4:A:422:PX4:H42	0.46	1.88	9	1
4:A:393:PX4:H33	4:A:394:PX4:H34	0.46	1.88	10	1
4:A:367:PX4:H28	4:A:424:PX4:H52	0.46	1.88	12	1
4:A:380:PX4:H62	4:A:387:PX4:H66	0.46	1.88	14	1
1:A:167:ALA:O	4:A:307:PX4:H6	0.46	2.10	8	2
4:A:325:PX4:H66	4:A:340:PX4:H66	0.46	1.87	8	1
4:A:330:PX4:H17	4:A:348:PX4:C27	0.46	2.41	14	1
4:A:405:PX4:H22	4:A:406:PX4:H22	0.46	1.86	4	1
4:A:376:PX4:H53	4:A:377:PX4:H25	0.46	1.87	5	1
4:A:399:PX4:H10	4:A:399:PX4:O2	0.46	2.11	5	1
1:A:153:ASN:O	4:A:331:PX4:H11	0.46	2.11	8	1
4:A:367:PX4:H48	4:A:412:PX4:H18	0.46	1.87	8	1
4:A:409:PX4:H51	4:A:415:PX4:H29	0.46	1.87	8	1
4:A:362:PX4:H64	4:A:413:PX4:H69	0.46	1.85	10	1
4:A:407:PX4:C7	4:A:414:PX4:H49	0.46	2.40	10	1
4:A:422:PX4:H22	4:A:425:PX4:H69	0.46	1.88	10	1
4:A:412:PX4:H64	4:A:428:PX4:H45	0.46	1.87	12	1
4:A:374:PX4:H29	4:A:427:PX4:H45	0.46	1.88	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:312:PX4:H19	4:A:366:PX4:H17	0.46	1.88	4	1
4:A:322:PX4:H33	4:A:424:PX4:H69	0.46	1.88	4	1
4:A:378:PX4:H9	4:A:417:PX4:H53	0.46	1.88	5	1
4:A:400:PX4:H24	4:A:400:PX4:H59	0.46	1.87	5	1
4:A:332:PX4:H4	4:A:356:PX4:O3	0.46	2.11	7	1
4:A:387:PX4:H17	4:A:411:PX4:H55	0.46	1.88	12	2
4:A:377:PX4:H46	4:A:378:PX4:H24	0.46	1.87	13	1
4:A:388:PX4:H23	4:A:396:PX4:H9	0.46	1.86	13	1
4:A:316:PX4:H52	4:A:333:PX4:H63	0.46	1.87	1	1
4:A:366:PX4:H34	4:A:427:PX4:H60	0.46	1.89	5	1
4:A:354:PX4:H47	4:A:360:PX4:H21	0.46	1.87	7	1
4:A:367:PX4:H47	4:A:412:PX4:H53	0.46	1.87	7	1
4:A:400:PX4:H10	4:A:409:PX4:O6	0.46	2.10	7	1
4:A:400:PX4:H60	4:A:422:PX4:H71	0.46	1.87	12	1
4:A:373:PX4:H21	4:A:381:PX4:H21	0.46	1.86	13	1
4:A:307:PX4:H34	4:A:321:PX4:H68	0.45	1.88	2	1
4:A:321:PX4:H55	4:A:354:PX4:H34	0.45	1.87	4	1
4:A:353:PX4:H29	4:A:357:PX4:H57	0.45	1.85	4	1
4:A:378:PX4:O3	4:A:378:PX4:H18	0.45	2.11	4	1
4:A:392:PX4:H35	4:A:399:PX4:H61	0.45	1.87	5	1
4:A:334:PX4:H61	4:A:356:PX4:H39	0.45	1.88	7	1
4:A:348:PX4:H43	4:A:402:PX4:H41	0.45	1.88	7	1
4:A:416:PX4:H63	4:A:422:PX4:H65	0.45	1.88	8	1
4:A:388:PX4:H51	4:A:411:PX4:H31	0.45	1.88	9	1
4:A:315:PX4:H41	4:A:323:PX4:H65	0.45	1.88	10	1
4:A:361:PX4:H38	4:A:362:PX4:H40	0.45	1.88	10	1
4:A:422:PX4:H17	4:A:425:PX4:H64	0.45	1.88	10	1
4:A:378:PX4:H18	4:A:378:PX4:H1	0.45	1.88	11	1
4:A:413:PX4:H57	4:A:430:PX4:H32	0.45	1.88	11	1
4:A:371:PX4:H10	4:A:371:PX4:O6	0.45	2.11	13	1
4:A:329:PX4:H46	4:A:336:PX4:H20	0.45	1.88	3	1
4:A:339:PX4:C11	4:A:347:PX4:H53	0.45	2.42	3	1
4:A:361:PX4:H37	4:A:409:PX4:H68	0.45	1.89	3	1
4:A:325:PX4:H18	4:A:334:PX4:H11	0.45	1.88	6	1
4:A:332:PX4:O6	4:A:332:PX4:H1	0.45	2.11	7	1
4:A:322:PX4:H71	4:A:430:PX4:H65	0.45	1.89	8	1
4:A:408:PX4:O3	4:A:409:PX4:H2	0.45	2.11	8	1
4:A:328:PX4:H33	4:A:359:PX4:H40	0.45	1.87	10	1
4:A:385:PX4:H66	4:A:399:PX4:H63	0.45	1.89	10	1
4:A:338:PX4:H52	4:A:345:PX4:H59	0.45	1.88	11	1
4:A:330:PX4:H34	4:A:343:PX4:H60	0.45	1.88	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:337:PX4:O1	4:A:338:PX4:H8	0.45	2.11	12	1
4:A:421:PX4:H45	4:A:430:PX4:H40	0.45	1.86	14	1
4:A:377:PX4:H51	4:A:378:PX4:H23	0.45	1.89	5	1
4:A:399:PX4:H39	4:A:407:PX4:H31	0.45	1.89	7	1
4:A:367:PX4:H34	4:A:428:PX4:H48	0.45	1.88	9	1
4:A:379:PX4:H24	4:A:384:PX4:H21	0.45	1.86	9	1
4:A:316:PX4:H41	4:A:368:PX4:H25	0.45	1.88	10	1
4:A:321:PX4:H8	4:A:362:PX4:O1	0.45	2.12	13	1
4:A:322:PX4:H69	4:A:413:PX4:H58	0.45	1.89	1	1
4:A:370:PX4:H40	4:A:404:PX4:H41	0.45	1.87	4	1
4:A:406:PX4:H31	4:A:424:PX4:H45	0.45	1.89	4	1
4:A:375:PX4:H27	4:A:382:PX4:H28	0.45	1.89	6	1
4:A:357:PX4:H49	4:A:357:PX4:H28	0.45	1.88	7	1
4:A:403:PX4:H54	4:A:419:PX4:H59	0.45	1.88	8	1
4:A:338:PX4:H23	4:A:348:PX4:H53	0.45	1.88	11	1
4:A:331:PX4:H61	4:A:339:PX4:H62	0.45	1.87	12	1
4:A:336:PX4:H34	4:A:339:PX4:H36	0.45	1.87	12	1
4:A:368:PX4:H50	4:A:369:PX4:H22	0.45	1.89	14	1
4:A:399:PX4:H10	4:A:399:PX4:H14	0.45	1.88	1	1
4:A:307:PX4:H12	4:A:361:PX4:O6	0.45	2.12	3	1
4:A:317:PX4:H54	4:A:342:PX4:H19	0.45	1.88	3	1
4:A:396:PX4:H52	4:A:398:PX4:H56	0.45	1.88	4	1
4:A:355:PX4:H61	4:A:405:PX4:H41	0.45	1.88	6	1
4:A:380:PX4:O8	4:A:381:PX4:H51	0.45	2.11	6	1
4:A:386:PX4:H58	4:A:411:PX4:H60	0.45	1.88	6	1
4:A:408:PX4:H29	4:A:415:PX4:H48	0.45	1.89	7	1
4:A:413:PX4:H70	4:A:430:PX4:H60	0.45	1.89	8	1
4:A:338:PX4:H69	4:A:346:PX4:H61	0.45	1.89	10	1
4:A:368:PX4:H51	4:A:369:PX4:H16	0.45	1.86	13	1
4:A:321:PX4:H47	4:A:354:PX4:H20	0.45	1.88	14	1
4:A:318:PX4:H53	4:A:336:PX4:H54	0.45	1.88	2	1
4:A:408:PX4:H51	4:A:415:PX4:H23	0.45	1.88	2	1
4:A:349:PX4:H71	4:A:356:PX4:H65	0.45	1.88	3	1
4:A:326:PX4:H40	4:A:350:PX4:H32	0.45	1.89	4	1
4:A:316:PX4:H46	4:A:319:PX4:H46	0.45	1.89	5	1
4:A:328:PX4:O6	4:A:328:PX4:H9	0.45	2.11	5	1
4:A:420:PX4:H48	4:A:427:PX4:H19	0.45	1.88	5	1
4:A:340:PX4:H54	4:A:341:PX4:H51	0.45	1.88	1	1
4:A:395:PX4:H59	4:A:406:PX4:H58	0.45	1.87	9	1
1:A:237:PHE:CD1	1:A:238:PRO:HD2	0.45	2.46	10	1
4:A:363:PX4:H23	4:A:364:PX4:H24	0.45	1.88	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:H54	4:A:324:PX4:H24	0.45	1.88	13	1
4:A:322:PX4:H68	4:A:430:PX4:H67	0.45	1.89	13	1
4:A:384:PX4:H7	4:A:386:PX4:O2	0.45	2.12	13	1
4:A:367:PX4:H23	4:A:368:PX4:H72	0.45	1.89	1	1
4:A:400:PX4:O2	4:A:409:PX4:H14	0.45	2.12	1	1
4:A:321:PX4:H25	4:A:322:PX4:H54	0.45	1.89	2	1
4:A:330:PX4:H28	4:A:344:PX4:H25	0.45	1.89	2	1
4:A:393:PX4:H32	4:A:394:PX4:H67	0.45	1.87	2	1
4:A:332:PX4:H35	4:A:355:PX4:H39	0.45	1.89	3	1
4:A:396:PX4:H45	4:A:398:PX4:H34	0.45	1.89	7	1
4:A:421:PX4:H42	4:A:423:PX4:H44	0.45	1.89	7	1
4:A:334:PX4:H70	4:A:406:PX4:H43	0.45	1.89	10	1
4:A:404:PX4:H10	4:A:430:PX4:O6	0.45	2.11	10	1
4:A:315:PX4:H29	4:A:425:PX4:H37	0.45	1.88	2	1
4:A:380:PX4:H19	4:A:381:PX4:H20	0.45	1.88	2	1
4:A:315:PX4:H64	4:A:316:PX4:H62	0.45	1.88	3	1
4:A:338:PX4:H59	4:A:345:PX4:H61	0.45	1.87	4	1
4:A:400:PX4:H59	4:A:400:PX4:H26	0.45	1.88	4	1
4:A:380:PX4:H52	4:A:386:PX4:H49	0.45	1.88	6	1
4:A:367:PX4:O5	4:A:428:PX4:H17	0.45	2.11	7	1
4:A:368:PX4:H24	4:A:390:PX4:H56	0.45	1.87	7	1
4:A:413:PX4:H22	4:A:430:PX4:H19	0.45	1.88	7	1
4:A:313:PX4:H52	4:A:328:PX4:H48	0.45	1.89	8	1
4:A:347:PX4:H41	4:A:348:PX4:H68	0.45	1.87	8	1
4:A:361:PX4:H29	4:A:362:PX4:H35	0.45	1.89	8	1
4:A:307:PX4:H13	4:A:361:PX4:O6	0.45	2.12	11	1
4:A:383:PX4:H22	4:A:399:PX4:H48	0.45	1.89	13	1
4:A:378:PX4:H3	4:A:410:PX4:O8	0.45	2.12	1	1
4:A:346:PX4:H14	4:A:362:PX4:H3	0.45	1.88	3	1
4:A:348:PX4:H1	4:A:355:PX4:H14	0.45	1.88	3	1
4:A:366:PX4:H34	4:A:427:PX4:H72	0.45	1.87	6	1
4:A:374:PX4:H17	4:A:382:PX4:H51	0.45	1.89	6	1
4:A:358:PX4:H22	4:A:365:PX4:H26	0.45	1.89	9	1
4:A:307:PX4:H42	4:A:364:PX4:H68	0.45	1.87	10	1
4:A:366:PX4:H43	4:A:412:PX4:H40	0.45	1.87	11	1
4:A:402:PX4:H67	4:A:421:PX4:H55	0.45	1.88	12	1
4:A:330:PX4:H53	4:A:338:PX4:C11	0.44	2.42	4	1
4:A:357:PX4:H20	4:A:358:PX4:H16	0.44	1.88	4	2
4:A:380:PX4:H16	4:A:381:PX4:H48	0.44	1.90	6	1
4:A:334:PX4:H52	4:A:349:PX4:H20	0.44	1.88	7	1
4:A:350:PX4:H22	4:A:363:PX4:H55	0.44	1.89	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H19	4:A:401:PX4:H23	0.44	1.89	14	1
4:A:374:PX4:H17	4:A:382:PX4:H50	0.44	1.90	1	1
4:A:317:PX4:H19	4:A:325:PX4:H46	0.44	1.87	2	1
4:A:341:PX4:H70	4:A:407:PX4:H41	0.44	1.88	2	1
4:A:391:PX4:H35	4:A:415:PX4:H65	0.44	1.88	2	1
4:A:321:PX4:H59	4:A:354:PX4:H35	0.44	1.90	4	1
4:A:373:PX4:H36	4:A:396:PX4:H30	0.44	1.89	4	1
4:A:361:PX4:H30	4:A:362:PX4:H39	0.44	1.88	12	1
4:A:313:PX4:H31	4:A:360:PX4:H26	0.44	1.88	13	1
4:A:346:PX4:H21	4:A:362:PX4:H51	0.44	1.90	4	1
4:A:346:PX4:H20	4:A:362:PX4:H2	0.44	1.89	7	1
4:A:367:PX4:H68	4:A:428:PX4:H21	0.44	1.88	8	1
4:A:308:PX4:H41	4:A:310:PX4:H41	0.44	1.89	3	1
4:A:331:PX4:H24	4:A:331:PX4:H58	0.44	1.88	5	1
4:A:357:PX4:H35	4:A:358:PX4:H33	0.44	1.89	5	1
4:A:340:PX4:H2	4:A:340:PX4:O6	0.44	2.13	6	1
4:A:421:PX4:H19	4:A:430:PX4:H16	0.44	1.88	6	1
4:A:311:PX4:H10	4:A:320:PX4:H22	0.44	1.89	10	1
4:A:328:PX4:H17	4:A:360:PX4:H39	0.44	1.88	10	1
4:A:419:PX4:H56	4:A:427:PX4:H51	0.44	1.88	13	1
4:A:400:PX4:H22	4:A:408:PX4:H66	0.44	1.89	2	1
4:A:389:PX4:H57	4:A:390:PX4:H35	0.44	1.88	3	1
4:A:367:PX4:H62	4:A:430:PX4:H34	0.44	1.89	6	1
4:A:368:PX4:H52	4:A:369:PX4:H28	0.44	1.90	12	1
4:A:371:PX4:H14	4:A:377:PX4:H4	0.44	1.89	12	1
4:A:398:PX4:H32	4:A:398:PX4:H52	0.44	1.88	12	1
4:A:322:PX4:H70	4:A:421:PX4:H69	0.44	1.90	1	1
4:A:308:PX4:H24	4:A:364:PX4:H52	0.44	1.89	4	1
4:A:373:PX4:H38	4:A:402:PX4:H33	0.44	1.89	6	1
4:A:374:PX4:H27	4:A:427:PX4:H22	0.44	1.90	6	1
4:A:358:PX4:H40	4:A:366:PX4:H70	0.44	1.88	8	1
4:A:395:PX4:H62	4:A:406:PX4:H71	0.44	1.89	8	1
4:A:357:PX4:H23	4:A:358:PX4:H23	0.44	1.89	9	1
4:A:355:PX4:H17	4:A:356:PX4:H49	0.44	1.89	10	1
4:A:336:PX4:H39	4:A:389:PX4:H68	0.44	1.89	12	1
4:A:374:PX4:H27	4:A:428:PX4:H35	0.44	1.90	14	1
4:A:328:PX4:H28	4:A:360:PX4:H40	0.44	1.89	2	1
4:A:366:PX4:H43	4:A:419:PX4:H30	0.44	1.90	2	1
4:A:367:PX4:H19	4:A:368:PX4:H67	0.44	1.88	2	1
4:A:402:PX4:H17	4:A:411:PX4:H22	0.44	1.90	2	1
4:A:366:PX4:H37	4:A:412:PX4:H35	0.44	1.90	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:353:PX4:H57	4:A:354:PX4:H56	0.44	1.89	6	1
4:A:412:PX4:H27	4:A:419:PX4:H47	0.44	1.89	6	1
4:A:332:PX4:H1	4:A:356:PX4:O3	0.44	2.12	10	1
4:A:307:PX4:H52	4:A:314:PX4:H17	0.44	1.90	1	1
4:A:377:PX4:H60	4:A:418:PX4:H66	0.44	1.89	1	1
4:A:321:PX4:H7	4:A:354:PX4:O4	0.44	2.12	2	1
4:A:317:PX4:H26	4:A:325:PX4:H52	0.44	1.90	3	1
4:A:418:PX4:C13	4:A:425:PX4:H24	0.44	2.38	4	1
4:A:341:PX4:H70	4:A:393:PX4:H70	0.44	1.90	5	1
4:A:396:PX4:H62	4:A:398:PX4:H45	0.44	1.88	8	1
4:A:346:PX4:H39	4:A:355:PX4:H59	0.44	1.90	11	1
4:A:402:PX4:H59	4:A:404:PX4:H54	0.44	1.88	11	1
4:A:313:PX4:H6	4:A:359:PX4:O2	0.44	2.13	13	1
4:A:373:PX4:H27	4:A:396:PX4:H22	0.44	1.89	14	1
4:A:316:PX4:H25	4:A:320:PX4:H33	0.44	1.90	1	1
4:A:322:PX4:H19	4:A:323:PX4:H21	0.44	1.89	6	1
4:A:322:PX4:H36	4:A:333:PX4:H36	0.44	1.90	9	1
4:A:410:PX4:H31	4:A:416:PX4:H39	0.44	1.89	12	1
4:A:345:PX4:H46	4:A:348:PX4:H7	0.44	1.89	13	1
4:A:409:PX4:H66	4:A:409:PX4:H60	0.44	1.45	14	1
4:A:338:PX4:H62	4:A:345:PX4:H65	0.43	1.89	2	1
4:A:371:PX4:H10	4:A:377:PX4:O6	0.43	2.13	2	1
4:A:326:PX4:H37	4:A:414:PX4:H38	0.43	1.88	3	1
4:A:324:PX4:H68	4:A:325:PX4:H34	0.43	1.90	5	1
4:A:368:PX4:C27	4:A:424:PX4:H48	0.43	2.43	5	1
4:A:314:PX4:H50	4:A:361:PX4:H26	0.43	1.89	6	1
4:A:331:PX4:H24	4:A:340:PX4:C8	0.43	2.43	7	1
4:A:337:PX4:H27	4:A:357:PX4:H37	0.43	1.88	8	1
4:A:402:PX4:H67	4:A:411:PX4:H44	0.43	1.90	8	1
4:A:355:PX4:H68	4:A:422:PX4:C21	0.43	2.42	9	1
4:A:306:PX4:H69	4:A:354:PX4:H22	0.43	1.90	10	1
4:A:308:PX4:H53	4:A:311:PX4:H14	0.43	1.90	10	1
4:A:399:PX4:H51	4:A:407:PX4:H31	0.43	1.89	10	1
4:A:360:PX4:H62	4:A:366:PX4:H68	0.43	1.89	11	1
4:A:424:PX4:H58	4:A:428:PX4:C31	0.43	2.43	1	1
4:A:317:PX4:H65	4:A:342:PX4:H62	0.43	1.90	2	1
4:A:383:PX4:C18	4:A:407:PX4:H26	0.43	2.42	3	1
4:A:403:PX4:H12	4:A:403:PX4:O6	0.43	2.13	4	1
4:A:337:PX4:H27	4:A:337:PX4:H22	0.43	1.55	5	1
1:A:165:ARG:NH1	4:A:354:PX4:O1	0.43	2.52	6	2
4:A:360:PX4:H57	4:A:366:PX4:H20	0.43	1.90	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H17	4:A:333:PX4:H44	0.43	1.89	10	1
4:A:420:PX4:H22	4:A:427:PX4:H27	0.43	1.90	12	1
4:A:334:PX4:H44	4:A:347:PX4:H65	0.43	1.89	14	1
4:A:308:PX4:H17	4:A:364:PX4:O1	0.43	2.12	1	1
4:A:334:PX4:H21	4:A:356:PX4:H10	0.43	1.89	12	2
4:A:421:PX4:H19	4:A:430:PX4:H21	0.43	1.90	5	1
4:A:316:PX4:H38	4:A:368:PX4:H30	0.43	1.89	8	1
4:A:335:PX4:H35	4:A:337:PX4:H37	0.43	1.91	8	1
4:A:343:PX4:H18	4:A:352:PX4:H57	0.43	1.91	10	1
4:A:370:PX4:H54	4:A:403:PX4:H26	0.43	1.90	10	1
4:A:314:PX4:O8	4:A:364:PX4:H4	0.43	2.13	11	1
4:A:325:PX4:H58	4:A:325:PX4:H26	0.43	1.90	12	1
4:A:385:PX4:H49	4:A:385:PX4:H54	0.43	1.54	12	1
4:A:353:PX4:O6	4:A:357:PX4:H46	0.43	2.13	14	1
4:A:311:PX4:H60	4:A:311:PX4:H27	0.43	1.89	2	1
4:A:308:PX4:H56	4:A:308:PX4:H63	0.43	1.47	4	1
4:A:370:PX4:H61	4:A:411:PX4:H54	0.43	1.90	4	1
4:A:392:PX4:H54	4:A:414:PX4:H47	0.43	1.89	4	1
4:A:315:PX4:H40	4:A:368:PX4:H45	0.43	1.91	6	1
4:A:316:PX4:H65	4:A:333:PX4:H72	0.43	1.90	6	1
4:A:370:PX4:H35	4:A:404:PX4:H27	0.43	1.89	8	1
4:A:405:PX4:H23	4:A:406:PX4:H17	0.43	1.89	8	1
4:A:424:PX4:H61	4:A:424:PX4:H66	0.43	1.54	9	1
4:A:326:PX4:H68	4:A:415:PX4:H42	0.43	1.90	10	1
4:A:331:PX4:H45	4:A:341:PX4:H68	0.43	1.90	10	1
4:A:380:PX4:H53	4:A:387:PX4:H57	0.43	1.91	10	1
4:A:336:PX4:H22	4:A:344:PX4:H55	0.43	1.90	11	1
4:A:400:PX4:H1	4:A:409:PX4:O4	0.43	2.13	11	1
4:A:422:PX4:C8	4:A:425:PX4:H56	0.43	2.33	13	1
4:A:315:PX4:H29	4:A:418:PX4:H42	0.43	1.91	14	1
4:A:314:PX4:H71	4:A:416:PX4:H38	0.43	1.90	1	1
4:A:409:PX4:H59	4:A:415:PX4:H34	0.43	1.91	1	1
4:A:318:PX4:H15	4:A:327:PX4:H15	0.43	1.91	3	1
4:A:348:PX4:H10	4:A:355:PX4:O2	0.43	2.13	4	1
4:A:330:PX4:H45	4:A:347:PX4:H38	0.43	1.90	5	1
4:A:367:PX4:H58	4:A:430:PX4:H26	0.43	1.90	6	1
4:A:428:PX4:H12	4:A:428:PX4:O2	0.43	2.14	6	1
4:A:400:PX4:H13	4:A:401:PX4:O1	0.43	2.13	10	1
4:A:360:PX4:H51	4:A:366:PX4:H18	0.43	1.89	11	1
4:A:361:PX4:H63	4:A:369:PX4:H34	0.43	1.90	11	1
4:A:310:PX4:C22	4:A:351:PX4:H66	0.43	2.43	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:330:PX4:H68	4:A:380:PX4:H44	0.43	1.90	12	1
4:A:356:PX4:H61	4:A:356:PX4:H66	0.43	1.59	12	1
4:A:349:PX4:H71	4:A:356:PX4:H55	0.43	1.88	13	1
4:A:354:PX4:H67	4:A:366:PX4:C27	0.43	2.43	13	1
4:A:338:PX4:O8	4:A:345:PX4:H49	0.43	2.13	2	1
4:A:380:PX4:C26	4:A:381:PX4:H55	0.43	2.44	2	1
4:A:372:PX4:C35	4:A:393:PX4:H41	0.43	2.44	3	1
4:A:378:PX4:H53	4:A:410:PX4:H58	0.43	1.90	3	1
4:A:369:PX4:H30	4:A:429:PX4:H57	0.43	1.91	6	1
4:A:375:PX4:H23	4:A:382:PX4:H24	0.43	1.89	6	1
4:A:410:PX4:H27	4:A:410:PX4:H34	0.43	1.58	14	2
4:A:331:PX4:H51	4:A:332:PX4:H21	0.43	1.89	10	1
4:A:334:PX4:H21	4:A:334:PX4:H53	0.43	1.91	11	1
4:A:351:PX4:H23	4:A:352:PX4:H17	0.43	1.91	12	1
4:A:406:PX4:H49	4:A:421:PX4:H49	0.43	1.91	13	1
4:A:417:PX4:H47	4:A:426:PX4:H52	0.43	1.89	13	1
4:A:326:PX4:H65	4:A:350:PX4:H37	0.43	1.91	1	1
4:A:388:PX4:H66	4:A:388:PX4:H38	0.43	1.91	4	1
4:A:404:PX4:H55	4:A:413:PX4:H25	0.43	1.90	4	1
4:A:330:PX4:H65	4:A:343:PX4:H65	0.43	1.90	6	1
4:A:373:PX4:H25	4:A:397:PX4:H23	0.43	1.90	8	1
4:A:388:PX4:H46	4:A:395:PX4:H47	0.43	1.90	8	1
4:A:392:PX4:H48	4:A:399:PX4:H56	0.43	1.89	8	1
4:A:337:PX4:H31	4:A:352:PX4:H54	0.43	1.89	9	1
4:A:391:PX4:C20	4:A:405:PX4:H69	0.43	2.40	9	1
4:A:321:PX4:H28	4:A:329:PX4:H72	0.43	1.89	10	1
4:A:385:PX4:H50	4:A:392:PX4:H16	0.43	1.90	13	1
4:A:317:PX4:H65	4:A:342:PX4:H60	0.43	1.89	14	1
4:A:375:PX4:H55	4:A:382:PX4:H71	0.43	1.89	14	1
4:A:318:PX4:H56	4:A:318:PX4:H63	0.43	1.60	1	1
4:A:403:PX4:H20	4:A:404:PX4:H22	0.43	1.89	2	1
4:A:370:PX4:H50	4:A:411:PX4:H59	0.43	1.90	7	1
4:A:422:PX4:H52	4:A:425:PX4:H48	0.43	1.90	8	1
4:A:317:PX4:H50	4:A:342:PX4:H47	0.43	1.90	9	1
4:A:327:PX4:H23	4:A:329:PX4:H36	0.43	1.91	9	1
4:A:367:PX4:H66	4:A:412:PX4:H63	0.43	1.91	11	1
4:A:306:PX4:H45	4:A:329:PX4:H55	0.43	1.91	13	1
4:A:369:PX4:O2	4:A:425:PX4:H10	0.43	2.14	1	1
4:A:411:PX4:H62	4:A:411:PX4:H69	0.43	1.47	3	1
4:A:306:PX4:H31	4:A:329:PX4:H60	0.43	1.90	6	1
4:A:310:PX4:H54	4:A:364:PX4:H23	0.43	1.91	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H15	4:A:401:PX4:H20	0.43	1.91	7	1
4:A:322:PX4:H41	4:A:323:PX4:H71	0.43	1.89	8	1
4:A:316:PX4:H23	4:A:418:PX4:H36	0.43	1.91	9	1
4:A:406:PX4:H28	4:A:423:PX4:H58	0.43	1.89	9	1
4:A:370:PX4:H19	4:A:370:PX4:H25	0.43	1.59	11	1
4:A:331:PX4:H49	4:A:336:PX4:H28	0.43	1.91	12	1
4:A:389:PX4:H26	4:A:397:PX4:H31	0.43	1.90	12	1
4:A:378:PX4:C25	4:A:417:PX4:H67	0.43	2.43	13	1
4:A:395:PX4:H41	4:A:406:PX4:H67	0.43	1.91	14	1
4:A:325:PX4:H38	4:A:326:PX4:H30	0.43	1.91	2	1
4:A:381:PX4:H61	4:A:396:PX4:H27	0.43	1.90	3	1
4:A:332:PX4:H62	4:A:414:PX4:H36	0.43	1.90	5	1
4:A:350:PX4:H41	4:A:414:PX4:H39	0.43	1.89	7	1
4:A:346:PX4:H16	4:A:362:PX4:H4	0.43	1.89	8	1
4:A:307:PX4:H56	4:A:349:PX4:H7	0.43	1.90	9	1
4:A:368:PX4:H53	4:A:424:PX4:H48	0.43	1.91	11	1
4:A:395:PX4:H61	4:A:406:PX4:H67	0.43	1.90	11	1
4:A:346:PX4:H52	4:A:362:PX4:H54	0.43	1.91	12	1
4:A:332:PX4:H15	4:A:334:PX4:H19	0.43	1.91	13	1
4:A:315:PX4:H60	4:A:323:PX4:H59	0.43	1.91	14	1
4:A:324:PX4:H42	4:A:372:PX4:H70	0.42	1.91	3	1
4:A:401:PX4:H66	4:A:401:PX4:H61	0.42	1.44	6	1
4:A:423:PX4:H19	4:A:425:PX4:H48	0.42	1.91	7	1
4:A:330:PX4:H39	4:A:344:PX4:H72	0.42	1.91	9	1
4:A:404:PX4:H28	4:A:419:PX4:H48	0.42	1.91	10	1
4:A:405:PX4:H48	4:A:414:PX4:H20	0.42	1.90	11	1
4:A:345:PX4:H31	4:A:357:PX4:H54	0.42	1.90	12	1
4:A:390:PX4:H45	4:A:407:PX4:H27	0.42	1.90	12	1
4:A:345:PX4:H33	4:A:354:PX4:H66	0.42	1.90	1	1
4:A:307:PX4:H22	4:A:361:PX4:H19	0.42	1.91	4	1
4:A:345:PX4:H53	4:A:346:PX4:H51	0.42	1.91	5	1
4:A:394:PX4:H2	4:A:401:PX4:O2	0.42	2.14	6	1
4:A:421:PX4:H23	4:A:430:PX4:H48	0.42	1.91	6	1
4:A:325:PX4:H35	4:A:341:PX4:H72	0.42	1.91	8	1
4:A:404:PX4:H13	4:A:430:PX4:O6	0.42	2.14	9	1
4:A:367:PX4:H50	4:A:419:PX4:H26	0.42	1.91	10	1
4:A:330:PX4:H56	4:A:357:PX4:H64	0.42	1.90	12	1
4:A:400:PX4:C31	4:A:422:PX4:H71	0.42	2.44	12	1
4:A:312:PX4:H31	4:A:366:PX4:H46	0.42	1.89	1	1
4:A:327:PX4:H30	4:A:359:PX4:H25	0.42	1.91	4	1
4:A:332:PX4:H44	4:A:340:PX4:H45	0.42	1.91	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:H44	4:A:367:PX4:C22	0.42	2.45	5	1
4:A:345:PX4:H9	4:A:353:PX4:O2	0.42	2.14	5	1
4:A:382:PX4:H45	4:A:397:PX4:H44	0.42	1.91	5	1
4:A:355:PX4:H30	4:A:356:PX4:H62	0.42	1.91	7	1
4:A:370:PX4:H67	4:A:403:PX4:H38	0.42	1.92	7	1
4:A:368:PX4:C34	4:A:424:PX4:H17	0.42	2.44	8	1
4:A:400:PX4:H44	4:A:400:PX4:H38	0.42	1.77	8	1
4:A:308:PX4:H29	4:A:416:PX4:H33	0.42	1.92	9	1
4:A:395:PX4:H36	4:A:406:PX4:H60	0.42	1.91	9	1
4:A:329:PX4:H64	4:A:329:PX4:H72	0.42	1.41	11	1
4:A:350:PX4:H54	4:A:363:PX4:H50	0.42	1.91	13	1
4:A:400:PX4:H62	4:A:400:PX4:H69	0.42	1.51	13	1
4:A:407:PX4:H27	4:A:407:PX4:H22	0.42	1.63	13	1
4:A:307:PX4:H18	4:A:314:PX4:H49	0.42	1.91	14	1
4:A:314:PX4:H36	4:A:356:PX4:H25	0.42	1.91	14	1
4:A:390:PX4:H59	4:A:390:PX4:H64	0.42	1.59	1	1
4:A:386:PX4:H59	4:A:387:PX4:H72	0.42	1.92	2	1
4:A:392:PX4:H59	4:A:407:PX4:H29	0.42	1.91	2	1
4:A:322:PX4:C18	4:A:424:PX4:H69	0.42	2.44	4	1
4:A:359:PX4:H10	4:A:359:PX4:O8	0.42	2.15	4	1
4:A:389:PX4:H47	4:A:398:PX4:H17	0.42	1.90	5	2
4:A:353:PX4:H70	4:A:424:PX4:H43	0.42	1.92	10	1
4:A:340:PX4:H56	4:A:341:PX4:H20	0.42	1.91	12	1
4:A:417:PX4:H46	4:A:426:PX4:H58	0.42	1.91	12	1
4:A:355:PX4:H5	4:A:362:PX4:O8	0.42	2.14	13	1
4:A:386:PX4:H48	4:A:387:PX4:H48	0.42	1.92	13	1
4:A:410:PX4:H23	4:A:410:PX4:H30	0.42	1.48	3	1
4:A:422:PX4:H22	4:A:425:PX4:H66	0.42	1.92	4	1
4:A:330:PX4:H46	4:A:337:PX4:H17	0.42	1.90	5	2
4:A:357:PX4:H39	4:A:358:PX4:H37	0.42	1.90	5	1
4:A:370:PX4:H32	4:A:404:PX4:H27	0.42	1.90	5	1
4:A:317:PX4:H29	4:A:317:PX4:H36	0.42	1.50	8	1
1:A:163:PHE:HZ	1:A:212:LEU:HD11	0.42	1.74	9	1
4:A:336:PX4:H25	4:A:344:PX4:H60	0.42	1.90	9	1
4:A:391:PX4:H26	4:A:414:PX4:H17	0.42	1.90	10	1
4:A:376:PX4:H14	4:A:377:PX4:O2	0.42	2.15	11	1
4:A:320:PX4:H43	4:A:376:PX4:H31	0.42	1.90	13	1
4:A:330:PX4:H16	4:A:343:PX4:H5	0.42	1.90	14	1
4:A:353:PX4:H36	4:A:413:PX4:H43	0.42	1.89	14	1
4:A:330:PX4:H51	4:A:337:PX4:H53	0.42	1.91	3	1
4:A:422:PX4:H20	4:A:422:PX4:H26	0.42	1.69	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H64	4:A:429:PX4:H59	0.42	1.92	3	1
4:A:335:PX4:H42	4:A:344:PX4:H37	0.42	1.92	5	1
4:A:328:PX4:H19	4:A:360:PX4:H21	0.42	1.92	10	1
4:A:306:PX4:H58	4:A:306:PX4:H65	0.42	1.65	11	1
4:A:332:PX4:H49	4:A:334:PX4:H32	0.42	1.92	11	1
4:A:334:PX4:H70	4:A:349:PX4:H61	0.42	1.92	1	1
4:A:388:PX4:H50	4:A:397:PX4:H58	0.42	1.91	1	1
4:A:384:PX4:H23	4:A:385:PX4:H24	0.42	1.91	3	1
1:A:116:TYR:CD2	1:A:138:PHE:CE2	0.42	3.07	4	1
4:A:322:PX4:H36	4:A:323:PX4:H57	0.42	1.91	4	1
4:A:315:PX4:H44	4:A:315:PX4:H64	0.42	1.91	8	1
4:A:346:PX4:H22	4:A:354:PX4:H20	0.42	1.91	8	1
4:A:322:PX4:H17	4:A:333:PX4:C22	0.42	2.44	10	1
1:A:165:ARG:NH1	4:A:354:PX4:H10	0.42	2.30	12	1
4:A:314:PX4:H63	4:A:314:PX4:H56	0.42	1.62	1	1
4:A:388:PX4:H56	4:A:402:PX4:H57	0.42	1.91	1	1
4:A:424:PX4:H54	4:A:428:PX4:H61	0.42	1.92	1	1
4:A:319:PX4:H37	4:A:319:PX4:H31	0.42	1.73	2	1
4:A:391:PX4:H63	4:A:391:PX4:H56	0.42	1.60	2	1
4:A:315:PX4:H29	4:A:425:PX4:H44	0.42	1.92	3	1
4:A:309:PX4:H54	4:A:316:PX4:H57	0.42	1.92	4	1
4:A:370:PX4:H36	4:A:404:PX4:H37	0.42	1.91	4	1
4:A:340:PX4:H49	4:A:340:PX4:H54	0.42	1.70	5	1
4:A:346:PX4:H6	4:A:360:PX4:O8	0.42	2.15	7	1
4:A:349:PX4:H32	4:A:349:PX4:H37	0.42	1.60	8	1
4:A:395:PX4:H58	4:A:406:PX4:H66	0.42	1.90	8	1
4:A:320:PX4:H37	4:A:378:PX4:H39	0.42	1.91	9	1
4:A:332:PX4:H63	4:A:415:PX4:H63	0.42	1.91	9	1
4:A:395:PX4:H19	4:A:405:PX4:H16	0.42	1.92	9	1
4:A:331:PX4:C21	4:A:332:PX4:H42	0.42	2.45	11	1
4:A:368:PX4:H10	4:A:418:PX4:O1	0.42	2.15	12	1
4:A:312:PX4:H65	4:A:312:PX4:H58	0.42	1.68	13	1
4:A:396:PX4:H47	4:A:405:PX4:H47	0.42	1.91	2	1
4:A:417:PX4:H34	4:A:426:PX4:H65	0.42	1.92	2	1
4:A:404:PX4:H12	4:A:419:PX4:O1	0.42	2.15	3	1
4:A:355:PX4:O8	4:A:355:PX4:H3	0.42	2.14	5	1
4:A:400:PX4:H28	4:A:400:PX4:H63	0.42	1.92	5	1
4:A:328:PX4:H7	4:A:354:PX4:O8	0.42	2.15	6	1
4:A:429:PX4:H51	4:A:429:PX4:H56	0.42	1.63	6	1
4:A:363:PX4:H19	4:A:364:PX4:H36	0.42	1.90	7	1
4:A:408:PX4:H65	4:A:409:PX4:H28	0.42	1.91	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:415:PX4:H24	4:A:425:PX4:H66	0.42	1.91	11	1
4:A:329:PX4:H53	4:A:329:PX4:H59	0.42	1.62	12	1
4:A:333:PX4:H27	4:A:333:PX4:H21	0.42	1.45	14	1
4:A:380:PX4:H8	4:A:402:PX4:O6	0.42	2.15	14	1
4:A:315:PX4:H40	4:A:361:PX4:C3	0.42	2.44	1	1
4:A:306:PX4:H38	4:A:328:PX4:H37	0.42	1.92	3	1
4:A:346:PX4:O8	4:A:362:PX4:H9	0.42	2.14	3	1
4:A:321:PX4:H68	4:A:425:PX4:H37	0.42	1.90	4	1
4:A:394:PX4:H55	4:A:394:PX4:H49	0.42	1.73	4	1
4:A:420:PX4:H17	4:A:427:PX4:H22	0.42	1.90	4	1
4:A:306:PX4:H18	4:A:322:PX4:H50	0.42	1.92	5	1
4:A:321:PX4:H48	4:A:354:PX4:H30	0.42	1.91	5	1
4:A:355:PX4:H11	4:A:362:PX4:O8	0.42	2.15	7	1
4:A:374:PX4:H25	4:A:412:PX4:H56	0.42	1.91	7	1
4:A:417:PX4:H25	4:A:417:PX4:H20	0.42	1.48	9	1
4:A:333:PX4:H59	4:A:333:PX4:H52	0.42	1.57	11	1
4:A:421:PX4:H24	4:A:430:PX4:H21	0.42	1.91	11	1
4:A:307:PX4:H38	4:A:364:PX4:H58	0.42	1.91	12	1
4:A:416:PX4:H12	4:A:426:PX4:O2	0.42	2.15	12	1
4:A:307:PX4:H60	4:A:349:PX4:H5	0.41	1.92	1	1
4:A:337:PX4:H59	4:A:338:PX4:H58	0.41	1.92	1	1
4:A:370:PX4:H64	4:A:370:PX4:H59	0.41	1.59	3	1
4:A:345:PX4:H35	4:A:353:PX4:H32	0.41	1.92	4	1
4:A:425:PX4:H32	4:A:425:PX4:H38	0.41	1.56	4	1
4:A:307:PX4:H70	4:A:350:PX4:H58	0.41	1.91	6	1
4:A:354:PX4:H36	4:A:355:PX4:H72	0.41	1.92	6	1
4:A:380:PX4:H23	4:A:381:PX4:H21	0.41	1.92	6	1
4:A:347:PX4:H24	4:A:348:PX4:H51	0.41	1.92	7	1
4:A:339:PX4:H20	4:A:347:PX4:H48	0.41	1.90	9	1
4:A:421:PX4:O6	4:A:423:PX4:H46	0.41	2.15	9	1
4:A:313:PX4:H53	4:A:359:PX4:C12	0.41	2.42	10	1
4:A:313:PX4:H57	4:A:359:PX4:H26	0.41	1.92	10	1
4:A:335:PX4:H26	4:A:335:PX4:H19	0.41	1.54	10	1
4:A:319:PX4:H23	4:A:320:PX4:H43	0.41	1.91	12	1
4:A:320:PX4:H70	4:A:371:PX4:H67	0.41	1.92	12	1
4:A:331:PX4:H37	4:A:331:PX4:H31	0.41	1.55	12	1
4:A:391:PX4:H57	4:A:391:PX4:H62	0.41	1.65	12	1
4:A:326:PX4:H35	4:A:340:PX4:H38	0.41	1.91	13	1
1:A:191:ILE:O	4:A:314:PX4:H7	0.41	2.16	14	1
4:A:308:PX4:H52	4:A:308:PX4:H59	0.41	1.72	4	1
4:A:388:PX4:H33	4:A:406:PX4:H64	0.41	1.93	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:312:PX4:H48	4:A:312:PX4:H55	0.41	1.65	6	1
4:A:314:PX4:H42	4:A:355:PX4:H11	0.41	1.91	7	1
4:A:322:PX4:H11	4:A:361:PX4:O8	0.41	2.15	7	1
4:A:330:PX4:H55	4:A:337:PX4:H52	0.41	1.91	7	1
4:A:325:PX4:H32	4:A:341:PX4:H67	0.41	1.91	8	1
4:A:426:PX4:H39	4:A:426:PX4:H34	0.41	1.75	10	1
4:A:347:PX4:C29	4:A:355:PX4:H25	0.41	2.24	11	1
4:A:379:PX4:H33	4:A:379:PX4:H28	0.41	1.60	11	1
4:A:307:PX4:H51	4:A:356:PX4:H37	0.41	1.92	12	1
4:A:319:PX4:H55	4:A:319:PX4:H22	0.41	1.92	13	1
4:A:366:PX4:H53	4:A:366:PX4:H47	0.41	1.69	14	1
4:A:402:PX4:H48	4:A:411:PX4:H25	0.41	1.92	14	1
1:A:191:ILE:O	4:A:314:PX4:H3	0.41	2.15	1	1
4:A:367:PX4:H52	4:A:430:PX4:H50	0.41	1.90	2	1
4:A:369:PX4:H27	4:A:369:PX4:H21	0.41	1.70	2	1
4:A:330:PX4:H22	4:A:343:PX4:H8	0.41	1.91	3	1
4:A:336:PX4:H39	4:A:428:PX4:H42	0.41	1.92	3	1
4:A:388:PX4:H36	4:A:406:PX4:H60	0.41	1.91	3	1
4:A:400:PX4:H64	4:A:417:PX4:H29	0.41	1.90	4	1
4:A:405:PX4:H33	4:A:415:PX4:H64	0.41	1.91	4	1
4:A:401:PX4:H63	4:A:401:PX4:H56	0.41	1.53	5	1
4:A:360:PX4:H47	4:A:366:PX4:H18	0.41	1.93	6	1
4:A:387:PX4:H55	4:A:411:PX4:H50	0.41	1.92	7	1
4:A:409:PX4:H59	4:A:409:PX4:H52	0.41	1.60	7	1
4:A:314:PX4:H43	4:A:349:PX4:H47	0.41	1.92	8	1
4:A:367:PX4:H46	4:A:367:PX4:H53	0.41	1.55	8	1
4:A:389:PX4:H52	4:A:398:PX4:H65	0.41	1.91	9	1
4:A:405:PX4:H30	4:A:422:PX4:H33	0.41	1.93	10	1
4:A:405:PX4:H52	4:A:405:PX4:H59	0.41	1.69	11	1
4:A:388:PX4:H55	4:A:402:PX4:H28	0.41	1.91	12	1
4:A:392:PX4:H54	4:A:407:PX4:H21	0.41	1.91	12	1
4:A:404:PX4:H23	4:A:419:PX4:H46	0.41	1.90	12	1
4:A:307:PX4:H20	4:A:307:PX4:H25	0.41	1.66	13	1
4:A:329:PX4:H45	4:A:359:PX4:H23	0.41	1.92	1	1
4:A:349:PX4:H71	4:A:355:PX4:H71	0.41	1.91	1	1
4:A:346:PX4:H33	4:A:362:PX4:H25	0.41	1.92	2	1
4:A:368:PX4:H17	4:A:390:PX4:H48	0.41	1.92	2	1
4:A:311:PX4:H26	4:A:311:PX4:H56	0.41	1.91	6	1
4:A:309:PX4:O1	4:A:319:PX4:H18	0.41	2.15	7	1
4:A:395:PX4:H21	4:A:406:PX4:C26	0.41	2.43	10	1
4:A:417:PX4:H47	4:A:417:PX4:H52	0.41	1.67	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:368:PX4:H3	4:A:369:PX4:O3	0.41	2.14	11	1
4:A:398:PX4:H27	4:A:398:PX4:H52	0.41	1.92	11	1
4:A:408:PX4:H24	4:A:415:PX4:H17	0.41	1.92	12	1
4:A:410:PX4:H54	4:A:426:PX4:H51	0.41	1.91	12	1
4:A:318:PX4:H71	4:A:318:PX4:H65	0.41	1.56	14	1
4:A:428:PX4:H49	4:A:429:PX4:H21	0.41	1.92	1	1
4:A:306:PX4:O8	4:A:322:PX4:H9	0.41	2.15	2	1
4:A:322:PX4:H19	4:A:333:PX4:H37	0.41	1.91	2	1
4:A:368:PX4:H50	4:A:369:PX4:H30	0.41	1.92	2	1
4:A:391:PX4:H47	4:A:391:PX4:H53	0.41	1.60	2	1
4:A:339:PX4:H65	4:A:339:PX4:H58	0.41	1.68	3	1
4:A:346:PX4:H26	4:A:354:PX4:H25	0.41	1.90	4	1
4:A:384:PX4:H22	4:A:385:PX4:H24	0.41	1.92	8	1
4:A:307:PX4:H41	4:A:425:PX4:H30	0.41	1.91	9	1
4:A:336:PX4:H35	4:A:336:PX4:H30	0.41	1.62	11	1
4:A:390:PX4:H25	4:A:390:PX4:H19	0.41	1.64	12	1
4:A:319:PX4:H46	4:A:333:PX4:H54	0.41	1.92	13	1
4:A:334:PX4:H26	4:A:334:PX4:H59	0.41	1.91	13	1
4:A:356:PX4:H31	4:A:356:PX4:H25	0.41	1.78	13	1
4:A:312:PX4:O1	4:A:366:PX4:H18	0.41	2.16	1	1
4:A:353:PX4:H50	4:A:353:PX4:H57	0.41	1.62	1	1
4:A:325:PX4:H55	4:A:325:PX4:H49	0.41	1.66	2	1
4:A:351:PX4:H19	4:A:351:PX4:H26	0.41	1.66	4	1
4:A:353:PX4:H27	4:A:365:PX4:H51	0.41	1.92	4	1
4:A:385:PX4:H8	4:A:393:PX4:O1	0.41	2.16	5	1
4:A:365:PX4:H16	4:A:366:PX4:H5	0.41	1.93	8	2
4:A:371:PX4:H25	4:A:377:PX4:C11	0.41	2.45	8	1
4:A:325:PX4:H62	4:A:325:PX4:H33	0.41	1.91	10	1
4:A:307:PX4:H18	4:A:314:PX4:O8	0.41	2.15	12	1
4:A:406:PX4:H61	4:A:421:PX4:H71	0.41	1.93	12	1
4:A:315:PX4:H59	4:A:368:PX4:H44	0.41	1.93	13	1
4:A:373:PX4:O6	4:A:397:PX4:H1	0.41	2.16	14	1
4:A:322:PX4:H16	4:A:323:PX4:H49	0.41	1.91	1	1
4:A:408:PX4:H37	4:A:425:PX4:H62	0.41	1.93	1	1
4:A:321:PX4:O1	4:A:328:PX4:H10	0.41	2.15	2	1
4:A:321:PX4:H61	4:A:361:PX4:H30	0.41	1.91	2	1
4:A:336:PX4:C36	4:A:344:PX4:H35	0.41	2.46	5	1
4:A:321:PX4:H62	4:A:425:PX4:H43	0.41	1.92	6	1
4:A:360:PX4:H17	4:A:366:PX4:O6	0.41	2.16	6	1
4:A:388:PX4:H14	4:A:395:PX4:O1	0.41	2.15	6	1
4:A:360:PX4:H68	4:A:413:PX4:H35	0.41	1.91	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:421:PX4:H30	4:A:421:PX4:H35	0.41	1.67	11	1
4:A:310:PX4:H70	4:A:364:PX4:H52	0.41	1.92	12	1
4:A:405:PX4:H17	4:A:414:PX4:H24	0.41	1.93	12	1
4:A:406:PX4:H33	4:A:425:PX4:H63	0.41	1.92	12	1
4:A:314:PX4:H55	4:A:364:PX4:H46	0.41	1.92	13	1
4:A:330:PX4:H36	4:A:347:PX4:H37	0.41	1.92	13	1
4:A:331:PX4:H15	4:A:332:PX4:O6	0.41	2.15	14	1
4:A:379:PX4:H53	4:A:379:PX4:H46	0.41	1.60	14	1
4:A:343:PX4:H44	4:A:343:PX4:H38	0.41	1.73	1	1
4:A:317:PX4:H56	4:A:324:PX4:H40	0.41	1.93	2	1
4:A:383:PX4:H49	4:A:392:PX4:H26	0.41	1.93	2	1
4:A:339:PX4:H21	4:A:348:PX4:H50	0.41	1.91	3	1
4:A:379:PX4:H68	4:A:379:PX4:H41	0.41	1.91	3	1
4:A:430:PX4:H52	4:A:430:PX4:H47	0.41	1.63	3	1
4:A:316:PX4:H69	4:A:368:PX4:H30	0.41	1.91	4	1
4:A:334:PX4:H52	4:A:349:PX4:H21	0.41	1.93	4	1
4:A:376:PX4:H39	4:A:377:PX4:H61	0.41	1.93	4	1
4:A:400:PX4:H50	4:A:416:PX4:H34	0.41	1.91	4	1
4:A:325:PX4:O6	4:A:334:PX4:H7	0.41	2.16	5	1
4:A:347:PX4:H58	4:A:355:PX4:H23	0.41	1.91	6	1
4:A:353:PX4:H50	4:A:353:PX4:H56	0.41	1.67	8	1
4:A:348:PX4:H42	4:A:388:PX4:H69	0.41	1.93	9	1
4:A:390:PX4:H38	4:A:390:PX4:H44	0.41	1.48	10	1
4:A:325:PX4:H43	4:A:393:PX4:H63	0.41	1.92	11	1
4:A:332:PX4:H4	4:A:356:PX4:O1	0.41	2.16	11	1
4:A:343:PX4:C24	4:A:352:PX4:H56	0.41	2.45	11	1
4:A:354:PX4:H39	4:A:423:PX4:H41	0.41	1.92	11	1
4:A:374:PX4:H33	4:A:428:PX4:H44	0.41	1.93	12	1
4:A:384:PX4:H19	4:A:386:PX4:O6	0.41	2.16	12	1
4:A:359:PX4:H54	4:A:359:PX4:H48	0.41	1.49	13	1
4:A:330:PX4:H58	4:A:357:PX4:H61	0.41	1.93	1	1
4:A:416:PX4:H18	4:A:425:PX4:H15	0.41	1.93	1	1
4:A:317:PX4:H16	4:A:342:PX4:O6	0.41	2.16	2	1
4:A:392:PX4:H47	4:A:392:PX4:H52	0.41	1.69	3	1
4:A:392:PX4:H15	4:A:392:PX4:H12	0.41	1.92	3	1
4:A:313:PX4:H47	4:A:327:PX4:H25	0.41	1.93	5	1
4:A:335:PX4:H46	4:A:343:PX4:H23	0.41	1.91	5	1
4:A:310:PX4:H37	4:A:364:PX4:H36	0.41	1.92	6	1
4:A:397:PX4:H60	4:A:406:PX4:H71	0.41	1.92	6	1
4:A:411:PX4:H31	4:A:411:PX4:H26	0.41	1.67	6	1
4:A:306:PX4:H19	4:A:360:PX4:H42	0.41	1.93	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:312:PX4:O2	4:A:312:PX4:H9	0.41	2.16	7	1
4:A:316:PX4:H69	4:A:377:PX4:H38	0.41	1.92	8	1
4:A:369:PX4:O1	4:A:425:PX4:H2	0.41	2.16	8	1
4:A:413:PX4:H71	4:A:424:PX4:H33	0.41	1.92	8	1
4:A:421:PX4:H20	4:A:430:PX4:H16	0.41	1.92	8	1
4:A:329:PX4:H62	4:A:428:PX4:H62	0.41	1.93	9	1
4:A:388:PX4:H64	4:A:402:PX4:H36	0.41	1.93	9	1
4:A:317:PX4:O8	4:A:342:PX4:H4	0.41	2.16	10	1
4:A:378:PX4:H63	4:A:378:PX4:H56	0.41	1.50	10	1
4:A:315:PX4:O7	4:A:316:PX4:H16	0.41	2.15	11	1
4:A:337:PX4:H69	4:A:395:PX4:H67	0.41	1.90	11	1
4:A:372:PX4:H36	4:A:372:PX4:H41	0.41	1.73	11	1
4:A:383:PX4:H17	4:A:392:PX4:H22	0.41	1.92	12	1
4:A:416:PX4:H21	4:A:425:PX4:O7	0.41	2.16	12	1
4:A:361:PX4:H30	4:A:364:PX4:H72	0.41	1.92	13	1
4:A:373:PX4:H38	4:A:373:PX4:H44	0.41	1.55	13	1
4:A:390:PX4:H5	4:A:407:PX4:O1	0.41	2.16	13	1
4:A:374:PX4:H28	4:A:427:PX4:H25	0.41	1.92	14	1
4:A:393:PX4:H55	4:A:399:PX4:H63	0.41	1.93	3	1
4:A:428:PX4:H51	4:A:429:PX4:H22	0.41	1.92	3	1
4:A:360:PX4:H49	4:A:360:PX4:H22	0.41	1.93	5	1
4:A:316:PX4:H72	4:A:316:PX4:C19	0.41	2.43	6	1
4:A:350:PX4:H63	4:A:363:PX4:H58	0.41	1.92	6	1
4:A:416:PX4:H27	4:A:426:PX4:H21	0.41	1.91	6	1
4:A:392:PX4:H60	4:A:393:PX4:H63	0.41	1.92	7	1
4:A:314:PX4:H67	4:A:314:PX4:H60	0.41	1.70	8	1
4:A:395:PX4:C19	4:A:415:PX4:H62	0.41	2.45	9	1
4:A:326:PX4:H55	4:A:363:PX4:H48	0.41	1.91	10	1
4:A:410:PX4:H58	4:A:426:PX4:H51	0.41	1.91	11	1
1:A:153:ASN:O	4:A:331:PX4:H12	0.41	2.16	14	1
4:A:306:PX4:H22	4:A:322:PX4:H57	0.41	1.90	14	1
4:A:384:PX4:H34	4:A:384:PX4:H40	0.41	1.72	14	1
4:A:416:PX4:H17	4:A:426:PX4:H25	0.41	1.91	14	1
4:A:396:PX4:H67	4:A:398:PX4:H65	0.40	1.93	1	1
4:A:348:PX4:H42	4:A:398:PX4:H45	0.40	1.91	3	1
4:A:393:PX4:H3	4:A:394:PX4:P1	0.40	2.56	4	1
4:A:428:PX4:H54	4:A:429:PX4:H48	0.40	1.93	4	1
4:A:330:PX4:O8	4:A:337:PX4:H10	0.40	2.16	5	1
4:A:322:PX4:H60	4:A:361:PX4:H52	0.40	1.92	7	1
4:A:334:PX4:H58	4:A:349:PX4:H48	0.40	1.92	7	1
4:A:337:PX4:H4	4:A:337:PX4:O6	0.40	2.16	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:330:PX4:H26	4:A:330:PX4:H31	0.40	1.59	8	1
4:A:333:PX4:H60	4:A:340:PX4:H60	0.40	1.92	8	1
4:A:306:PX4:H22	4:A:329:PX4:H63	0.40	1.92	10	1
4:A:349:PX4:H24	4:A:350:PX4:H52	0.40	1.93	10	1
4:A:385:PX4:H54	4:A:385:PX4:H48	0.40	1.59	11	1
4:A:423:PX4:H52	4:A:423:PX4:H47	0.40	1.69	11	1
4:A:355:PX4:H9	4:A:356:PX4:O6	0.40	2.16	12	1
4:A:378:PX4:H52	4:A:378:PX4:H47	0.40	1.76	12	1
4:A:325:PX4:H61	4:A:341:PX4:H29	0.40	1.93	13	1
4:A:389:PX4:O6	4:A:397:PX4:H8	0.40	2.16	13	1
4:A:367:PX4:H17	4:A:430:PX4:H50	0.40	1.91	14	1
4:A:389:PX4:H56	4:A:389:PX4:H51	0.40	1.63	14	1
4:A:325:PX4:H23	4:A:325:PX4:H30	0.40	1.29	2	1
4:A:315:PX4:H27	4:A:315:PX4:H21	0.40	1.73	3	1
4:A:399:PX4:H14	4:A:399:PX4:H6	0.40	1.94	3	1
4:A:321:PX4:H60	4:A:321:PX4:H67	0.40	1.45	6	1
4:A:392:PX4:H30	4:A:392:PX4:H35	0.40	1.73	6	1
4:A:327:PX4:H55	4:A:327:PX4:H48	0.40	1.54	9	1
4:A:328:PX4:H68	4:A:328:PX4:H62	0.40	1.73	9	1
4:A:345:PX4:H23	4:A:345:PX4:H30	0.40	1.74	11	1
4:A:313:PX4:H27	4:A:360:PX4:H21	0.40	1.93	12	1
1:A:125:MET:HE3	1:A:205:THR:HG23	0.40	1.92	13	1
4:A:307:PX4:H37	4:A:361:PX4:H55	0.40	1.92	13	1
4:A:317:PX4:H17	4:A:324:PX4:H52	0.40	1.93	14	1
4:A:379:PX4:H12	4:A:385:PX4:O1	0.40	2.16	14	1
4:A:395:PX4:H22	4:A:395:PX4:H27	0.40	1.68	14	1
4:A:307:PX4:H41	4:A:315:PX4:H28	0.40	1.93	1	1
4:A:322:PX4:H72	4:A:413:PX4:H63	0.40	1.92	2	1
4:A:331:PX4:H3	4:A:347:PX4:H46	0.40	1.93	2	1
4:A:370:PX4:H66	4:A:411:PX4:H31	0.40	1.93	4	1
4:A:375:PX4:H47	4:A:389:PX4:H21	0.40	1.93	4	1
4:A:422:PX4:H40	4:A:423:PX4:H69	0.40	1.93	5	1
4:A:346:PX4:H67	4:A:362:PX4:H68	0.40	1.92	6	1
1:A:160:LEU:CD2	4:A:356:PX4:H23	0.40	2.47	8	1
4:A:340:PX4:H20	4:A:341:PX4:H55	0.40	1.92	10	1
1:A:123:PRO:HB3	4:A:345:PX4:H4	0.40	1.93	13	1
4:A:346:PX4:H46	4:A:355:PX4:C4	0.40	2.46	13	1
4:A:369:PX4:O2	4:A:425:PX4:H2	0.40	2.16	13	1
4:A:359:PX4:H29	4:A:359:PX4:H24	0.40	1.64	14	1
4:A:345:PX4:H46	4:A:348:PX4:H6	0.40	1.94	1	1
4:A:349:PX4:H32	4:A:350:PX4:H35	0.40	1.92	2	1

Continued on next page...

Continued from previous page...

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

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	151±2 (93±1%)	10±2 (6±1%)	2±1 (1±1%)	15	65
All	All	2268/2296 (99%)	2109 (93%)	136 (6%)	23 (1%)	15	65

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	173	ALA	11
1	A	179	GLY	4
1	A	172	HIS	2
1	A	170	ASP	2
1	A	109	TRP	1
1	A	107	PRO	1
1	A	171	PHE	1
1	A	110	ARG	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/131 (99%)	123±1 (95±1%)	7±1 (5±1%)	22	72
All	All	1820/1834 (99%)	1723 (95%)	97 (5%)	22	72

All 36 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	165	ARG	14
1	A	172	HIS	11
1	A	199	GLU	11
1	A	170	ASP	11
1	A	253	ASP	5
1	A	244	ASP	4
1	A	191	ILE	3
1	A	129	ASP	2
1	A	159	ILE	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	102	GLU	2
1	A	201	GLU	2
1	A	115	THR	2
1	A	136	LYS	2
1	A	260	SER	2
1	A	110	ARG	2
1	A	101	ARG	2
1	A	239	THR	1
1	A	189	SER	1
1	A	230	SER	1
1	A	108	VAL	1
1	A	261	LEU	1
1	A	131	ASP	1
1	A	222	HIS	1
1	A	224	LEU	1
1	A	251	SER	1
1	A	223	SER	1
1	A	140	VAL	1
1	A	162	VAL	1
1	A	114	ILE	1
1	A	109	TRP	1
1	A	236	MET	1
1	A	124	ASP	1
1	A	144	VAL	1
1	A	200	ASP	1
1	A	258	ILE	1
1	A	243	VAL	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	326	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	410	-	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	387	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	363	-	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	362	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	405	-	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	372	-	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	367	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	388	-	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	421	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	403	-	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	320	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	384	-	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	323	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	424	-	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	329	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.65±0.03	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	390	-	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	306	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	427	-	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	349	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	411	-	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	404	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	413	-	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	354	-	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	430	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	332	-	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	376	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	336	-	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	333	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.66±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	385	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	374	-	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	381	-	45,45,45	0.65±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	326	-	51,53,53	1.47±0.15	8±2 (16±3%)
4	PX4	A	416	-	51,53,53	1.56±0.15	10±2 (19±4%)
4	PX4	A	410	-	51,53,53	1.46±0.16	9±2 (17±4%)
4	PX4	A	334	-	51,53,53	1.46±0.13	9±2 (16±3%)
4	PX4	A	387	-	51,53,53	1.46±0.19	8±3 (16±5%)
4	PX4	A	347	-	51,53,53	1.51±0.19	9±3 (18±5%)
4	PX4	A	316	-	51,53,53	1.39±0.12	8±2 (14±3%)
4	PX4	A	339	-	51,53,53	1.55±0.15	10±3 (19±5%)
4	PX4	A	422	-	51,53,53	1.49±0.16	9±3 (17±5%)
4	PX4	A	423	-	51,53,53	1.51±0.11	8±2 (16±3%)
4	PX4	A	408	-	51,53,53	1.55±0.16	10±3 (19±6%)
4	PX4	A	419	-	51,53,53	1.45±0.10	8±2 (16±4%)
4	PX4	A	319	-	51,53,53	1.42±0.10	8±2 (14±3%)
4	PX4	A	412	-	51,53,53	1.54±0.18	10±3 (19±5%)
4	PX4	A	361	-	51,53,53	1.60±0.14	10±2 (20±4%)
4	PX4	A	379	-	51,53,53	1.64±0.17	10±3 (19±5%)
4	PX4	A	342	-	51,53,53	1.48±0.15	9±2 (17±3%)
4	PX4	A	420	-	51,53,53	1.54±0.16	10±3 (20±5%)
4	PX4	A	395	-	51,53,53	1.45±0.11	8±2 (16±3%)
4	PX4	A	380	-	51,53,53	1.52±0.16	10±2 (19±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	359	-	51,53,53	1.49±0.12	9±2 (17±3%)
4	PX4	A	321	-	51,53,53	1.57±0.14	9±2 (18±3%)
4	PX4	A	337	-	51,53,53	1.45±0.13	8±2 (14±4%)
4	PX4	A	389	-	51,53,53	1.51±0.09	9±2 (16±4%)
4	PX4	A	401	-	51,53,53	1.44±0.16	8±2 (16±4%)
4	PX4	A	363	-	51,53,53	1.57±0.08	10±2 (20±3%)
4	PX4	A	307	-	51,53,53	1.46±0.19	8±3 (16±6%)
4	PX4	A	362	-	51,53,53	1.46±0.12	8±2 (16±4%)
4	PX4	A	358	-	51,53,53	1.37±0.10	7±2 (14±4%)
4	PX4	A	405	-	51,53,53	1.40±0.14	8±2 (14±3%)
4	PX4	A	371	-	51,53,53	1.50±0.15	9±3 (17±5%)
4	PX4	A	372	-	51,53,53	1.44±0.20	8±4 (16±6%)
4	PX4	A	367	-	51,53,53	1.48±0.10	8±2 (16±3%)
4	PX4	A	392	-	51,53,53	1.47±0.10	9±2 (17±3%)
4	PX4	A	426	-	51,53,53	1.49±0.14	10±2 (18±4%)
4	PX4	A	388	-	51,53,53	1.54±0.11	10±2 (20±4%)
4	PX4	A	428	-	51,53,53	1.51±0.13	9±2 (17±4%)
4	PX4	A	421	-	51,53,53	1.52±0.16	9±3 (18±5%)
4	PX4	A	311	-	51,53,53	1.52±0.15	10±2 (19±4%)
4	PX4	A	330	-	51,53,53	1.43±0.16	8±3 (15±5%)
4	PX4	A	312	-	51,53,53	1.51±0.12	8±1 (16±2%)
4	PX4	A	338	-	51,53,53	1.47±0.11	8±2 (16±4%)
4	PX4	A	322	-	51,53,53	1.48±0.10	9±2 (18±3%)
4	PX4	A	365	-	51,53,53	1.43±0.09	8±2 (14±4%)
4	PX4	A	403	-	51,53,53	1.52±0.16	9±2 (18±4%)
4	PX4	A	383	-	51,53,53	1.43±0.12	8±2 (16±3%)
4	PX4	A	320	-	51,53,53	1.52±0.12	10±2 (18±4%)
4	PX4	A	429	-	51,53,53	1.47±0.15	9±2 (16±4%)
4	PX4	A	384	-	51,53,53	1.45±0.13	8±2 (16±4%)
4	PX4	A	317	-	51,53,53	1.46±0.11	8±1 (16±2%)
4	PX4	A	323	-	51,53,53	1.49±0.14	9±2 (18±4%)
4	PX4	A	318	-	51,53,53	1.45±0.14	8±2 (16±3%)
4	PX4	A	409	-	51,53,53	1.46±0.17	8±2 (16±4%)
4	PX4	A	309	-	51,53,53	1.53±0.14	10±3 (18±5%)
4	PX4	A	364	-	51,53,53	1.48±0.13	8±3 (16±5%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	324	-	51,53,53	1.42±0.12	7±2 (14±4%)
4	PX4	A	327	-	51,53,53	1.48±0.14	9±3 (17±5%)
4	PX4	A	355	-	51,53,53	1.48±0.17	9±2 (16±4%)
4	PX4	A	308	-	51,53,53	1.54±0.11	10±2 (18±3%)
4	PX4	A	344	-	51,53,53	1.55±0.10	9±2 (16±4%)
4	PX4	A	424	-	51,53,53	1.47±0.16	8±2 (15±3%)
4	PX4	A	418	-	51,53,53	1.49±0.12	8±1 (15±2%)
4	PX4	A	329	-	51,53,53	1.48±0.15	9±3 (17±5%)
4	PX4	A	341	-	51,53,53	1.46±0.12	7±3 (14±5%)
4	PX4	A	398	-	51,53,53	1.55±0.16	10±3 (18±5%)
4	PX4	A	400	-	51,53,53	1.47±0.16	9±2 (17±4%)
4	PX4	A	351	-	51,53,53	1.45±0.12	8±2 (16±3%)
4	PX4	A	399	-	51,53,53	1.48±0.09	9±2 (17±4%)
4	PX4	A	393	-	51,53,53	1.44±0.13	8±2 (15±4%)
4	PX4	A	386	-	51,53,53	1.52±0.14	9±2 (17±3%)
4	PX4	A	314	-	51,53,53	1.57±0.12	9±1 (17±2%)
4	PX4	A	340	-	51,53,53	1.45±0.13	9±2 (16±4%)
4	PX4	A	375	-	51,53,53	1.54±0.22	10±4 (19±7%)
4	PX4	A	331	-	51,53,53	1.46±0.12	8±2 (16±3%)
4	PX4	A	390	-	51,53,53	1.49±0.11	8±2 (16±4%)
4	PX4	A	306	-	51,53,53	1.43±0.13	8±3 (14±5%)
4	PX4	A	414	-	51,53,53	1.52±0.15	9±2 (17±4%)
4	PX4	A	368	-	51,53,53	1.48±0.15	8±2 (16±4%)
4	PX4	A	350	-	51,53,53	1.46±0.11	9±2 (16±3%)
4	PX4	A	357	-	51,53,53	1.53±0.09	9±2 (17±3%)
4	PX4	A	366	-	51,53,53	1.57±0.16	10±2 (18±3%)
4	PX4	A	382	-	51,53,53	1.53±0.12	10±2 (20±4%)
4	PX4	A	313	-	51,53,53	1.50±0.13	9±3 (16±5%)
4	PX4	A	391	-	51,53,53	1.49±0.14	8±3 (16±6%)
4	PX4	A	360	-	51,53,53	1.52±0.13	9±2 (17±3%)
4	PX4	A	417	-	51,53,53	1.52±0.16	10±3 (19±5%)
4	PX4	A	427	-	51,53,53	1.59±0.12	10±2 (18±3%)
4	PX4	A	310	-	51,53,53	1.49±0.12	9±2 (17±4%)
4	PX4	A	349	-	51,53,53	1.51±0.11	9±2 (18±4%)
4	PX4	A	335	-	51,53,53	1.54±0.15	9±2 (18±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	394	-	51,53,53	1.43±0.14	8±2 (15±4%)
4	PX4	A	411	-	51,53,53	1.56±0.23	10±4 (19±7%)
4	PX4	A	345	-	51,53,53	1.36±0.09	7±1 (13±2%)
4	PX4	A	404	-	51,53,53	1.51±0.14	7±2 (14±3%)
4	PX4	A	373	-	51,53,53	1.49±0.11	9±2 (17±3%)
4	PX4	A	415	-	51,53,53	1.54±0.14	9±3 (18±5%)
4	PX4	A	356	-	51,53,53	1.47±0.13	8±2 (16±4%)
4	PX4	A	407	-	51,53,53	1.53±0.12	9±2 (17±4%)
4	PX4	A	325	-	51,53,53	1.50±0.14	8±2 (15±3%)
4	PX4	A	397	-	51,53,53	1.48±0.15	8±2 (15±4%)
4	PX4	A	369	-	51,53,53	1.53±0.09	9±1 (17±2%)
4	PX4	A	353	-	51,53,53	1.51±0.12	9±2 (18±3%)
4	PX4	A	413	-	51,53,53	1.57±0.15	10±2 (19±4%)
4	PX4	A	396	-	51,53,53	1.45±0.15	8±2 (14±4%)
4	PX4	A	354	-	51,53,53	1.62±0.11	11±3 (21±5%)
4	PX4	A	370	-	51,53,53	1.53±0.17	9±2 (17±4%)
4	PX4	A	430	-	51,53,53	1.50±0.11	9±2 (17±3%)
4	PX4	A	402	-	51,53,53	1.58±0.16	9±2 (18±3%)
4	PX4	A	425	-	51,53,53	1.49±0.14	9±2 (17±3%)
4	PX4	A	332	-	51,53,53	1.51±0.14	9±2 (18±4%)
4	PX4	A	348	-	51,53,53	1.43±0.17	8±3 (15±4%)
4	PX4	A	376	-	51,53,53	1.50±0.16	10±2 (19±4%)
4	PX4	A	328	-	51,53,53	1.48±0.14	9±2 (17±4%)
4	PX4	A	377	-	51,53,53	1.45±0.13	9±2 (16±3%)
4	PX4	A	336	-	51,53,53	1.41±0.09	8±3 (16±5%)
4	PX4	A	346	-	51,53,53	1.47±0.13	9±2 (17±4%)
4	PX4	A	333	-	51,53,53	1.48±0.16	10±3 (18±5%)
4	PX4	A	315	-	51,53,53	1.43±0.09	8±2 (16±4%)
4	PX4	A	385	-	51,53,53	1.50±0.13	9±3 (18±5%)
4	PX4	A	378	-	51,53,53	1.56±0.14	10±2 (18±3%)
4	PX4	A	406	-	51,53,53	1.46±0.13	8±2 (16±4%)
4	PX4	A	343	-	51,53,53	1.50±0.15	9±2 (18±3%)
4	PX4	A	374	-	51,53,53	1.46±0.14	8±2 (16±4%)
4	PX4	A	352	-	51,53,53	1.49±0.16	9±2 (16±3%)
4	PX4	A	381	-	51,53,53	1.51±0.16	10±2 (18±4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	371	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	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	356	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	C8-C7-C6	7.84	93.49	111.78	5	5
4	A	341	PX4	C7-O7-C23	7.69	136.20	117.80	2	10
4	A	314	PX4	C8-C7-C6	7.65	93.95	111.78	11	10
4	A	378	PX4	C8-C7-C6	7.60	94.07	111.78	2	10
4	A	371	PX4	C8-C7-C6	7.45	94.42	111.78	3	12
4	A	416	PX4	C8-C7-C6	7.44	94.43	111.78	6	11
4	A	323	PX4	C8-C7-C6	7.33	94.70	111.78	12	10
4	A	380	PX4	O7-C23-C24	7.15	126.95	111.48	10	5
4	A	400	PX4	C8-C7-C6	7.08	95.28	111.78	6	10
4	A	379	PX4	O3-P1-O2	6.83	81.85	108.94	3	7
4	A	350	PX4	O5-C8-C7	6.71	127.73	108.40	4	5
4	A	427	PX4	C8-C7-C6	6.69	96.20	111.78	3	7
4	A	313	PX4	C8-C7-C6	6.57	96.47	111.78	8	10
4	A	372	PX4	O7-C23-C24	6.53	125.60	111.48	3	8
4	A	420	PX4	C8-C7-C6	6.50	96.63	111.78	1	6
4	A	318	PX4	C8-C7-C6	6.50	96.64	111.78	5	10
4	A	405	PX4	O7-C23-C24	6.46	125.46	111.48	9	4
4	A	376	PX4	C8-C7-C6	6.46	96.72	111.78	3	10
4	A	333	PX4	C8-C7-C6	6.43	96.80	111.78	1	10
4	A	338	PX4	O5-C8-C7	6.39	126.83	108.40	4	5
4	A	413	PX4	C8-C7-C6	6.33	97.01	111.78	3	9
4	A	353	PX4	O7-C23-C24	6.19	124.88	111.48	13	9
4	A	402	PX4	C8-C7-C6	6.19	97.34	111.78	6	13
4	A	321	PX4	O5-C8-C7	6.19	126.24	108.40	13	7
4	A	408	PX4	O3-P1-O2	6.18	84.43	108.94	2	10
4	A	426	PX4	C7-O7-C23	6.18	132.58	117.80	8	3
4	A	353	PX4	O7-C23-O8	6.17	109.28	123.70	13	4
4	A	337	PX4	C8-C7-C6	6.16	97.43	111.78	7	6
4	A	326	PX4	O7-C23-C24	6.12	124.73	111.48	11	8
4	A	355	PX4	C8-C7-C6	6.10	97.56	111.78	14	11
4	A	423	PX4	O7-C23-O8	6.08	109.49	123.70	3	2
4	A	335	PX4	O7-C23-C24	6.08	124.63	111.48	3	9
4	A	311	PX4	O7-C23-O8	6.07	109.52	123.70	3	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PX4	C8-C7-C6	6.07	97.64	111.78	4	7
4	A	342	PX4	O7-C23-C24	6.04	124.54	111.48	8	3
4	A	331	PX4	O5-C8-C7	5.99	125.67	108.40	14	10
4	A	347	PX4	C8-C7-C6	5.97	97.86	111.78	9	11
4	A	396	PX4	C8-C7-C6	5.93	97.95	111.78	13	10
4	A	416	PX4	O5-C8-C7	5.92	125.48	108.40	8	7
4	A	347	PX4	O5-C8-C7	5.90	125.40	108.40	14	8
4	A	414	PX4	O7-C23-C24	5.90	124.23	111.48	5	9
4	A	399	PX4	C8-C7-C6	5.86	98.13	111.78	11	11
4	A	354	PX4	C7-O7-C23	5.81	131.70	117.80	13	9
4	A	332	PX4	O7-C23-C24	5.79	124.02	111.48	9	10
4	A	415	PX4	O3-P1-O2	5.77	86.07	108.94	13	7
4	A	359	PX4	O5-C9-O6	5.74	109.26	123.63	13	5
4	A	390	PX4	C7-O7-C23	5.74	131.53	117.80	10	6
4	A	381	PX4	O7-C23-C24	5.73	123.87	111.48	5	9
4	A	386	PX4	O3-P1-O2	5.72	86.26	108.94	13	4
4	A	317	PX4	C8-C7-C6	5.71	98.48	111.78	9	9
4	A	325	PX4	C8-C7-C6	5.69	98.52	111.78	14	7
4	A	361	PX4	O5-C8-C7	5.69	124.79	108.40	3	8
4	A	401	PX4	O7-C23-C24	5.65	123.70	111.48	6	5
4	A	389	PX4	O7-C23-C24	5.64	123.69	111.48	10	9
4	A	393	PX4	C8-C7-C6	5.62	98.67	111.78	13	7
4	A	344	PX4	C8-C7-C6	5.62	98.68	111.78	1	10
4	A	320	PX4	O7-C23-C24	5.62	123.64	111.48	3	8
4	A	376	PX4	O3-P1-O2	5.62	86.67	108.94	13	6
4	A	413	PX4	C7-O7-C23	5.60	104.39	117.80	5	3
4	A	410	PX4	C8-C7-C6	5.59	98.74	111.78	9	7
4	A	379	PX4	C8-C7-C6	5.59	98.75	111.78	9	10
4	A	312	PX4	O5-C8-C7	5.58	124.49	108.40	3	13
4	A	412	PX4	C8-C7-C6	5.58	98.77	111.78	4	11
4	A	369	PX4	O1-P1-O3	5.58	82.28	107.57	13	1
4	A	368	PX4	O5-C8-C7	5.57	124.46	108.40	3	10
4	A	398	PX4	O7-C23-C24	5.56	123.51	111.48	2	9
4	A	418	PX4	O7-C23-C24	5.56	123.51	111.48	13	7
4	A	355	PX4	C4-N1-C3	5.55	94.39	108.98	2	5
4	A	313	PX4	O5-C8-C7	5.55	124.40	108.40	7	9
4	A	310	PX4	O5-C9-O6	5.54	109.77	123.63	5	3
4	A	309	PX4	C8-C7-C6	5.54	98.88	111.78	9	8
4	A	306	PX4	C7-O7-C23	5.53	131.02	117.80	11	3
4	A	404	PX4	C8-C7-C6	5.52	98.91	111.78	3	8
4	A	424	PX4	O7-C23-C24	5.51	123.41	111.48	9	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	316	PX4	O7-C7-C8	5.51	128.12	108.34	4	9
4	A	309	PX4	O7-C23-C24	5.50	123.38	111.48	4	7
4	A	386	PX4	C5-N1-C3	5.49	94.57	108.98	5	3
4	A	334	PX4	C8-C7-C6	5.48	99.00	111.78	3	9
4	A	308	PX4	C8-C7-C6	5.47	99.02	111.78	10	7
4	A	422	PX4	O3-P1-O2	5.47	87.27	108.94	1	3
4	A	366	PX4	C8-C7-C6	5.46	99.05	111.78	8	9
4	A	367	PX4	O5-C8-C7	5.45	124.12	108.40	1	11
4	A	327	PX4	C8-C7-C6	5.45	99.07	111.78	8	9
4	A	341	PX4	O7-C7-C8	5.45	127.88	108.34	3	8
4	A	375	PX4	O3-P1-O2	5.44	87.39	108.94	8	5
4	A	348	PX4	O7-C23-C24	5.43	123.22	111.48	3	6
4	A	415	PX4	C8-C7-C6	5.43	99.13	111.78	7	8
4	A	363	PX4	O7-C23-C24	5.42	123.21	111.48	5	9
4	A	357	PX4	C8-C7-C6	5.40	99.19	111.78	4	8
4	A	387	PX4	O1-P1-O3	5.40	83.11	107.57	12	2
4	A	321	PX4	C8-C7-C6	5.36	99.29	111.78	3	8
4	A	430	PX4	O7-C23-C24	5.36	123.08	111.48	7	6
4	A	317	PX4	P1-O3-C1	5.36	95.77	121.26	6	10
4	A	356	PX4	P1-O3-C1	5.35	95.78	121.26	7	9
4	A	330	PX4	O5-C8-C7	5.35	123.81	108.40	9	8
4	A	312	PX4	C8-C7-C6	5.33	99.36	111.78	4	7
4	A	421	PX4	O7-C23-C24	5.33	123.00	111.48	14	5
4	A	371	PX4	C4-N1-C3	5.32	94.99	108.98	6	3
4	A	344	PX4	O5-C8-C7	5.32	123.73	108.40	6	9
4	A	360	PX4	O5-C8-C7	5.32	123.73	108.40	5	12
4	A	332	PX4	C8-C7-C6	5.31	99.41	111.78	4	3
4	A	384	PX4	P1-O3-C1	5.31	96.00	121.26	4	9
4	A	335	PX4	O7-C23-O8	5.30	111.31	123.70	3	6
4	A	367	PX4	C8-C7-C6	5.30	99.42	111.78	6	9
4	A	403	PX4	C8-C7-C6	5.30	99.44	111.78	11	9
4	A	373	PX4	O5-C8-C7	5.29	123.63	108.40	7	11
4	A	375	PX4	C8-C7-C6	5.28	99.47	111.78	4	8
4	A	306	PX4	C8-C7-C6	5.28	99.48	111.78	14	6
4	A	411	PX4	C8-C7-C6	5.28	99.49	111.78	1	10
4	A	337	PX4	O7-C23-O8	5.27	111.38	123.70	2	6
4	A	356	PX4	O7-C23-C24	5.27	122.88	111.48	10	7
4	A	417	PX4	O1-P1-O3	5.27	83.69	107.57	14	3
4	A	409	PX4	C8-C7-C6	5.25	99.54	111.78	1	12
4	A	327	PX4	O7-C23-C24	5.25	122.84	111.48	11	8
4	A	395	PX4	C8-C7-C6	5.25	99.55	111.78	4	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	415	PX4	O7-C23-O8	5.24	111.47	123.70	4	7
4	A	366	PX4	O5-C8-C7	5.23	123.48	108.40	2	11
4	A	311	PX4	C8-C7-C6	5.23	99.59	111.78	8	11
4	A	369	PX4	C7-O7-C23	5.23	130.32	117.80	7	4
4	A	370	PX4	O5-C9-O6	5.23	110.55	123.63	3	7
4	A	360	PX4	O7-C23-C24	5.23	122.79	111.48	11	9
4	A	380	PX4	C8-C7-C6	5.23	99.60	111.78	9	9
4	A	320	PX4	C8-C7-C6	5.22	99.61	111.78	11	11
4	A	400	PX4	O5-C8-C7	5.22	123.43	108.40	5	9
4	A	361	PX4	C7-O7-C23	5.21	130.27	117.80	11	4
4	A	329	PX4	O7-C23-C24	5.20	122.73	111.48	2	6
4	A	324	PX4	C8-C7-C6	5.20	99.67	111.78	14	11
4	A	417	PX4	C8-C7-C6	5.20	99.67	111.78	4	9
4	A	362	PX4	C7-O7-C23	5.19	130.23	117.80	11	6
4	A	418	PX4	O5-C8-C7	5.19	123.37	108.40	1	6
4	A	387	PX4	C8-C7-C6	5.19	99.69	111.78	6	8
4	A	331	PX4	O7-C7-C8	5.19	126.95	108.34	3	8
4	A	366	PX4	O7-C23-C24	5.18	122.68	111.48	12	7
4	A	390	PX4	C8-C7-C6	5.18	99.72	111.78	8	8
4	A	309	PX4	C7-O7-C23	5.17	130.17	117.80	8	6
4	A	332	PX4	O5-C8-C7	5.17	123.30	108.40	6	8
4	A	429	PX4	C7-O7-C23	5.16	130.15	117.80	1	2
4	A	409	PX4	O5-C8-C7	5.14	123.23	108.40	9	8
4	A	352	PX4	C8-C7-C6	5.14	99.80	111.78	2	12
4	A	368	PX4	C8-C7-C6	5.14	99.80	111.78	6	11
4	A	397	PX4	O5-C8-C7	5.14	123.21	108.40	10	5
4	A	378	PX4	O7-C23-C24	5.14	122.59	111.48	13	8
4	A	389	PX4	C8-C7-C6	5.12	99.84	111.78	5	7
4	A	328	PX4	C8-C7-C6	5.11	99.86	111.78	2	12
4	A	319	PX4	C7-O7-C23	5.11	130.02	117.80	12	3
4	A	411	PX4	C5-N1-C3	5.11	95.56	108.98	1	3
4	A	333	PX4	O5-C8-C7	5.10	123.11	108.40	11	9
4	A	343	PX4	O5-C8-C7	5.09	123.07	108.40	11	7
4	A	406	PX4	C8-C7-C6	5.09	99.92	111.78	1	8
4	A	353	PX4	O5-C9-O6	5.08	110.91	123.63	6	5
4	A	410	PX4	O7-C23-C24	5.09	122.48	111.48	4	9
4	A	397	PX4	O7-C23-O8	5.08	111.82	123.70	14	4
4	A	349	PX4	O7-C23-C24	5.08	122.47	111.48	2	9
4	A	402	PX4	C1-C2-N1	5.08	132.12	115.82	2	4
4	A	394	PX4	O7-C23-C24	5.08	122.46	111.48	6	5
4	A	370	PX4	C8-C7-C6	5.06	99.98	111.78	4	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	331	PX4	O7-C23-C24	5.06	122.42	111.48	8	5
4	A	394	PX4	O5-C8-C7	5.06	122.98	108.40	3	8
4	A	420	PX4	P1-O3-C1	5.05	97.20	121.26	14	9
4	A	398	PX4	C5-N1-C4	5.05	95.71	108.98	9	7
4	A	421	PX4	O5-C8-C7	5.05	122.96	108.40	13	8
4	A	414	PX4	O1-P1-O2	5.04	135.91	112.44	11	10
4	A	424	PX4	O5-C8-C7	5.04	122.93	108.40	13	11
4	A	322	PX4	C8-C7-C6	5.03	100.05	111.78	9	11
4	A	365	PX4	P1-O3-C1	5.03	97.31	121.26	4	12
4	A	319	PX4	O5-C8-C7	5.03	122.88	108.40	6	9
4	A	328	PX4	P1-O3-C1	5.03	97.33	121.26	5	12
4	A	334	PX4	O5-C8-C7	5.03	122.88	108.40	13	6
4	A	330	PX4	O7-C23-C24	5.01	122.33	111.48	11	7
4	A	342	PX4	C8-C7-C6	5.01	100.09	111.78	2	11
4	A	309	PX4	O5-C8-C7	5.01	122.84	108.40	7	8
4	A	337	PX4	O5-C8-C7	5.01	122.83	108.40	12	9
4	A	354	PX4	C8-C7-C6	5.00	100.13	111.78	11	9
4	A	425	PX4	P1-O4-C6	5.00	92.71	121.35	10	10
4	A	412	PX4	O7-C23-C24	4.99	122.28	111.48	7	7
4	A	351	PX4	C8-C7-C6	4.99	100.14	111.78	6	8
4	A	386	PX4	C8-C7-C6	4.99	100.16	111.78	12	11
4	A	413	PX4	P1-O3-C1	4.99	97.52	121.26	11	12
4	A	324	PX4	O5-C8-C7	4.99	122.77	108.40	14	7
4	A	329	PX4	C7-O7-C23	4.99	129.73	117.80	4	3
4	A	346	PX4	O5-C8-C7	4.99	122.77	108.40	3	6
4	A	340	PX4	C8-C7-C6	4.98	100.16	111.78	2	9
4	A	319	PX4	O3-P1-O2	4.98	89.20	108.94	2	3
4	A	392	PX4	C5-N1-C4	4.98	95.90	108.98	8	3
4	A	419	PX4	P1-O3-C1	4.98	97.57	121.26	7	9
4	A	359	PX4	C8-C7-C6	4.97	100.19	111.78	14	11
4	A	411	PX4	P1-O3-C1	4.97	97.59	121.26	5	11
4	A	346	PX4	C7-O7-C23	4.97	129.69	117.80	9	5
4	A	415	PX4	P1-O3-C1	4.97	97.61	121.26	12	12
4	A	426	PX4	O1-P1-O3	4.96	85.09	107.57	8	3
4	A	344	PX4	O7-C23-C24	4.95	122.20	111.48	8	9
4	A	397	PX4	O7-C23-C24	4.95	122.19	111.48	14	6
4	A	382	PX4	O7-C23-C24	4.95	122.18	111.48	3	4
4	A	420	PX4	C5-N1-C3	4.94	95.99	108.98	7	4
4	A	422	PX4	O7-C23-C24	4.94	122.17	111.48	5	3
4	A	361	PX4	O5-C9-O6	4.94	111.27	123.63	10	3
4	A	367	PX4	C26-C25-C24	4.94	94.99	113.13	9	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	421	PX4	C8-C7-C6	4.93	100.28	111.78	14	10
4	A	363	PX4	O5-C8-C7	4.93	122.60	108.40	11	10
4	A	414	PX4	O5-C8-C7	4.92	122.59	108.40	6	10
4	A	335	PX4	O3-P1-O2	4.92	89.43	108.94	7	4
4	A	389	PX4	O5-C8-C7	4.92	122.58	108.40	13	10
4	A	362	PX4	C8-C7-C6	4.92	100.32	111.78	2	9
4	A	423	PX4	C8-C7-C6	4.92	100.32	111.78	13	11
4	A	381	PX4	O7-C7-C8	4.91	125.95	108.34	2	6
4	A	407	PX4	C7-O7-C23	4.91	129.54	117.80	2	4
4	A	422	PX4	C8-C7-C6	4.90	100.35	111.78	13	12
4	A	391	PX4	O5-C8-C7	4.90	122.53	108.40	4	9
4	A	407	PX4	C8-C7-C6	4.89	100.38	111.78	4	7
4	A	329	PX4	P1-O3-C1	4.88	98.03	121.26	7	11
4	A	419	PX4	C8-C7-C6	4.87	100.42	111.78	8	11
4	A	400	PX4	C4-N1-C3	4.87	96.18	108.98	2	4
4	A	328	PX4	O5-C8-C7	4.87	122.43	108.40	9	7
4	A	385	PX4	O5-C8-C7	4.87	122.43	108.40	12	8
4	A	370	PX4	O5-C8-C7	4.87	122.42	108.40	2	7
4	A	343	PX4	C7-O7-C23	4.86	129.44	117.80	5	3
4	A	402	PX4	O5-C8-C7	4.86	122.42	108.40	7	10
4	A	427	PX4	P1-O3-C1	4.85	98.16	121.26	12	10
4	A	426	PX4	O7-C23-C24	4.85	121.97	111.48	9	7
4	A	327	PX4	C7-O7-C23	4.85	129.40	117.80	14	6
4	A	383	PX4	O7-C7-C6	4.85	125.74	108.34	9	8
4	A	361	PX4	O1-P1-O3	4.84	85.61	107.57	14	6
4	A	430	PX4	C8-C7-C6	4.84	100.49	111.78	9	10
4	A	339	PX4	C4-N1-C3	4.84	121.69	108.98	5	3
4	A	355	PX4	C1-C2-N1	4.84	131.36	115.82	10	5
4	A	402	PX4	O7-C23-C24	4.83	121.93	111.48	12	7
4	A	398	PX4	C8-C7-C6	4.83	100.53	111.78	2	8
4	A	335	PX4	O5-C8-C7	4.83	122.31	108.40	3	8
4	A	379	PX4	O7-C23-O8	4.83	112.42	123.70	2	4
4	A	407	PX4	O7-C23-C24	4.83	121.92	111.48	12	10
4	A	340	PX4	O7-C23-C24	4.82	121.91	111.48	7	8
4	A	374	PX4	C8-C7-C6	4.82	100.55	111.78	7	9
4	A	340	PX4	P1-O3-C1	4.81	98.35	121.26	6	11
4	A	353	PX4	C7-O7-C23	4.81	106.28	117.80	2	5
4	A	415	PX4	O1-P1-O2	4.81	134.82	112.44	10	8
4	A	413	PX4	C1-C2-N1	4.81	131.25	115.82	4	3
4	A	428	PX4	C8-C7-C6	4.81	100.57	111.78	2	9
4	A	411	PX4	O7-C7-C8	4.81	125.58	108.34	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	413	PX4	O5-C8-C7	4.80	122.23	108.40	8	6
4	A	401	PX4	O5-C8-C7	4.80	122.23	108.40	12	10
4	A	308	PX4	O7-C23-C24	4.79	121.85	111.48	11	7
4	A	422	PX4	P1-O3-C1	4.79	98.45	121.26	3	10
4	A	355	PX4	C5-N1-C4	4.78	96.42	108.98	5	2
4	A	418	PX4	P1-O3-C1	4.78	98.51	121.26	6	14
4	A	312	PX4	O3-P1-O2	4.78	90.00	108.94	13	5
4	A	352	PX4	O5-C8-C7	4.78	122.17	108.40	2	6
4	A	361	PX4	O7-C7-C6	4.78	125.48	108.34	8	8
4	A	402	PX4	O3-P1-O2	4.78	90.01	108.94	4	6
4	A	404	PX4	P1-O3-C1	4.78	98.53	121.26	12	8
4	A	428	PX4	O5-C8-C7	4.78	122.17	108.40	5	8
4	A	359	PX4	P1-O3-C1	4.77	98.55	121.26	12	11
4	A	366	PX4	P1-O3-C1	4.77	98.55	121.26	10	11
4	A	374	PX4	C5-N1-C3	4.77	96.45	108.98	11	3
4	A	411	PX4	C7-O7-C23	4.77	106.38	117.80	11	6
4	A	425	PX4	C8-C7-C6	4.77	100.66	111.78	1	7
4	A	406	PX4	O5-C8-C7	4.76	122.12	108.40	2	4
4	A	335	PX4	C8-C7-C6	4.76	100.69	111.78	5	9
4	A	383	PX4	O7-C23-C24	4.75	121.77	111.48	4	5
4	A	388	PX4	O7-C23-C24	4.76	121.77	111.48	7	8
4	A	412	PX4	O7-C7-C8	4.75	125.40	108.34	6	6
4	A	351	PX4	O5-C8-C7	4.74	122.07	108.40	14	6
4	A	339	PX4	O7-C23-C24	4.74	121.74	111.48	3	7
4	A	374	PX4	O5-C8-C7	4.74	122.06	108.40	4	10
4	A	388	PX4	C8-C7-C6	4.74	100.73	111.78	8	11
4	A	384	PX4	C8-C7-C6	4.74	100.74	111.78	11	7
4	A	426	PX4	O5-C9-O6	4.73	111.78	123.63	14	5
4	A	362	PX4	C5-N1-C4	4.73	96.55	108.98	1	8
4	A	423	PX4	O7-C23-C24	4.73	121.72	111.48	11	8
4	A	369	PX4	O5-C8-C7	4.73	122.03	108.40	8	12
4	A	372	PX4	O5-C8-C7	4.73	122.03	108.40	1	4
4	A	354	PX4	C5-N1-C3	4.73	96.56	108.98	5	3
4	A	423	PX4	P1-O3-C1	4.72	98.80	121.26	6	11
4	A	323	PX4	O7-C7-C6	4.71	125.24	108.34	12	7
4	A	318	PX4	O7-C23-C24	4.71	121.67	111.48	11	8
4	A	356	PX4	C8-C7-C6	4.71	100.81	111.78	1	9
4	A	408	PX4	P1-O3-C1	4.71	98.86	121.26	6	11
4	A	418	PX4	C8-C7-C6	4.70	100.82	111.78	11	9
4	A	371	PX4	O7-C23-C24	4.69	121.63	111.48	13	10
4	A	423	PX4	C5-N1-C4	4.69	96.65	108.98	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	381	PX4	O5-C8-C7	4.68	121.89	108.40	4	8
4	A	325	PX4	O5-C8-C7	4.67	121.86	108.40	5	6
4	A	353	PX4	C8-C7-C6	4.67	100.89	111.78	7	9
4	A	309	PX4	C5-N1-C4	4.67	96.71	108.98	7	3
4	A	411	PX4	O5-C8-C7	4.67	121.85	108.40	1	8
4	A	410	PX4	C7-O7-C23	4.67	106.63	117.80	13	5
4	A	425	PX4	O7-C23-C24	4.66	121.56	111.48	2	6
4	A	316	PX4	C8-C7-C6	4.66	100.92	111.78	6	9
4	A	324	PX4	C7-O7-C23	4.66	128.94	117.80	1	3
4	A	372	PX4	C8-C7-C6	4.65	100.93	111.78	4	8
4	A	407	PX4	O7-C7-C8	4.65	125.03	108.34	14	2
4	A	308	PX4	O3-P1-O2	4.65	90.51	108.94	4	7
4	A	308	PX4	C4-N1-C3	4.65	96.77	108.98	4	3
4	A	412	PX4	O5-C8-C7	4.65	121.79	108.40	10	9
4	A	393	PX4	O5-C8-C7	4.65	121.79	108.40	9	6
4	A	420	PX4	O5-C8-C7	4.65	121.79	108.40	4	7
4	A	345	PX4	O7-C23-O8	4.64	112.85	123.70	6	3
4	A	399	PX4	O7-C23-C24	4.64	121.52	111.48	12	5
4	A	416	PX4	C5-N1-C4	4.64	96.79	108.98	6	2
4	A	354	PX4	O5-C9-O6	4.64	112.03	123.63	11	2
4	A	408	PX4	C8-C7-C6	4.63	100.98	111.78	5	9
4	A	425	PX4	O5-C9-O6	4.63	112.04	123.63	2	5
4	A	404	PX4	O7-C23-O8	4.63	112.88	123.70	7	4
4	A	394	PX4	O3-P1-O2	4.63	90.59	108.94	11	3
4	A	424	PX4	C12-C11-C10	4.63	96.11	113.13	6	2
4	A	378	PX4	C7-O7-C23	4.63	128.87	117.80	5	7
4	A	376	PX4	C8-O5-C9	4.63	100.21	117.12	11	2
4	A	388	PX4	O5-C8-C7	4.62	121.72	108.40	5	8
4	A	419	PX4	O5-C8-C7	4.62	121.72	108.40	8	7
4	A	348	PX4	C8-C7-C6	4.62	101.01	111.78	2	9
4	A	380	PX4	O5-C8-C7	4.62	121.72	108.40	3	8
4	A	389	PX4	O3-P1-O2	4.62	90.63	108.94	7	3
4	A	395	PX4	O5-C9-O6	4.62	112.08	123.63	9	3
4	A	374	PX4	P1-O3-C1	4.61	99.30	121.26	9	9
4	A	373	PX4	O7-C23-C24	4.61	121.46	111.48	13	9
4	A	362	PX4	O7-C23-C24	4.61	121.46	111.48	9	8
4	A	343	PX4	P1-O3-C1	4.61	99.33	121.26	8	9
4	A	422	PX4	O5-C9-O6	4.61	112.10	123.63	10	4
4	A	313	PX4	O7-C7-C8	4.61	124.87	108.34	9	6
4	A	341	PX4	O7-C23-C24	4.60	121.44	111.48	5	6
4	A	385	PX4	C8-C7-C6	4.60	101.06	111.78	1	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	391	PX4	P1-O3-C1	4.60	99.37	121.26	10	9
4	A	314	PX4	O7-C23-C24	4.60	121.42	111.48	13	9
4	A	314	PX4	O5-C8-C7	4.59	121.64	108.40	8	5
4	A	357	PX4	O5-C8-C7	4.60	121.64	108.40	7	8
4	A	346	PX4	O7-C23-C24	4.59	121.41	111.48	14	6
4	A	377	PX4	P1-O3-C1	4.58	99.44	121.26	6	11
4	A	325	PX4	O3-P1-O2	4.58	90.78	108.94	8	2
4	A	404	PX4	O7-C23-C24	4.58	121.39	111.48	7	7
4	A	346	PX4	P1-O3-C1	4.57	99.48	121.26	8	13
4	A	327	PX4	C5-N1-C4	4.57	96.97	108.98	3	2
4	A	347	PX4	O7-C7-C8	4.57	124.75	108.34	9	8
4	A	325	PX4	P1-O4-C6	4.57	95.19	121.35	10	11
4	A	349	PX4	O5-C9-O6	4.56	112.21	123.63	11	5
4	A	357	PX4	O7-C23-C24	4.56	121.34	111.48	1	10
4	A	330	PX4	C4-N1-C3	4.56	120.95	108.98	6	3
4	A	331	PX4	C4-N1-C3	4.56	97.01	108.98	13	4
4	A	350	PX4	O7-C23-C24	4.56	121.34	111.48	6	10
4	A	418	PX4	O7-C23-O8	4.55	113.06	123.70	8	8
4	A	392	PX4	O5-C8-C7	4.55	121.52	108.40	7	5
4	A	321	PX4	O7-C23-C24	4.55	121.32	111.48	11	4
4	A	343	PX4	C8-C7-C6	4.55	101.17	111.78	6	10
4	A	424	PX4	O7-C7-C6	4.55	124.67	108.34	13	4
4	A	321	PX4	C25-C24-C23	4.55	97.03	113.69	4	1
4	A	314	PX4	C7-O7-C23	4.54	128.67	117.80	11	3
4	A	428	PX4	O7-C23-C24	4.54	121.31	111.48	11	8
4	A	348	PX4	O5-C8-C7	4.54	121.49	108.40	12	7
4	A	364	PX4	C8-C7-C6	4.54	101.20	111.78	8	8
4	A	307	PX4	O5-C8-C7	4.54	121.48	108.40	1	10
4	A	319	PX4	C8-C7-C6	4.54	101.20	111.78	7	7
4	A	413	PX4	C11-C10-C9	4.54	97.06	113.69	11	2
4	A	421	PX4	C26-C25-C24	4.53	96.47	113.13	12	2
4	A	378	PX4	P1-O3-C1	4.53	99.69	121.26	5	9
4	A	398	PX4	C5-N1-C3	4.53	120.88	108.98	7	4
4	A	427	PX4	O1-P1-O3	4.53	87.04	107.57	5	3
4	A	404	PX4	C7-O7-C23	4.52	128.61	117.80	5	6
4	A	386	PX4	O7-C23-C24	4.52	121.25	111.48	12	8
4	A	405	PX4	C1-C2-N1	4.52	130.32	115.82	4	6
4	A	427	PX4	O5-C8-C7	4.52	121.42	108.40	12	10
4	A	326	PX4	O3-P1-O2	4.51	91.07	108.94	11	4
4	A	352	PX4	P1-O3-C1	4.51	99.80	121.26	6	10
4	A	314	PX4	P1-O3-C1	4.51	99.81	121.26	7	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	418	PX4	C5-N1-C3	4.51	97.14	108.98	2	6
4	A	310	PX4	O7-C23-C24	4.50	121.22	111.48	9	7
4	A	401	PX4	C4-N1-C3	4.50	97.15	108.98	2	4
4	A	311	PX4	P1-O3-C1	4.49	99.89	121.26	3	13
4	A	369	PX4	C8-C7-C6	4.49	101.32	111.78	14	7
4	A	395	PX4	P1-O3-C1	4.49	99.90	121.26	9	9
4	A	416	PX4	C11-C10-C9	4.49	130.14	113.69	9	1
4	A	413	PX4	O7-C7-C8	4.48	124.43	108.34	12	7
4	A	324	PX4	O7-C7-C8	4.48	124.41	108.34	12	7
4	A	312	PX4	C5-N1-C4	4.48	97.21	108.98	3	4
4	A	326	PX4	P1-O3-C1	4.48	99.95	121.26	1	6
4	A	396	PX4	P1-O4-C6	4.47	95.71	121.35	9	9
4	A	424	PX4	C8-C7-C6	4.47	101.36	111.78	7	11
4	A	387	PX4	O5-C8-C7	4.47	121.28	108.40	3	8
4	A	402	PX4	O1-P1-O4	4.47	127.82	107.57	8	3
4	A	391	PX4	O7-C23-C24	4.47	121.14	111.48	3	7
4	A	328	PX4	O5-C9-O6	4.46	112.46	123.63	3	6
4	A	330	PX4	P1-O3-C1	4.47	100.00	121.26	3	11
4	A	352	PX4	O7-C23-C24	4.46	121.13	111.48	7	7
4	A	320	PX4	O7-C7-C8	4.46	124.34	108.34	6	5
4	A	376	PX4	P1-O4-C6	4.46	95.80	121.35	5	14
4	A	411	PX4	O3-P1-O2	4.45	91.28	108.94	12	6
4	A	415	PX4	O7-C7-C8	4.45	124.29	108.34	3	8
4	A	338	PX4	C8-C7-C6	4.44	101.42	111.78	14	10
4	A	425	PX4	C7-O7-C23	4.44	107.17	117.80	9	3
4	A	403	PX4	P1-O3-C1	4.44	100.13	121.26	3	9
4	A	369	PX4	O7-C23-C24	4.43	121.06	111.48	9	5
4	A	405	PX4	C7-O7-C23	4.43	128.40	117.80	11	4
4	A	317	PX4	O5-C9-O6	4.43	112.56	123.63	13	4
4	A	384	PX4	O5-C8-C7	4.43	121.16	108.40	4	9
4	A	397	PX4	C8-C7-C6	4.42	101.47	111.78	5	7
4	A	369	PX4	O1-P1-O2	4.42	133.01	112.44	13	9
4	A	419	PX4	C7-O7-C23	4.42	128.38	117.80	1	4
4	A	360	PX4	C7-O7-C23	4.42	107.22	117.80	6	3
4	A	422	PX4	O5-C8-C7	4.41	121.12	108.40	13	7
4	A	348	PX4	O7-C23-O8	4.41	113.39	123.70	5	4
4	A	332	PX4	O3-P1-O2	4.41	91.46	108.94	9	3
4	A	350	PX4	O3-P1-O2	4.41	91.46	108.94	11	5
4	A	370	PX4	O7-C23-C24	4.40	121.01	111.48	5	10
4	A	422	PX4	O4-P1-O2	4.40	126.39	108.94	1	1
4	A	379	PX4	O1-P1-O2	4.40	132.92	112.44	13	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	375	PX4	O5-C8-C7	4.40	121.08	108.40	7	8
4	A	370	PX4	C7-O7-C23	4.40	128.32	117.80	4	3
4	A	383	PX4	O4-P1-O2	4.39	126.35	108.94	9	3
4	A	308	PX4	O5-C8-C7	4.39	121.04	108.40	9	10
4	A	306	PX4	P1-O3-C1	4.38	100.39	121.26	6	10
4	A	406	PX4	O3-P1-O2	4.38	91.57	108.94	14	5
4	A	313	PX4	C4-N1-C3	4.38	97.48	108.98	1	3
4	A	399	PX4	P1-O3-C1	4.37	100.45	121.26	7	9
4	A	377	PX4	C8-C7-C6	4.37	101.60	111.78	13	9
4	A	331	PX4	P1-O3-C1	4.36	100.48	121.26	5	10
4	A	403	PX4	O7-C7-C6	4.36	124.00	108.34	6	6
4	A	404	PX4	O5-C9-O6	4.36	112.71	123.63	12	2
4	A	307	PX4	O7-C7-C6	4.36	124.00	108.34	5	9
4	A	421	PX4	P1-O3-C1	4.36	100.49	121.26	9	10
4	A	344	PX4	C5-N1-C4	4.36	97.52	108.98	9	3
4	A	376	PX4	O1-P1-O2	4.36	132.74	112.44	13	8
4	A	397	PX4	P1-O3-C1	4.36	100.50	121.26	1	10
4	A	382	PX4	O5-C8-C7	4.36	120.95	108.40	3	8
4	A	375	PX4	O7-C23-C24	4.35	120.90	111.48	14	8
4	A	407	PX4	O5-C9-O6	4.36	112.73	123.63	6	2
4	A	377	PX4	O7-C23-C24	4.35	120.89	111.48	2	6
4	A	371	PX4	P1-O3-C1	4.35	100.56	121.26	11	8
4	A	311	PX4	O5-C8-C7	4.35	120.93	108.40	2	10
4	A	369	PX4	P1-O3-C1	4.35	100.57	121.26	8	9
4	A	387	PX4	O5-C9-C10	4.35	125.09	111.83	9	4
4	A	317	PX4	O7-C23-C24	4.35	120.88	111.48	10	6
4	A	416	PX4	O3-P1-O2	4.35	91.71	108.94	14	7
4	A	323	PX4	O7-C23-C24	4.34	120.88	111.48	4	5
4	A	358	PX4	O5-C8-C7	4.34	120.92	108.40	9	6
4	A	384	PX4	O7-C7-C8	4.34	123.93	108.34	6	5
4	A	409	PX4	O7-C7-C8	4.34	123.93	108.34	8	6
4	A	423	PX4	O5-C8-C7	4.34	120.92	108.40	1	7
4	A	360	PX4	P1-O3-C1	4.34	100.58	121.26	9	11
4	A	361	PX4	O3-P1-O2	4.34	91.73	108.94	9	9
4	A	430	PX4	O5-C9-C10	4.34	125.07	111.83	12	2
4	A	400	PX4	P1-O3-C1	4.34	100.61	121.26	12	9
4	A	329	PX4	C8-C7-C6	4.34	101.67	111.78	5	9
4	A	381	PX4	C8-C7-C6	4.33	101.68	111.78	6	8
4	A	345	PX4	P1-O3-C1	4.33	100.63	121.26	8	9
4	A	408	PX4	C5-N1-C3	4.33	120.35	108.98	3	3
4	A	332	PX4	C5-N1-C3	4.33	120.35	108.98	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	379	PX4	O7-C7-C8	4.33	123.88	108.34	2	10
4	A	416	PX4	P1-O3-C1	4.33	100.66	121.26	3	10
4	A	352	PX4	C26-C25-C24	4.32	97.24	113.13	7	4
4	A	407	PX4	C5-N1-C4	4.33	97.62	108.98	5	3
4	A	379	PX4	P1-O3-C1	4.32	100.69	121.26	7	11
4	A	394	PX4	P1-O3-C1	4.32	100.69	121.26	5	12
4	A	416	PX4	O7-C23-C24	4.32	120.83	111.48	14	9
4	A	370	PX4	P1-O3-C1	4.32	100.71	121.26	11	9
4	A	398	PX4	O3-P1-O2	4.32	91.82	108.94	7	5
4	A	403	PX4	C7-O7-C23	4.32	128.13	117.80	14	5
4	A	357	PX4	C7-O7-C23	4.32	107.47	117.80	5	5
4	A	383	PX4	O5-C8-C7	4.32	120.84	108.40	11	7
4	A	429	PX4	C5-N1-C4	4.31	97.66	108.98	12	5
4	A	338	PX4	P1-O3-C1	4.31	100.76	121.26	2	11
4	A	429	PX4	O5-C9-O6	4.31	112.86	123.63	7	4
4	A	364	PX4	C5-N1-C4	4.31	97.67	108.98	9	2
4	A	389	PX4	O7-C23-O8	4.31	113.64	123.70	10	7
4	A	390	PX4	P1-O3-C1	4.30	100.78	121.26	6	11
4	A	310	PX4	P1-O4-C6	4.30	96.70	121.35	2	10
4	A	336	PX4	C12-C11-C10	4.30	97.33	113.13	6	3
4	A	333	PX4	P1-O4-C6	4.30	96.73	121.35	4	9
4	A	342	PX4	O1-P1-O2	4.30	132.43	112.44	14	5
4	A	401	PX4	O5-C9-C10	4.30	124.93	111.83	11	4
4	A	418	PX4	C7-O7-C23	4.30	128.08	117.80	4	3
4	A	325	PX4	C5-N1-C3	4.29	97.70	108.98	9	7
4	A	329	PX4	O5-C8-C7	4.29	120.77	108.40	4	7
4	A	412	PX4	O7-C23-O8	4.29	113.67	123.70	13	4
4	A	376	PX4	O5-C8-C7	4.29	120.77	108.40	4	7
4	A	349	PX4	P1-O3-C1	4.28	100.87	121.26	11	13
4	A	393	PX4	P1-O3-C1	4.28	100.87	121.26	10	8
4	A	334	PX4	O1-P1-O2	4.28	132.36	112.44	5	8
4	A	359	PX4	C7-O7-C23	4.28	128.04	117.80	2	7
4	A	361	PX4	C26-C25-C24	4.28	97.40	113.13	10	2
4	A	362	PX4	C4-N1-C3	4.28	120.22	108.98	6	4
4	A	326	PX4	O5-C9-C10	4.27	124.86	111.83	7	6
4	A	312	PX4	P1-O3-C1	4.27	100.93	121.26	3	8
4	A	389	PX4	P1-O3-C1	4.27	100.93	121.26	13	10
4	A	427	PX4	O7-C23-C24	4.27	120.71	111.48	11	8
4	A	363	PX4	C8-C7-C6	4.26	101.84	111.78	5	8
4	A	424	PX4	O7-C23-O8	4.26	113.74	123.70	1	4
4	A	316	PX4	O5-C8-C7	4.26	120.68	108.40	3	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	413	PX4	O1-P1-O4	4.26	126.87	107.57	8	4
4	A	412	PX4	P1-O3-C1	4.26	101.00	121.26	14	11
4	A	351	PX4	O7-C7-C8	4.25	123.61	108.34	13	7
4	A	411	PX4	C5-N1-C4	4.25	97.81	108.98	12	1
4	A	342	PX4	P1-O3-C1	4.25	101.04	121.26	8	10
4	A	323	PX4	P1-O3-C1	4.25	101.05	121.26	13	10
4	A	376	PX4	P1-O3-C1	4.25	101.04	121.26	9	11
4	A	314	PX4	P1-O4-C6	4.24	97.05	121.35	9	13
4	A	347	PX4	O7-C7-C6	4.24	123.55	108.34	14	3
4	A	358	PX4	P1-O3-C1	4.24	101.08	121.26	13	12
4	A	350	PX4	C5-N1-C3	4.24	97.85	108.98	7	4
4	A	358	PX4	C8-C7-C6	4.24	101.91	111.78	14	9
4	A	391	PX4	O3-P1-O2	4.24	92.15	108.94	12	6
4	A	426	PX4	O5-C8-C7	4.24	120.61	108.40	6	7
4	A	383	PX4	C5-N1-C4	4.23	97.86	108.98	14	2
4	A	404	PX4	O3-P1-O2	4.23	92.16	108.94	3	4
4	A	411	PX4	C4-N1-C3	4.23	97.86	108.98	5	3
4	A	402	PX4	O7-C7-C6	4.23	123.50	108.34	12	7
4	A	410	PX4	O7-C23-O8	4.22	113.83	123.70	5	8
4	A	350	PX4	P1-O4-C6	4.22	97.15	121.35	9	6
4	A	354	PX4	O5-C8-C7	4.22	120.57	108.40	7	6
4	A	426	PX4	C8-C7-C6	4.22	101.94	111.78	6	9
4	A	402	PX4	C8-O5-C9	4.22	132.54	117.12	1	3
4	A	408	PX4	O7-C23-C24	4.22	120.61	111.48	3	7
4	A	362	PX4	O4-P1-O2	4.22	125.65	108.94	11	6
4	A	379	PX4	O4-P1-O2	4.22	125.65	108.94	2	2
4	A	320	PX4	C5-N1-C3	4.21	120.05	108.98	12	5
4	A	421	PX4	O7-C23-O8	4.21	113.85	123.70	14	7
4	A	326	PX4	O7-C23-O8	4.21	113.86	123.70	2	5
4	A	405	PX4	C8-C7-C6	4.21	101.96	111.78	11	8
4	A	362	PX4	O5-C8-C7	4.21	120.54	108.40	13	4
4	A	430	PX4	O5-C9-O6	4.21	113.10	123.63	11	6
4	A	396	PX4	O7-C23-O8	4.20	113.88	123.70	9	6
4	A	339	PX4	C5-N1-C3	4.20	97.94	108.98	4	3
4	A	352	PX4	C7-O7-C23	4.20	127.85	117.80	1	4
4	A	399	PX4	O5-C9-O6	4.20	113.12	123.63	5	2
4	A	343	PX4	O7-C23-C24	4.20	120.57	111.48	13	9
4	A	347	PX4	O7-C23-C24	4.20	120.57	111.48	7	6
4	A	322	PX4	O7-C23-C24	4.20	120.56	111.48	13	8
4	A	334	PX4	O7-C23-C24	4.20	120.56	111.48	14	8
4	A	307	PX4	O7-C23-O8	4.20	113.90	123.70	12	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	O1-P1-O3	4.20	88.55	107.57	5	3
4	A	310	PX4	P1-O3-C1	4.19	101.29	121.26	11	11
4	A	339	PX4	C5-N1-C4	4.19	97.97	108.98	5	3
4	A	315	PX4	O7-C23-C24	4.19	120.54	111.48	8	9
4	A	320	PX4	P1-O4-C6	4.19	97.36	121.35	9	9
4	A	307	PX4	O7-C23-C24	4.19	120.54	111.48	11	9
4	A	351	PX4	P1-O3-C1	4.19	101.33	121.26	9	11
4	A	428	PX4	P1-O4-C6	4.18	97.37	121.35	11	10
4	A	368	PX4	O1-P1-O2	4.18	131.90	112.44	4	7
4	A	377	PX4	O5-C8-C7	4.18	120.44	108.40	7	8
4	A	383	PX4	C8-C7-C6	4.18	102.04	111.78	13	10
4	A	427	PX4	P1-O4-C6	4.18	97.40	121.35	6	13
4	A	381	PX4	O1-P1-O2	4.17	131.86	112.44	3	10
4	A	394	PX4	C5-N1-C4	4.17	98.01	108.98	7	3
4	A	313	PX4	O1-P1-O2	4.17	131.85	112.44	5	9
4	A	339	PX4	C8-C7-C6	4.17	102.06	111.78	6	8
4	A	361	PX4	O7-C23-C24	4.17	120.50	111.48	1	10
4	A	365	PX4	O7-C23-O8	4.17	113.96	123.70	1	6
4	A	427	PX4	C1-C2-N1	4.17	129.20	115.82	4	6
4	A	373	PX4	C8-C7-C6	4.17	102.07	111.78	5	9
4	A	315	PX4	P1-O3-C1	4.16	101.44	121.26	5	8
4	A	397	PX4	C5-N1-C4	4.16	98.04	108.98	3	3
4	A	331	PX4	C8-C7-C6	4.16	102.08	111.78	9	8
4	A	332	PX4	P1-O3-C1	4.16	101.45	121.26	8	9
4	A	379	PX4	C25-C24-C23	4.16	98.44	113.69	12	4
4	A	336	PX4	O7-C23-C24	4.16	120.48	111.48	1	11
4	A	336	PX4	O3-P1-O2	4.16	92.45	108.94	12	5
4	A	390	PX4	O7-C23-C24	4.16	120.48	111.48	6	8
4	A	392	PX4	P1-O4-C6	4.16	97.52	121.35	9	10
4	A	362	PX4	O7-C7-C8	4.16	123.25	108.34	2	8
4	A	398	PX4	P1-O3-C1	4.15	101.49	121.26	1	10
4	A	361	PX4	C4-N1-C3	4.15	98.07	108.98	7	2
4	A	326	PX4	O5-C8-C7	4.15	120.36	108.40	9	4
4	A	344	PX4	P1-O3-C1	4.15	101.52	121.26	12	10
4	A	339	PX4	O1-P1-O2	4.15	131.73	112.44	4	7
4	A	405	PX4	C8-O5-C9	4.15	101.96	117.12	13	3
4	A	363	PX4	O7-C7-C8	4.14	123.21	108.34	1	4
4	A	426	PX4	C5-N1-C3	4.14	98.09	108.98	13	3
4	A	357	PX4	P1-O3-C1	4.14	101.55	121.26	3	11
4	A	312	PX4	O7-C7-C8	4.14	123.19	108.34	1	5
4	A	349	PX4	C31-C30-C29	4.14	93.46	114.37	9	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	341	PX4	P1-O3-C1	4.13	101.58	121.26	8	10
4	A	361	PX4	C5-N1-C3	4.14	119.84	108.98	8	6
4	A	388	PX4	O1-P1-O3	4.14	88.82	107.57	1	2
4	A	378	PX4	O7-C23-O8	4.13	114.04	123.70	13	6
4	A	404	PX4	O5-C8-C7	4.13	120.31	108.40	12	10
4	A	327	PX4	C1-C2-N1	4.13	129.09	115.82	4	3
4	A	342	PX4	O7-C23-O8	4.13	114.04	123.70	7	6
4	A	379	PX4	O1-P1-O3	4.13	88.84	107.57	13	5
4	A	415	PX4	C4-N1-C3	4.13	98.12	108.98	1	3
4	A	344	PX4	C1-C2-N1	4.13	129.08	115.82	10	4
4	A	406	PX4	C26-C25-C24	4.13	97.96	113.13	11	3
4	A	424	PX4	P1-O3-C1	4.13	101.61	121.26	13	7
4	A	338	PX4	O7-C23-C24	4.12	120.40	111.48	6	8
4	A	335	PX4	P1-O3-C1	4.12	101.63	121.26	2	10
4	A	407	PX4	O5-C8-C7	4.12	120.28	108.40	2	5
4	A	392	PX4	O7-C7-C6	4.12	123.13	108.34	9	7
4	A	376	PX4	O7-C23-O8	4.12	114.08	123.70	5	3
4	A	411	PX4	C1-C2-N1	4.12	129.04	115.82	14	4
4	A	321	PX4	O5-C9-O6	4.11	113.34	123.63	8	4
4	A	360	PX4	O7-C23-O8	4.11	114.08	123.70	2	7
4	A	361	PX4	O7-C7-C8	4.12	123.11	108.34	13	5
4	A	396	PX4	O5-C8-C7	4.11	120.26	108.40	7	8
4	A	327	PX4	O7-C7-C8	4.11	123.10	108.34	13	5
4	A	367	PX4	O5-C9-C10	4.11	124.38	111.83	11	7
4	A	391	PX4	C8-C7-C6	4.11	102.19	111.78	14	9
4	A	308	PX4	O5-C9-O6	4.11	113.35	123.63	3	3
4	A	321	PX4	O1-P1-O2	4.11	131.56	112.44	7	7
4	A	386	PX4	P1-O3-C1	4.11	101.70	121.26	7	10
4	A	397	PX4	O5-C9-O6	4.11	113.35	123.63	8	6
4	A	354	PX4	O7-C23-O8	4.11	114.10	123.70	14	5
4	A	359	PX4	O1-P1-O2	4.11	131.55	112.44	4	8
4	A	340	PX4	O7-C7-C8	4.11	123.07	108.34	12	8
4	A	382	PX4	O5-C9-C10	4.10	124.35	111.83	1	7
4	A	412	PX4	O7-C7-C6	4.11	123.07	108.34	5	7
4	A	327	PX4	P1-O3-C1	4.10	101.72	121.26	14	13
4	A	345	PX4	C8-C7-C6	4.10	102.22	111.78	3	7
4	A	335	PX4	C5-N1-C4	4.10	98.20	108.98	12	3
4	A	320	PX4	P1-O3-C1	4.10	101.74	121.26	1	7
4	A	315	PX4	C8-C7-C6	4.10	102.23	111.78	14	7
4	A	336	PX4	O5-C8-C7	4.10	120.21	108.40	4	5
4	A	390	PX4	O7-C7-C8	4.10	123.05	108.34	4	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	385	PX4	C7-O7-C23	4.10	127.60	117.80	1	5
4	A	390	PX4	P1-O4-C6	4.10	97.87	121.35	5	10
4	A	322	PX4	O7-C23-O8	4.09	114.14	123.70	7	5
4	A	366	PX4	O1-P1-O2	4.09	131.49	112.44	2	12
4	A	417	PX4	C5-N1-C4	4.09	119.73	108.98	8	3
4	A	333	PX4	C25-C24-C23	4.09	98.70	113.69	2	3
4	A	339	PX4	O4-P1-O2	4.09	125.15	108.94	14	3
4	A	347	PX4	C5-N1-C4	4.09	119.72	108.98	10	3
4	A	417	PX4	C1-C2-N1	4.09	128.95	115.82	3	5
4	A	405	PX4	C5-N1-C3	4.09	98.23	108.98	13	3
4	A	327	PX4	O7-C23-O8	4.08	114.16	123.70	9	6
4	A	354	PX4	O7-C23-C24	4.08	120.32	111.48	7	6
4	A	396	PX4	O7-C7-C8	4.08	123.00	108.34	10	5
4	A	429	PX4	O7-C23-C24	4.08	120.32	111.48	1	7
4	A	310	PX4	O5-C9-C10	4.08	124.28	111.83	5	4
4	A	395	PX4	O1-P1-O2	4.08	131.44	112.44	5	9
4	A	411	PX4	O5-C9-O6	4.08	113.42	123.63	10	5
4	A	307	PX4	O7-C7-C8	4.08	122.98	108.34	9	4
4	A	317	PX4	O5-C8-C7	4.08	96.64	108.40	4	8
4	A	428	PX4	O7-C23-O8	4.08	114.17	123.70	1	6
4	A	330	PX4	C7-O7-C23	4.07	127.55	117.80	5	4
4	A	333	PX4	O7-C23-C24	4.08	120.30	111.48	1	6
4	A	323	PX4	O5-C8-C7	4.07	120.14	108.40	2	8
4	A	331	PX4	O7-C23-O8	4.07	114.18	123.70	1	4
4	A	344	PX4	O7-C23-O8	4.07	114.18	123.70	12	7
4	A	346	PX4	C8-C7-C6	4.07	102.29	111.78	3	4
4	A	384	PX4	O7-C23-C24	4.07	120.29	111.48	5	8
4	A	428	PX4	P1-O3-C1	4.07	101.87	121.26	13	11
4	A	430	PX4	C7-O7-C23	4.07	108.04	117.80	5	5
4	A	314	PX4	C4-N1-C3	4.07	98.28	108.98	4	4
4	A	351	PX4	C5-N1-C3	4.07	98.28	108.98	2	3
4	A	315	PX4	C7-O7-C23	4.07	108.06	117.80	14	5
4	A	395	PX4	C7-O7-C23	4.07	127.54	117.80	11	3
4	A	339	PX4	P1-O3-C1	4.07	101.90	121.26	5	13
4	A	429	PX4	O1-P1-O3	4.07	89.13	107.57	9	4
4	A	310	PX4	O1-P1-O2	4.07	131.35	112.44	1	6
4	A	364	PX4	O5-C8-C7	4.06	120.11	108.40	5	9
4	A	394	PX4	C8-C7-C6	4.06	102.31	111.78	4	8
4	A	321	PX4	P1-O3-C1	4.06	101.94	121.26	12	11
4	A	321	PX4	P1-O4-C6	4.06	98.10	121.35	4	10
4	A	353	PX4	O5-C8-C7	4.06	120.09	108.40	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	310	PX4	C4-N1-C3	4.06	98.32	108.98	8	3
4	A	348	PX4	C4-N1-C3	4.06	98.32	108.98	5	3
4	A	358	PX4	C31-C30-C29	4.06	93.86	114.37	12	1
4	A	321	PX4	O7-C7-C6	4.06	122.89	108.34	2	4
4	A	339	PX4	O3-P1-O2	4.05	92.86	108.94	14	6
4	A	363	PX4	C1-C2-N1	4.06	128.84	115.82	8	5
4	A	382	PX4	O7-C7-C6	4.05	122.88	108.34	12	6
4	A	392	PX4	O7-C23-C24	4.05	120.25	111.48	9	6
4	A	415	PX4	O7-C23-C24	4.05	120.25	111.48	1	8
4	A	410	PX4	P1-O3-C1	4.05	101.97	121.26	6	10
4	A	380	PX4	P1-O3-C1	4.05	101.98	121.26	11	13
4	A	428	PX4	C5-N1-C3	4.05	98.34	108.98	4	2
4	A	387	PX4	P1-O4-C6	4.05	98.16	121.35	14	10
4	A	360	PX4	C8-C7-C6	4.04	102.36	111.78	4	7
4	A	339	PX4	O5-C8-C7	4.04	120.05	108.40	3	6
4	A	403	PX4	O7-C23-C24	4.04	120.22	111.48	6	6
4	A	389	PX4	O1-P1-O2	4.04	131.23	112.44	8	6
4	A	403	PX4	C5-N1-C3	4.04	98.37	108.98	3	7
4	A	429	PX4	P1-O3-C1	4.04	102.05	121.26	10	12
4	A	380	PX4	O1-P1-O3	4.03	89.29	107.57	7	4
4	A	413	PX4	C20-C19-C18	4.03	93.98	114.37	13	1
4	A	369	PX4	O3-P1-O2	4.03	92.96	108.94	6	5
4	A	419	PX4	C5-N1-C4	4.03	98.39	108.98	8	3
4	A	392	PX4	C4-N1-C3	4.03	98.39	108.98	7	2
4	A	421	PX4	P1-O4-C6	4.03	98.26	121.35	8	8
4	A	375	PX4	P1-O3-C1	4.03	102.09	121.26	1	10
4	A	315	PX4	O7-C7-C8	4.03	122.79	108.34	14	7
4	A	386	PX4	O5-C9-O6	4.03	113.56	123.63	13	4
4	A	407	PX4	P1-O3-C1	4.03	102.09	121.26	8	9
4	A	386	PX4	O5-C9-C10	4.03	124.11	111.83	4	2
4	A	365	PX4	O7-C23-C24	4.02	120.19	111.48	2	7
4	A	365	PX4	C5-N1-C3	4.02	98.41	108.98	14	3
4	A	346	PX4	P1-O4-C6	4.02	98.32	121.35	5	9
4	A	414	PX4	O7-C7-C6	4.02	122.77	108.34	9	5
4	A	322	PX4	P1-O3-C1	4.02	102.13	121.26	6	11
4	A	417	PX4	C4-N1-C3	4.02	98.42	108.98	14	7
4	A	352	PX4	P1-O4-C6	4.02	98.33	121.35	9	6
4	A	372	PX4	O7-C7-C8	4.01	122.74	108.34	4	7
4	A	417	PX4	O4-P1-O2	4.01	124.84	108.94	1	2
4	A	430	PX4	C1-C2-N1	4.01	128.70	115.82	13	2
4	A	339	PX4	O5-C9-O6	4.01	113.59	123.63	13	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	O7-C23-C24	4.01	120.16	111.48	1	4
4	A	406	PX4	O7-C23-O8	4.01	114.33	123.70	14	5
4	A	382	PX4	C8-C7-C6	4.01	102.44	111.78	12	10
4	A	395	PX4	P1-O4-C6	4.01	98.39	121.35	4	10
4	A	402	PX4	O7-C7-C8	4.01	122.71	108.34	7	6
4	A	419	PX4	O7-C23-C24	4.01	120.15	111.48	3	7
4	A	425	PX4	O5-C8-C7	4.01	119.94	108.40	12	8
4	A	406	PX4	O4-P1-O2	4.00	124.80	108.94	11	3
4	A	424	PX4	O1-P1-O2	4.00	131.05	112.44	4	10
4	A	346	PX4	O5-C9-O6	4.00	113.63	123.63	13	2
4	A	375	PX4	C4-N1-C3	3.99	98.48	108.98	12	2
4	A	395	PX4	O7-C7-C6	3.99	122.67	108.34	2	7
4	A	369	PX4	O7-C7-C8	3.99	122.67	108.34	1	5
4	A	430	PX4	O5-C8-C7	3.99	119.90	108.40	5	9
4	A	355	PX4	P1-O4-C6	3.99	98.49	121.35	14	7
4	A	326	PX4	C8-C7-C6	3.99	102.49	111.78	5	8
4	A	324	PX4	O7-C7-C6	3.99	122.64	108.34	11	7
4	A	366	PX4	C7-O7-C23	3.99	127.34	117.80	10	7
4	A	405	PX4	O5-C8-C7	3.98	119.88	108.40	8	9
4	A	397	PX4	C1-C2-N1	3.98	128.61	115.82	7	5
4	A	406	PX4	C1-C2-N1	3.98	128.61	115.82	14	6
4	A	318	PX4	O5-C8-C7	3.98	119.87	108.40	4	7
4	A	356	PX4	C7-O7-C23	3.98	127.33	117.80	11	3
4	A	404	PX4	O4-P1-O2	3.98	124.72	108.94	13	3
4	A	387	PX4	P1-O3-C1	3.98	102.32	121.26	11	7
4	A	325	PX4	O1-P1-O4	3.98	125.59	107.57	8	1
4	A	385	PX4	O7-C23-C24	3.98	120.09	111.48	4	6
4	A	393	PX4	O7-C23-C24	3.97	120.08	111.48	2	9
4	A	398	PX4	O5-C9-O6	3.98	113.68	123.63	11	5
4	A	400	PX4	C5-N1-C3	3.97	98.53	108.98	14	3
4	A	401	PX4	P1-O3-C1	3.98	102.33	121.26	2	12
4	A	404	PX4	C5-N1-C4	3.98	98.53	108.98	6	4
4	A	413	PX4	O7-C23-C24	3.98	120.08	111.48	8	9
4	A	421	PX4	O1-P1-O4	3.97	125.58	107.57	13	2
4	A	387	PX4	O5-C9-O6	3.97	113.69	123.63	13	3
4	A	411	PX4	O7-C23-C24	3.97	120.08	111.48	8	3
4	A	426	PX4	O7-C7-C8	3.97	122.58	108.34	11	6
4	A	348	PX4	P1-O3-C1	3.97	102.38	121.26	4	11
4	A	413	PX4	C5-N1-C3	3.96	119.39	108.98	6	2
4	A	414	PX4	P1-O4-C6	3.96	98.63	121.35	12	8
4	A	353	PX4	O3-P1-O2	3.96	93.23	108.94	14	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	368	PX4	O7-C7-C8	3.96	122.56	108.34	8	5
4	A	354	PX4	P1-O3-C1	3.96	102.40	121.26	9	10
4	A	382	PX4	O1-P1-O2	3.96	130.88	112.44	6	8
4	A	385	PX4	C5-N1-C4	3.96	98.57	108.98	6	5
4	A	309	PX4	P1-O3-C1	3.96	102.42	121.26	13	11
4	A	311	PX4	C7-O7-C23	3.96	127.27	117.80	14	7
4	A	337	PX4	O4-P1-O2	3.96	124.61	108.94	10	2
4	A	357	PX4	O7-C7-C8	3.96	122.53	108.34	12	7
4	A	364	PX4	P1-O3-C1	3.96	102.43	121.26	9	9
4	A	415	PX4	O1-P1-O4	3.96	125.50	107.57	11	2
4	A	417	PX4	P1-O3-C1	3.96	102.43	121.26	4	13
4	A	357	PX4	O7-C23-O8	3.95	114.46	123.70	13	8
4	A	367	PX4	P1-O4-C6	3.95	98.69	121.35	14	9
4	A	396	PX4	C5-N1-C3	3.95	98.59	108.98	13	3
4	A	386	PX4	O5-C8-C7	3.95	119.79	108.40	1	7
4	A	399	PX4	P1-O4-C6	3.95	98.71	121.35	6	11
4	A	340	PX4	C12-C11-C10	3.95	98.61	113.13	11	2
4	A	400	PX4	O7-C7-C6	3.95	122.52	108.34	2	8
4	A	429	PX4	O5-C9-C10	3.95	123.88	111.83	9	5
4	A	318	PX4	O7-C7-C6	3.95	122.51	108.34	13	4
4	A	402	PX4	O7-C23-O8	3.95	114.48	123.70	5	4
4	A	325	PX4	O7-C23-C24	3.94	120.01	111.48	6	6
4	A	325	PX4	O7-C7-C6	3.95	122.50	108.34	10	3
4	A	394	PX4	P1-O4-C6	3.95	98.74	121.35	2	12
4	A	313	PX4	P1-O3-C1	3.94	102.49	121.26	4	12
4	A	349	PX4	C8-C7-C6	3.94	102.59	111.78	4	8
4	A	350	PX4	O7-C7-C8	3.94	122.50	108.34	14	5
4	A	399	PX4	O4-P1-O2	3.94	124.55	108.94	9	2
4	A	401	PX4	C8-C7-C6	3.94	102.60	111.78	1	6
4	A	318	PX4	O7-C23-O8	3.93	114.51	123.70	10	3
4	A	374	PX4	P1-O4-C6	3.93	98.80	121.35	1	12
4	A	325	PX4	P1-O3-C1	3.93	102.56	121.26	5	7
4	A	413	PX4	P1-O4-C6	3.93	98.84	121.35	13	9
4	A	429	PX4	O5-C8-C7	3.93	119.72	108.40	10	7
4	A	323	PX4	C26-C25-C24	3.93	98.70	113.13	14	1
4	A	405	PX4	P1-O4-C6	3.92	98.86	121.35	6	8
4	A	407	PX4	O3-P1-O2	3.93	93.38	108.94	3	6
4	A	312	PX4	O7-C23-C24	3.92	119.96	111.48	2	6
4	A	320	PX4	C7-O7-C23	3.92	127.18	117.80	8	2
4	A	327	PX4	C11-C10-C9	3.92	99.33	113.69	10	1
4	A	359	PX4	O7-C23-C24	3.92	119.97	111.48	13	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	324	PX4	P1-O3-C1	3.92	102.61	121.26	9	11
4	A	391	PX4	O4-P1-O2	3.92	124.47	108.94	9	4
4	A	400	PX4	C5-N1-C4	3.92	98.68	108.98	5	2
4	A	407	PX4	O7-C23-O8	3.92	114.54	123.70	2	6
4	A	354	PX4	O7-C7-C8	3.92	122.39	108.34	12	10
4	A	385	PX4	P1-O3-C1	3.91	102.62	121.26	8	12
4	A	392	PX4	C1-C2-N1	3.92	128.39	115.82	10	3
4	A	333	PX4	C7-O7-C23	3.91	108.43	117.80	10	7
4	A	325	PX4	O7-C23-O8	3.91	114.56	123.70	6	7
4	A	343	PX4	P1-O4-C6	3.91	98.93	121.35	9	11
4	A	382	PX4	P1-O3-C1	3.91	102.64	121.26	1	12
4	A	416	PX4	O1-P1-O2	3.91	130.65	112.44	8	12
4	A	325	PX4	O1-P1-O3	3.90	89.88	107.57	11	3
4	A	352	PX4	O1-P1-O2	3.90	130.59	112.44	8	8
4	A	389	PX4	P1-O4-C6	3.90	99.00	121.35	1	12
4	A	398	PX4	O5-C9-C10	3.90	123.73	111.83	2	7
4	A	408	PX4	O7-C7-C8	3.90	122.33	108.34	7	4
4	A	415	PX4	C1-C2-N1	3.90	128.34	115.82	5	4
4	A	352	PX4	C5-N1-C4	3.90	119.21	108.98	6	2
4	A	364	PX4	O1-P1-O3	3.90	89.91	107.57	6	2
4	A	375	PX4	C1-C2-N1	3.90	128.33	115.82	2	6
4	A	324	PX4	O7-C23-C24	3.89	119.91	111.48	2	6
4	A	342	PX4	O5-C8-C7	3.89	119.62	108.40	4	8
4	A	388	PX4	C7-O7-C23	3.90	127.12	117.80	7	3
4	A	425	PX4	O7-C7-C8	3.89	122.31	108.34	3	8
4	A	391	PX4	O1-P1-O2	3.89	130.54	112.44	10	11
4	A	426	PX4	C5-N1-C4	3.89	98.76	108.98	1	5
4	A	350	PX4	C8-C7-C6	3.89	102.72	111.78	13	8
4	A	320	PX4	O1-P1-O2	3.89	130.52	112.44	10	10
4	A	308	PX4	O4-P1-O2	3.88	124.32	108.94	12	4
4	A	346	PX4	C4-N1-C3	3.88	98.78	108.98	6	4
4	A	430	PX4	O7-C7-C8	3.88	122.27	108.34	6	5
4	A	328	PX4	O7-C23-C24	3.88	119.87	111.48	11	5
4	A	349	PX4	C7-O7-C23	3.88	127.08	117.80	1	7
4	A	376	PX4	O1-P1-O3	3.88	89.98	107.57	13	3
4	A	390	PX4	O7-C23-O8	3.88	114.64	123.70	10	3
4	A	358	PX4	P1-O4-C6	3.88	99.14	121.35	11	8
4	A	345	PX4	P1-O4-C6	3.87	99.15	121.35	9	9
4	A	356	PX4	O7-C7-C8	3.87	122.24	108.34	5	7
4	A	386	PX4	O1-P1-O2	3.87	130.46	112.44	13	7
4	A	344	PX4	C7-O7-C23	3.87	127.06	117.80	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	390	PX4	O5-C9-O6	3.87	113.94	123.63	12	6
4	A	411	PX4	P1-O4-C6	3.87	99.17	121.35	1	7
4	A	380	PX4	O5-C9-C10	3.87	123.64	111.83	5	6
4	A	416	PX4	O7-C23-O8	3.87	114.66	123.70	6	9
4	A	338	PX4	O7-C7-C8	3.87	122.22	108.34	5	4
4	A	342	PX4	O5-C9-C10	3.87	123.63	111.83	6	3
4	A	421	PX4	O3-P1-O2	3.87	93.61	108.94	10	6
4	A	307	PX4	P1-O3-C1	3.86	102.86	121.26	10	8
4	A	376	PX4	O5-C9-C10	3.87	123.62	111.83	5	5
4	A	344	PX4	O1-P1-O4	3.86	125.08	107.57	7	3
4	A	371	PX4	C5-N1-C3	3.86	98.83	108.98	8	2
4	A	345	PX4	O1-P1-O2	3.86	130.41	112.44	13	10
4	A	359	PX4	O7-C7-C8	3.86	122.20	108.34	6	5
4	A	360	PX4	P1-O4-C6	3.86	99.23	121.35	7	6
4	A	363	PX4	O7-C23-O8	3.86	114.68	123.70	11	7
4	A	384	PX4	P1-O4-C6	3.86	99.23	121.35	1	8
4	A	363	PX4	C20-C19-C18	3.86	94.86	114.37	5	2
4	A	389	PX4	C5-N1-C3	3.86	119.10	108.98	13	2
4	A	372	PX4	C5-N1-C4	3.85	98.86	108.98	13	3
4	A	316	PX4	P1-O3-C1	3.85	102.93	121.26	6	6
4	A	342	PX4	C26-C25-C24	3.85	98.97	113.13	13	3
4	A	392	PX4	C26-C25-C24	3.85	99.00	113.13	12	4
4	A	357	PX4	C20-C19-C18	3.84	94.94	114.37	8	2
4	A	376	PX4	C5-N1-C3	3.84	119.07	108.98	4	3
4	A	333	PX4	O5-C9-O6	3.84	114.02	123.63	2	4
4	A	337	PX4	O7-C23-C24	3.84	119.79	111.48	4	3
4	A	308	PX4	O1-P1-O3	3.84	90.18	107.57	8	2
4	A	413	PX4	O1-P1-O3	3.84	90.18	107.57	8	4
4	A	428	PX4	O5-C9-C10	3.84	123.53	111.83	1	5
4	A	329	PX4	O7-C23-O8	3.83	114.74	123.70	11	7
4	A	339	PX4	C34-C33-C32	3.83	95.01	114.37	2	1
4	A	366	PX4	O7-C7-C8	3.83	122.08	108.34	3	8
4	A	382	PX4	O7-C23-O8	3.83	114.75	123.70	2	5
4	A	420	PX4	O5-C9-O6	3.83	114.05	123.63	14	2
4	A	355	PX4	P1-O3-C1	3.83	103.03	121.26	12	9
4	A	392	PX4	O7-C7-C8	3.83	122.08	108.34	11	6
4	A	384	PX4	C1-C2-N1	3.83	128.11	115.82	8	3
4	A	307	PX4	P1-O4-C6	3.83	99.42	121.35	14	7
4	A	361	PX4	C8-C7-C6	3.83	102.86	111.78	13	8
4	A	310	PX4	C7-O7-C23	3.82	126.95	117.80	7	3
4	A	343	PX4	C5-N1-C4	3.82	98.93	108.98	10	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	309	PX4	O7-C7-C6	3.82	122.05	108.34	9	5
4	A	413	PX4	C4-N1-C3	3.82	98.94	108.98	8	3
4	A	332	PX4	O7-C7-C8	3.82	122.03	108.34	9	11
4	A	358	PX4	C5-N1-C3	3.81	98.96	108.98	11	3
4	A	404	PX4	P1-O4-C6	3.81	99.49	121.35	1	6
4	A	376	PX4	O7-C23-C24	3.81	119.73	111.48	5	7
4	A	383	PX4	C26-C25-C24	3.81	99.12	113.13	10	2
4	A	408	PX4	C7-O7-C23	3.81	126.92	117.80	6	5
4	A	334	PX4	O5-C9-C10	3.81	123.45	111.83	7	2
4	A	330	PX4	C8-C7-C6	3.81	102.90	111.78	1	7
4	A	400	PX4	P1-O4-C6	3.81	99.52	121.35	6	12
4	A	320	PX4	O5-C8-C7	3.81	119.37	108.40	4	8
4	A	321	PX4	O3-P1-O2	3.81	93.85	108.94	6	6
4	A	363	PX4	O1-P1-O2	3.80	130.14	112.44	5	10
4	A	421	PX4	C7-O7-C23	3.80	126.90	117.80	1	3
4	A	421	PX4	C5-N1-C4	3.80	98.99	108.98	5	4
4	A	382	PX4	C7-O7-C23	3.80	126.88	117.80	11	3
4	A	393	PX4	C4-N1-C3	3.80	99.00	108.98	14	3
4	A	417	PX4	O5-C8-C7	3.80	119.34	108.40	5	7
4	A	308	PX4	P1-O3-C1	3.79	103.20	121.26	13	11
4	A	362	PX4	C5-N1-C3	3.79	99.01	108.98	13	1
4	A	374	PX4	O5-C9-O6	3.79	114.14	123.63	3	2
4	A	315	PX4	O7-C23-O8	3.79	114.84	123.70	8	6
4	A	339	PX4	O1-P1-O3	3.79	90.39	107.57	3	6
4	A	354	PX4	P1-O4-C6	3.79	99.63	121.35	13	8
4	A	384	PX4	O1-P1-O2	3.79	130.08	112.44	3	5
4	A	306	PX4	O7-C23-C24	3.79	119.68	111.48	9	8
4	A	398	PX4	C7-O7-C23	3.79	126.86	117.80	5	6
4	A	347	PX4	P1-O3-C1	3.79	103.23	121.26	13	11
4	A	381	PX4	O3-P1-O2	3.79	93.93	108.94	6	5
4	A	385	PX4	C5-N1-C3	3.78	99.04	108.98	13	5
4	A	420	PX4	O7-C23-C24	3.78	119.67	111.48	9	9
4	A	321	PX4	O7-C23-O8	3.78	114.86	123.70	5	4
4	A	357	PX4	O1-P1-O2	3.78	130.04	112.44	3	8
4	A	408	PX4	C11-C10-C9	3.78	99.83	113.69	13	3
4	A	368	PX4	C7-O7-C23	3.78	126.84	117.80	1	4
4	A	426	PX4	O5-C9-C10	3.78	123.35	111.83	3	5
4	A	340	PX4	O7-C7-C6	3.77	121.88	108.34	1	3
4	A	347	PX4	O5-C9-C10	3.77	123.33	111.83	14	5
4	A	349	PX4	C5-N1-C3	3.77	99.07	108.98	13	1
4	A	425	PX4	P1-O3-C1	3.77	103.30	121.26	3	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	429	PX4	C8-C7-C6	3.77	102.99	111.78	3	9
4	A	388	PX4	O7-C7-C8	3.77	121.86	108.34	12	5
4	A	348	PX4	C5-N1-C3	3.76	118.86	108.98	8	1
4	A	388	PX4	O7-C23-O8	3.76	114.90	123.70	3	6
4	A	310	PX4	C8-C7-C6	3.76	103.01	111.78	8	10
4	A	311	PX4	O7-C23-C24	3.76	119.62	111.48	11	8
4	A	427	PX4	O7-C7-C8	3.76	121.84	108.34	10	6
4	A	398	PX4	O7-C23-O8	3.76	114.92	123.70	9	3
4	A	319	PX4	P1-O3-C1	3.76	103.38	121.26	10	8
4	A	425	PX4	C25-C24-C23	3.76	99.92	113.69	14	1
4	A	364	PX4	O7-C23-C24	3.76	119.61	111.48	13	7
4	A	380	PX4	O1-P1-O2	3.76	129.92	112.44	3	10
4	A	369	PX4	C5-N1-C4	3.75	99.11	108.98	12	5
4	A	378	PX4	C5-N1-C4	3.75	99.11	108.98	10	3
4	A	408	PX4	O5-C8-C7	3.75	119.22	108.40	12	7
4	A	337	PX4	O7-C7-C8	3.75	121.81	108.34	3	3
4	A	318	PX4	O1-P1-O2	3.75	129.90	112.44	4	8
4	A	338	PX4	C1-C2-N1	3.75	127.87	115.82	5	4
4	A	382	PX4	O7-C7-C8	3.75	121.80	108.34	6	6
4	A	355	PX4	O4-P1-O2	3.75	123.80	108.94	2	2
4	A	312	PX4	O4-P1-O2	3.75	94.08	108.94	9	2
4	A	368	PX4	O3-P1-O2	3.75	94.08	108.94	4	3
4	A	383	PX4	P1-O4-C6	3.75	99.88	121.35	14	9
4	A	406	PX4	O7-C7-C8	3.75	121.79	108.34	4	3
4	A	380	PX4	O7-C23-O8	3.74	114.95	123.70	13	5
4	A	382	PX4	P1-O4-C6	3.74	99.90	121.35	2	7
4	A	398	PX4	O1-P1-O2	3.74	129.85	112.44	4	8
4	A	349	PX4	O7-C7-C8	3.74	121.76	108.34	3	5
4	A	426	PX4	P1-O4-C6	3.74	99.91	121.35	14	8
4	A	327	PX4	O5-C8-C7	3.74	119.17	108.40	11	9
4	A	366	PX4	C11-C10-C9	3.74	99.99	113.69	7	4
4	A	374	PX4	O7-C23-O8	3.74	114.96	123.70	12	5
4	A	333	PX4	C8-O5-C9	3.73	103.47	117.12	3	1
4	A	420	PX4	C7-O7-C23	3.73	126.73	117.80	6	3
4	A	401	PX4	C5-N1-C3	3.73	118.78	108.98	7	3
4	A	414	PX4	O7-C23-O8	3.73	114.98	123.70	5	4
4	A	319	PX4	O5-C9-C10	3.73	123.21	111.83	11	3
4	A	427	PX4	O7-C23-O8	3.73	114.99	123.70	11	4
4	A	386	PX4	O7-C23-O8	3.72	115.00	123.70	7	3
4	A	392	PX4	P1-O3-C1	3.72	103.54	121.26	10	9
4	A	398	PX4	O1-P1-O4	3.72	124.42	107.57	7	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	315	PX4	O1-P1-O2	3.72	129.74	112.44	10	7
4	A	416	PX4	O7-C7-C6	3.72	121.68	108.34	5	7
4	A	417	PX4	O7-C23-C24	3.72	119.52	111.48	7	8
4	A	393	PX4	O1-P1-O2	3.71	129.72	112.44	14	6
4	A	367	PX4	O7-C23-C24	3.71	119.51	111.48	2	6
4	A	399	PX4	O1-P1-O2	3.71	129.72	112.44	5	8
4	A	372	PX4	C5-N1-C3	3.71	99.22	108.98	11	1
4	A	419	PX4	O7-C7-C6	3.71	121.67	108.34	7	6
4	A	310	PX4	C8-O5-C9	3.71	130.68	117.12	5	2
4	A	392	PX4	C5-N1-C3	3.71	118.73	108.98	3	3
4	A	397	PX4	P1-O4-C6	3.71	100.08	121.35	1	5
4	A	333	PX4	O5-C9-C10	3.71	123.14	111.83	2	7
4	A	359	PX4	O5-C8-C7	3.71	119.08	108.40	10	7
4	A	366	PX4	O7-C23-O8	3.70	115.04	123.70	8	3
4	A	378	PX4	O1-P1-O2	3.70	129.67	112.44	7	9
4	A	406	PX4	O1-P1-O2	3.70	129.67	112.44	4	8
4	A	408	PX4	O7-C23-O8	3.70	115.05	123.70	5	3
4	A	410	PX4	C5-N1-C3	3.70	99.25	108.98	1	3
4	A	414	PX4	P1-O3-C1	3.70	103.63	121.26	10	12
4	A	376	PX4	C11-C10-C9	3.70	100.13	113.69	14	3
4	A	389	PX4	C5-N1-C4	3.70	99.25	108.98	9	3
4	A	414	PX4	O8-C23-C24	3.70	109.30	123.78	7	1
4	A	343	PX4	C4-N1-C3	3.70	118.70	108.98	4	3
4	A	355	PX4	O5-C8-C7	3.70	119.06	108.40	10	5
4	A	403	PX4	O5-C8-C7	3.70	119.06	108.40	8	5
4	A	319	PX4	O1-P1-O2	3.70	129.64	112.44	5	9
4	A	351	PX4	O7-C23-C24	3.70	119.48	111.48	6	4
4	A	318	PX4	O7-C7-C8	3.70	121.60	108.34	8	4
4	A	358	PX4	O1-P1-O2	3.69	129.63	112.44	12	9
4	A	388	PX4	C12-C11-C10	3.70	99.55	113.13	4	4
4	A	392	PX4	O5-C9-O6	3.69	114.39	123.63	12	3
4	A	353	PX4	P1-O4-C6	3.69	100.20	121.35	12	7
4	A	377	PX4	C26-C25-C24	3.69	99.56	113.13	7	1
4	A	323	PX4	O5-C9-O6	3.69	114.40	123.63	8	4
4	A	355	PX4	C7-O7-C23	3.69	126.63	117.80	2	4
4	A	379	PX4	C11-C10-C9	3.69	100.17	113.69	1	3
4	A	386	PX4	O7-C7-C8	3.69	121.58	108.34	3	6
4	A	420	PX4	O5-C9-C10	3.69	123.08	111.83	7	5
4	A	319	PX4	O7-C23-C24	3.69	119.45	111.48	4	9
4	A	335	PX4	C7-O7-C23	3.69	126.62	117.80	13	5
4	A	382	PX4	O3-P1-O2	3.68	94.33	108.94	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	403	PX4	P1-O4-C6	3.69	100.23	121.35	14	11
4	A	340	PX4	O5-C8-C7	3.68	119.02	108.40	9	7
4	A	382	PX4	C26-C25-C24	3.68	99.59	113.13	4	3
4	A	350	PX4	O7-C23-O8	3.68	115.10	123.70	14	4
4	A	399	PX4	O7-C7-C6	3.68	121.56	108.34	3	8
4	A	306	PX4	O7-C23-O8	3.68	115.10	123.70	9	8
4	A	321	PX4	O3-C1-C2	3.68	127.34	109.65	5	2
4	A	323	PX4	C5-N1-C4	3.68	99.31	108.98	1	4
4	A	423	PX4	C5-N1-C3	3.68	99.31	108.98	4	4
4	A	365	PX4	O1-P1-O2	3.68	129.55	112.44	14	7
4	A	396	PX4	O7-C23-C24	3.68	119.44	111.48	6	6
4	A	408	PX4	O1-P1-O3	3.67	90.94	107.57	2	4
4	A	409	PX4	P1-O4-C6	3.67	100.32	121.35	6	9
4	A	338	PX4	P1-O4-C6	3.67	100.34	121.35	13	8
4	A	429	PX4	P1-O4-C6	3.67	100.33	121.35	12	9
4	A	341	PX4	C12-C11-C10	3.67	99.66	113.13	8	2
4	A	409	PX4	O7-C23-O8	3.67	115.13	123.70	3	6
4	A	313	PX4	P1-O4-C6	3.66	100.35	121.35	8	7
4	A	392	PX4	C8-C7-C6	3.66	103.24	111.78	10	9
4	A	308	PX4	O7-C23-O8	3.66	115.14	123.70	12	5
4	A	360	PX4	C4-N1-C3	3.66	99.36	108.98	2	3
4	A	417	PX4	C25-C24-C23	3.66	100.28	113.69	13	3
4	A	325	PX4	C5-N1-C4	3.66	99.36	108.98	4	4
4	A	349	PX4	C1-C2-N1	3.66	127.57	115.82	7	2
4	A	325	PX4	C5-N1-C2	3.66	95.37	109.91	1	2
4	A	368	PX4	P1-O3-C1	3.66	103.84	121.26	10	8
4	A	370	PX4	C4-N1-C3	3.66	99.36	108.98	13	4
4	A	387	PX4	O3-P1-O2	3.66	94.43	108.94	1	4
4	A	422	PX4	O7-C7-C6	3.66	121.47	108.34	4	6
4	A	430	PX4	O4-P1-O2	3.66	123.44	108.94	14	2
4	A	335	PX4	C1-C2-N1	3.66	127.56	115.82	7	5
4	A	364	PX4	O3-P1-O2	3.66	94.44	108.94	2	4
4	A	372	PX4	P1-O3-C1	3.66	103.85	121.26	1	7
4	A	373	PX4	O1-P1-O2	3.66	129.46	112.44	2	9
4	A	417	PX4	O3-P1-O2	3.66	94.44	108.94	7	4
4	A	429	PX4	O7-C7-C6	3.66	121.46	108.34	2	7
4	A	341	PX4	O5-C9-O6	3.66	114.48	123.63	1	2
4	A	367	PX4	P1-O3-C1	3.66	103.86	121.26	14	9
4	A	368	PX4	C5-N1-C3	3.66	99.37	108.98	14	3
4	A	399	PX4	O5-C8-C7	3.65	118.93	108.40	5	6
4	A	405	PX4	O7-C7-C6	3.66	121.46	108.34	12	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	316	PX4	C4-N1-C3	3.65	118.57	108.98	3	2
4	A	416	PX4	C7-O7-C23	3.65	109.06	117.80	10	6
4	A	428	PX4	O3-P1-O2	3.65	94.46	108.94	5	5
4	A	349	PX4	C5-N1-C4	3.65	99.39	108.98	12	4
4	A	359	PX4	O7-C23-O8	3.65	115.17	123.70	2	2
4	A	418	PX4	O4-P1-O2	3.65	94.47	108.94	3	3
4	A	423	PX4	O7-C7-C6	3.64	121.42	108.34	13	6
4	A	317	PX4	C5-N1-C4	3.64	99.41	108.98	9	3
4	A	318	PX4	C3-N1-C2	3.64	124.39	109.91	7	3
4	A	336	PX4	C8-C7-C6	3.64	103.30	111.78	5	5
4	A	382	PX4	C5-N1-C3	3.64	99.41	108.98	10	5
4	A	379	PX4	O5-C8-C7	3.64	118.88	108.40	9	10
4	A	416	PX4	C4-N1-C3	3.64	118.53	108.98	3	1
4	A	417	PX4	O7-C7-C6	3.64	121.40	108.34	3	6
4	A	322	PX4	C5-N1-C4	3.64	99.43	108.98	13	4
4	A	308	PX4	O7-C7-C8	3.63	121.38	108.34	7	7
4	A	364	PX4	O7-C7-C6	3.63	121.38	108.34	12	6
4	A	421	PX4	O4-P1-O2	3.63	123.33	108.94	11	4
4	A	410	PX4	O5-C8-C7	3.63	118.86	108.40	5	9
4	A	420	PX4	P1-O4-C6	3.63	100.55	121.35	3	7
4	A	313	PX4	O4-P1-O2	3.63	123.32	108.94	10	3
4	A	348	PX4	O7-C7-C6	3.63	121.36	108.34	4	6
4	A	406	PX4	O5-C9-O6	3.63	114.55	123.63	4	3
4	A	420	PX4	O1-P1-O2	3.63	129.32	112.44	9	10
4	A	306	PX4	C15-C14-C13	3.63	96.04	114.37	1	2
4	A	310	PX4	O5-C8-C7	3.63	118.85	108.40	5	6
4	A	340	PX4	P1-O4-C6	3.63	100.58	121.35	8	8
4	A	425	PX4	C4-N1-C3	3.63	99.45	108.98	5	5
4	A	334	PX4	O7-C23-O8	3.62	115.25	123.70	2	4
4	A	395	PX4	O7-C23-C24	3.62	119.31	111.48	1	7
4	A	403	PX4	O5-C9-C10	3.62	122.86	111.83	5	4
4	A	391	PX4	C7-O7-C23	3.62	126.45	117.80	2	4
4	A	415	PX4	O5-C8-C7	3.61	118.81	108.40	6	6
4	A	358	PX4	O7-C7-C8	3.61	121.30	108.34	4	5
4	A	400	PX4	C26-C25-C24	3.61	99.86	113.13	6	2
4	A	368	PX4	O1-P1-O4	3.61	123.92	107.57	11	3
4	A	395	PX4	O5-C8-C7	3.61	118.80	108.40	14	5
4	A	325	PX4	O1-P1-O2	3.61	129.22	112.44	14	7
4	A	379	PX4	O7-C23-C24	3.61	119.28	111.48	7	6
4	A	409	PX4	O5-C9-O6	3.61	114.61	123.63	2	3
4	A	422	PX4	O5-C9-C10	3.61	122.83	111.83	10	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	C7-O7-C23	3.60	109.17	117.80	3	2
4	A	352	PX4	O7-C7-C8	3.60	121.28	108.34	3	5
4	A	414	PX4	O3-P1-O2	3.60	94.65	108.94	4	4
4	A	322	PX4	O1-P1-O2	3.60	129.20	112.44	12	7
4	A	331	PX4	O1-P1-O2	3.60	129.20	112.44	9	8
4	A	306	PX4	O7-C7-C8	3.60	121.26	108.34	2	7
4	A	412	PX4	P1-O4-C6	3.60	100.72	121.35	7	8
4	A	430	PX4	P1-O3-C1	3.60	104.12	121.26	6	12
4	A	387	PX4	C14-C13-C12	3.60	96.18	114.37	12	1
4	A	309	PX4	O3-P1-O2	3.60	94.68	108.94	11	2
4	A	356	PX4	C11-C10-C9	3.60	100.52	113.69	9	2
4	A	388	PX4	P1-O3-C1	3.60	104.14	121.26	1	11
4	A	308	PX4	O1-P1-O4	3.59	123.86	107.57	2	5
4	A	340	PX4	C4-N1-C3	3.59	99.54	108.98	14	2
4	A	326	PX4	P1-O4-C6	3.59	100.76	121.35	7	9
4	A	384	PX4	C8-O5-C9	3.59	103.99	117.12	3	1
4	A	386	PX4	O7-C7-C6	3.59	121.23	108.34	12	5
4	A	388	PX4	P1-O4-C6	3.59	100.76	121.35	4	9
4	A	426	PX4	P1-O3-C1	3.59	104.15	121.26	6	12
4	A	342	PX4	C7-O7-C23	3.59	126.39	117.80	8	4
4	A	396	PX4	C1-C2-N1	3.59	127.35	115.82	14	1
4	A	337	PX4	C1-C2-N1	3.59	127.34	115.82	8	4
4	A	377	PX4	P1-O4-C6	3.59	100.78	121.35	9	11
4	A	414	PX4	C5-N1-C4	3.59	99.55	108.98	7	3
4	A	367	PX4	O5-C9-O6	3.59	114.65	123.63	7	6
4	A	309	PX4	O7-C23-O8	3.59	115.32	123.70	7	7
4	A	324	PX4	C1-C2-N1	3.59	127.33	115.82	14	3
4	A	311	PX4	O7-C7-C8	3.58	121.20	108.34	11	12
4	A	391	PX4	C5-N1-C3	3.58	99.57	108.98	11	2
4	A	416	PX4	O5-C9-C10	3.58	122.76	111.83	7	3
4	A	426	PX4	O4-P1-O2	3.58	123.13	108.94	13	3
4	A	389	PX4	C4-N1-C3	3.58	99.57	108.98	12	5
4	A	398	PX4	P1-O4-C6	3.58	100.83	121.35	2	7
4	A	322	PX4	C15-C14-C13	3.58	96.27	114.37	8	1
4	A	398	PX4	C12-C11-C10	3.58	99.97	113.13	14	1
4	A	332	PX4	O4-P1-O2	3.58	123.12	108.94	7	8
4	A	317	PX4	O7-C7-C8	3.58	121.18	108.34	11	9
4	A	405	PX4	O4-P1-O2	3.58	94.76	108.94	9	2
4	A	408	PX4	C5-N1-C4	3.58	99.58	108.98	13	2
4	A	308	PX4	C12-C11-C10	3.58	99.99	113.13	5	1
4	A	329	PX4	O1-P1-O2	3.58	129.08	112.44	13	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	352	PX4	C1-C2-N1	3.58	127.30	115.82	3	4
4	A	314	PX4	O7-C23-O8	3.57	115.35	123.70	1	3
4	A	370	PX4	O5-C9-C10	3.57	122.73	111.83	4	2
4	A	381	PX4	P1-O3-C1	3.57	104.25	121.26	12	12
4	A	409	PX4	O5-C9-C10	3.57	122.73	111.83	5	4
4	A	308	PX4	O1-P1-O2	3.57	129.05	112.44	8	8
4	A	330	PX4	O5-C9-C10	3.57	122.72	111.83	13	4
4	A	326	PX4	O5-C9-O6	3.57	114.70	123.63	9	6
4	A	348	PX4	C13-C12-C11	3.57	96.33	114.37	13	3
4	A	348	PX4	C8-O5-C9	3.57	104.08	117.12	8	3
4	A	354	PX4	O1-P1-O4	3.57	123.74	107.57	3	4
4	A	355	PX4	O3-P1-O2	3.57	94.80	108.94	10	3
4	A	334	PX4	C7-O7-C23	3.56	109.26	117.80	5	4
4	A	378	PX4	O5-C8-C7	3.57	118.67	108.40	12	8
4	A	336	PX4	P1-O4-C6	3.56	100.93	121.35	14	7
4	A	361	PX4	O4-P1-O2	3.56	123.06	108.94	14	6
4	A	361	PX4	P1-O4-C6	3.56	100.94	121.35	13	9
4	A	378	PX4	O5-C9-O6	3.56	114.72	123.63	2	6
4	A	381	PX4	C5-N1-C4	3.56	118.33	108.98	8	5
4	A	344	PX4	P1-O4-C6	3.56	100.95	121.35	3	9
4	A	354	PX4	C5-N1-C4	3.56	99.63	108.98	10	3
4	A	373	PX4	P1-O3-C1	3.56	104.31	121.26	12	10
4	A	375	PX4	O5-C9-O6	3.56	114.72	123.63	4	5
4	A	419	PX4	C1-C2-N1	3.56	127.25	115.82	10	3
4	A	370	PX4	C5-N1-C4	3.56	99.63	108.98	4	4
4	A	399	PX4	C5-N1-C4	3.56	118.32	108.98	13	4
4	A	420	PX4	O1-P1-O3	3.56	91.44	107.57	10	8
4	A	339	PX4	O7-C23-O8	3.56	115.39	123.70	11	5
4	A	423	PX4	O3-P1-O2	3.56	94.84	108.94	8	4
4	A	306	PX4	O1-P1-O2	3.55	128.96	112.44	13	8
4	A	375	PX4	C20-C19-C18	3.55	96.43	114.37	3	2
4	A	332	PX4	O7-C23-O8	3.55	115.41	123.70	13	7
4	A	360	PX4	O5-C9-O6	3.54	114.76	123.63	8	5
4	A	403	PX4	C1-C2-N1	3.54	127.19	115.82	3	2
4	A	421	PX4	O7-C7-C6	3.54	121.06	108.34	9	4
4	A	371	PX4	C7-O7-C23	3.54	126.27	117.80	8	6
4	A	373	PX4	C1-C2-N1	3.54	127.19	115.82	3	3
4	A	382	PX4	C4-N1-C3	3.54	118.28	108.98	3	3
4	A	390	PX4	O1-P1-O2	3.54	128.91	112.44	14	4
4	A	335	PX4	C26-C25-C24	3.54	100.13	113.13	11	2
4	A	356	PX4	O1-P1-O2	3.54	128.91	112.44	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	356	PX4	O5-C8-C7	3.54	118.60	108.40	6	7
4	A	381	PX4	O7-C7-C6	3.54	121.04	108.34	11	4
4	A	407	PX4	P1-O4-C6	3.54	101.07	121.35	12	10
4	A	409	PX4	O7-C23-C24	3.54	119.14	111.48	8	7
4	A	407	PX4	O1-P1-O2	3.54	128.90	112.44	11	9
4	A	373	PX4	O3-P1-O2	3.54	94.92	108.94	8	4
4	A	424	PX4	O5-C9-C10	3.54	122.62	111.83	11	3
4	A	419	PX4	C15-C14-C13	3.53	96.51	114.37	6	1
4	A	429	PX4	O4-P1-O2	3.53	122.94	108.94	3	5
4	A	421	PX4	O7-C7-C8	3.53	121.02	108.34	4	3
4	A	315	PX4	O7-C7-C6	3.53	121.01	108.34	7	6
4	A	307	PX4	C19-C18-C17	3.53	96.53	114.37	7	1
4	A	390	PX4	O5-C8-C7	3.53	118.57	108.40	3	9
4	A	408	PX4	O1-P1-O2	3.53	128.87	112.44	11	8
4	A	313	PX4	O7-C23-C24	3.53	119.11	111.48	6	6
4	A	355	PX4	C5-N1-C2	3.53	123.94	109.91	12	3
4	A	341	PX4	P1-O4-C6	3.53	101.14	121.35	9	8
4	A	341	PX4	O5-C8-C7	3.53	118.56	108.40	11	6
4	A	351	PX4	C7-O7-C23	3.53	126.23	117.80	6	6
4	A	425	PX4	C12-C11-C10	3.53	100.17	113.13	11	1
4	A	318	PX4	C18-C17-C16	3.52	96.56	114.37	6	2
4	A	325	PX4	C34-C33-C32	3.52	96.57	114.37	13	2
4	A	349	PX4	O1-P1-O2	3.52	128.83	112.44	11	6
4	A	311	PX4	O5-C9-C10	3.52	122.57	111.83	2	5
4	A	403	PX4	C5-N1-C2	3.52	123.91	109.91	3	2
4	A	320	PX4	C19-C18-C17	3.52	96.58	114.37	8	2
4	A	364	PX4	C7-O7-C23	3.52	109.38	117.80	11	3
4	A	373	PX4	O1-P1-O4	3.52	123.51	107.57	1	2
4	A	385	PX4	P1-O4-C6	3.51	101.21	121.35	12	11
4	A	422	PX4	C4-N1-C3	3.52	99.74	108.98	12	5
4	A	337	PX4	P1-O4-C6	3.51	101.22	121.35	3	9
4	A	357	PX4	P1-O4-C6	3.51	101.22	121.35	12	10
4	A	355	PX4	C5-N1-C3	3.51	99.75	108.98	12	4
4	A	312	PX4	O1-P1-O2	3.51	128.77	112.44	5	9
4	A	332	PX4	P1-O4-C6	3.51	101.23	121.35	11	9
4	A	335	PX4	O7-C7-C8	3.51	120.94	108.34	12	8
4	A	350	PX4	P1-O3-C1	3.51	104.55	121.26	5	10
4	A	370	PX4	O7-C23-O8	3.51	115.50	123.70	6	2
4	A	403	PX4	O1-P1-O2	3.51	128.77	112.44	3	10
4	A	340	PX4	C33-C32-C31	3.51	96.64	114.37	2	2
4	A	364	PX4	O1-P1-O2	3.51	128.76	112.44	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	425	PX4	O5-C9-C10	3.51	122.53	111.83	10	3
4	A	332	PX4	C1-C2-N1	3.50	127.07	115.82	14	7
4	A	365	PX4	P1-O4-C6	3.51	101.26	121.35	5	10
4	A	395	PX4	C20-C19-C18	3.50	96.65	114.37	13	4
4	A	374	PX4	O7-C23-C24	3.50	119.06	111.48	7	5
4	A	346	PX4	O7-C23-O8	3.50	115.52	123.70	1	7
4	A	367	PX4	C1-C2-N1	3.50	127.06	115.82	7	2
4	A	321	PX4	O1-P1-O3	3.50	91.71	107.57	3	6
4	A	379	PX4	O5-C9-C10	3.50	122.50	111.83	5	5
4	A	405	PX4	P1-O3-C1	3.50	104.61	121.26	9	8
4	A	430	PX4	P1-O4-C6	3.50	101.30	121.35	14	11
4	A	313	PX4	C5-N1-C3	3.50	118.16	108.98	1	4
4	A	332	PX4	C11-C10-C9	3.50	100.88	113.69	13	1
4	A	430	PX4	C4-N1-C3	3.50	99.79	108.98	7	4
4	A	341	PX4	C5-N1-C4	3.49	99.80	108.98	14	2
4	A	369	PX4	C5-N1-C3	3.49	118.15	108.98	10	4
4	A	356	PX4	P1-O4-C6	3.49	101.34	121.35	6	11
4	A	386	PX4	C1-C2-N1	3.49	127.03	115.82	11	4
4	A	396	PX4	P1-O3-C1	3.49	104.64	121.26	14	11
4	A	415	PX4	P1-O4-C6	3.49	101.34	121.35	12	6
4	A	430	PX4	O7-C7-C6	3.49	120.87	108.34	11	4
4	A	383	PX4	O7-C7-C8	3.49	120.86	108.34	13	4
4	A	377	PX4	O3-P1-O2	3.49	95.11	108.94	10	4
4	A	323	PX4	C32-C31-C30	3.49	96.75	114.37	10	2
4	A	381	PX4	C5-N1-C3	3.49	99.82	108.98	8	4
4	A	317	PX4	C4-N1-C3	3.48	99.82	108.98	8	3
4	A	325	PX4	C8-O5-C9	3.48	104.38	117.12	10	3
4	A	348	PX4	P1-O4-C6	3.48	101.38	121.35	13	7
4	A	308	PX4	P1-O4-C6	3.48	101.40	121.35	7	9
4	A	344	PX4	O5-C9-O6	3.48	114.92	123.63	10	4
4	A	388	PX4	C5-N1-C3	3.48	118.12	108.98	8	4
4	A	397	PX4	O1-P1-O2	3.48	128.65	112.44	3	6
4	A	430	PX4	C20-C19-C18	3.48	96.76	114.37	3	1
4	A	362	PX4	O5-C9-C10	3.48	122.44	111.83	5	4
4	A	323	PX4	O7-C23-O8	3.48	115.58	123.70	10	5
4	A	324	PX4	P1-O4-C6	3.48	101.43	121.35	10	7
4	A	351	PX4	P1-O4-C6	3.48	101.43	121.35	12	6
4	A	353	PX4	C5-N1-C3	3.48	99.84	108.98	2	6
4	A	397	PX4	O5-C9-C10	3.48	122.44	111.83	10	4
4	A	306	PX4	C12-C11-C10	3.47	100.36	113.13	8	4
4	A	318	PX4	C26-C25-C24	3.48	100.36	113.13	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	322	PX4	O3-P1-O2	3.48	95.16	108.94	14	4
4	A	399	PX4	C5-N1-C3	3.48	99.85	108.98	9	4
4	A	418	PX4	O1-P1-O3	3.48	123.32	107.57	11	1
4	A	308	PX4	C5-N1-C3	3.47	99.86	108.98	12	2
4	A	318	PX4	P1-O4-C6	3.47	101.46	121.35	1	7
4	A	329	PX4	C4-N1-C2	3.47	96.12	109.91	14	1
4	A	345	PX4	O5-C8-C7	3.47	118.39	108.40	3	4
4	A	353	PX4	O1-P1-O2	3.47	128.58	112.44	1	9
4	A	388	PX4	O5-C9-O6	3.47	114.95	123.63	8	4
4	A	418	PX4	C5-N1-C2	3.47	123.70	109.91	2	2
4	A	406	PX4	P1-O4-C6	3.47	101.49	121.35	13	8
4	A	325	PX4	C3-N1-C2	3.46	123.68	109.91	2	3
4	A	398	PX4	O5-C8-C7	3.47	118.39	108.40	4	7
4	A	364	PX4	O1-P1-O4	3.46	123.27	107.57	7	1
4	A	308	PX4	C26-C25-C24	3.46	100.41	113.13	5	4
4	A	362	PX4	P1-O3-C1	3.46	104.78	121.26	7	7
4	A	340	PX4	O5-C9-O6	3.46	114.97	123.63	4	7
4	A	382	PX4	O5-C9-O6	3.46	114.97	123.63	14	4
4	A	387	PX4	C11-C10-C9	3.46	126.38	113.69	9	2
4	A	381	PX4	O1-P1-O3	3.46	91.89	107.57	5	4
4	A	410	PX4	O5-C9-C10	3.46	122.38	111.83	13	4
4	A	345	PX4	C4-N1-C3	3.46	99.90	108.98	8	3
4	A	361	PX4	O7-C23-O8	3.46	115.62	123.70	5	4
4	A	375	PX4	C26-C25-C24	3.46	100.43	113.13	14	5
4	A	415	PX4	O5-C9-O6	3.45	114.99	123.63	12	2
4	A	417	PX4	C7-O7-C23	3.46	126.07	117.80	14	5
4	A	378	PX4	O3-P1-O2	3.45	95.26	108.94	8	1
4	A	420	PX4	O3-P1-O2	3.45	95.26	108.94	7	6
4	A	425	PX4	C5-N1-C3	3.45	99.91	108.98	8	4
4	A	328	PX4	C7-O7-C23	3.45	126.05	117.80	12	3
4	A	344	PX4	O1-P1-O2	3.45	128.48	112.44	12	6
4	A	377	PX4	C4-N1-C3	3.45	99.92	108.98	6	6
4	A	388	PX4	O7-C7-C6	3.45	120.71	108.34	9	5
4	A	421	PX4	O5-C9-C10	3.45	122.35	111.83	7	5
4	A	319	PX4	C4-N1-C2	3.44	123.60	109.91	14	1
4	A	326	PX4	O7-C7-C8	3.45	120.70	108.34	7	4
4	A	378	PX4	P1-O4-C6	3.44	101.62	121.35	7	9
4	A	387	PX4	C1-C2-N1	3.44	126.86	115.82	11	5
4	A	414	PX4	C8-O5-C9	3.44	104.55	117.12	11	3
4	A	390	PX4	C4-N1-C3	3.44	99.95	108.98	1	4
4	A	336	PX4	O1-P1-O2	3.43	128.42	112.44	4	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	370	PX4	C1-C2-N1	3.43	126.85	115.82	6	7
4	A	412	PX4	C7-O7-C23	3.43	126.02	117.80	5	5
4	A	314	PX4	C28-C27-C26	3.43	97.01	114.37	12	1
4	A	354	PX4	O1-P1-O2	3.43	128.42	112.44	12	12
4	A	309	PX4	O1-P1-O2	3.43	128.40	112.44	11	10
4	A	338	PX4	O7-C23-O8	3.43	115.68	123.70	2	7
4	A	355	PX4	O7-C7-C8	3.43	120.65	108.34	1	8
4	A	378	PX4	O5-C9-C10	3.43	122.30	111.83	13	6
4	A	406	PX4	P1-O3-C1	3.43	104.93	121.26	4	10
4	A	427	PX4	O4-P1-O2	3.43	122.53	108.94	5	2
4	A	309	PX4	O5-C9-C10	3.43	122.28	111.83	8	3
4	A	332	PX4	C32-C31-C30	3.43	97.04	114.37	13	2
4	A	371	PX4	O5-C9-C10	3.43	122.29	111.83	10	4
4	A	382	PX4	C11-C10-C9	3.43	126.26	113.69	2	2
4	A	388	PX4	O1-P1-O2	3.43	128.39	112.44	3	8
4	A	424	PX4	O8-C23-C24	3.43	110.37	123.78	10	3
4	A	334	PX4	P1-O3-C1	3.43	104.95	121.26	13	11
4	A	345	PX4	O5-C9-O6	3.43	115.06	123.63	5	3
4	A	313	PX4	O7-C7-C6	3.42	120.63	108.34	1	6
4	A	316	PX4	C32-C31-C30	3.42	97.06	114.37	2	2
4	A	320	PX4	O3-P1-O2	3.42	95.36	108.94	6	2
4	A	360	PX4	C5-N1-C3	3.42	99.98	108.98	14	1
4	A	417	PX4	O5-C9-O6	3.42	115.06	123.63	7	4
4	A	306	PX4	P1-O4-C6	3.42	101.74	121.35	7	9
4	A	343	PX4	O7-C7-C8	3.42	120.62	108.34	7	8
4	A	350	PX4	O7-C7-C6	3.42	120.62	108.34	7	9
4	A	363	PX4	P1-O3-C1	3.42	104.97	121.26	8	12
4	A	360	PX4	O1-P1-O2	3.42	128.36	112.44	14	8
4	A	371	PX4	O7-C23-O8	3.42	115.71	123.70	13	3
4	A	424	PX4	C4-N1-C3	3.42	117.96	108.98	14	3
4	A	392	PX4	C30-C29-C28	3.42	97.09	114.37	11	1
4	A	409	PX4	O1-P1-O4	3.42	123.07	107.57	7	2
4	A	427	PX4	O7-C7-C6	3.42	120.60	108.34	1	2
4	A	421	PX4	C11-C10-C9	3.41	101.19	113.69	9	2
4	A	323	PX4	O7-C7-C8	3.41	120.58	108.34	7	9
4	A	310	PX4	C33-C32-C31	3.41	97.13	114.37	1	2
4	A	398	PX4	C1-C2-N1	3.41	126.77	115.82	10	1
4	A	313	PX4	C19-C18-C17	3.41	97.14	114.37	4	2
4	A	319	PX4	P1-O4-C6	3.41	101.82	121.35	14	8
4	A	306	PX4	O5-C8-C7	3.40	118.21	108.40	3	6
4	A	342	PX4	O7-C7-C8	3.40	120.56	108.34	10	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	388	PX4	C4-N1-C3	3.40	100.03	108.98	2	3
4	A	402	PX4	C5-N1-C4	3.40	100.03	108.98	11	2
4	A	322	PX4	C7-O7-C23	3.40	125.94	117.80	11	5
4	A	359	PX4	C13-C12-C11	3.40	97.18	114.37	7	1
4	A	363	PX4	P1-O4-C6	3.40	101.86	121.35	8	9
4	A	306	PX4	O7-C7-C6	3.40	120.54	108.34	6	4
4	A	367	PX4	O3-P1-O2	3.40	95.46	108.94	14	2
4	A	400	PX4	C25-C24-C23	3.40	101.25	113.69	11	2
4	A	416	PX4	C12-C11-C10	3.40	100.64	113.13	11	3
4	A	329	PX4	C11-C10-C9	3.39	101.26	113.69	4	2
4	A	336	PX4	P1-O3-C1	3.39	105.11	121.26	14	9
4	A	373	PX4	C33-C32-C31	3.39	97.22	114.37	3	1
4	A	413	PX4	O1-P1-O2	3.39	128.23	112.44	2	7
4	A	421	PX4	O1-P1-O3	3.39	92.18	107.57	8	3
4	A	427	PX4	O1-P1-O2	3.39	128.23	112.44	2	11
4	A	337	PX4	P1-O3-C1	3.39	105.12	121.26	14	10
4	A	396	PX4	C5-N1-C4	3.39	100.07	108.98	7	2
4	A	423	PX4	C25-C24-C23	3.39	101.27	113.69	14	3
4	A	424	PX4	O7-C7-C8	3.39	120.51	108.34	4	6
4	A	308	PX4	C5-N1-C4	3.39	100.08	108.98	10	4
4	A	353	PX4	C17-C16-C15	3.39	97.24	114.37	12	3
4	A	386	PX4	C5-N1-C2	3.39	96.44	109.91	6	2
4	A	319	PX4	C5-N1-C3	3.39	117.87	108.98	8	3
4	A	322	PX4	C26-C25-C24	3.39	100.68	113.13	8	3
4	A	318	PX4	P1-O3-C1	3.39	105.14	121.26	12	8
4	A	317	PX4	O3-P1-O2	3.38	95.52	108.94	3	1
4	A	346	PX4	O7-C7-C8	3.38	120.49	108.34	10	9
4	A	387	PX4	O4-P1-O2	3.38	122.35	108.94	2	6
4	A	402	PX4	O1-P1-O2	3.38	128.19	112.44	2	6
4	A	412	PX4	O1-P1-O2	3.38	128.19	112.44	5	11
4	A	366	PX4	P1-O4-C6	3.38	101.97	121.35	9	5
4	A	334	PX4	C4-N1-C3	3.38	117.86	108.98	1	4
4	A	380	PX4	O7-C7-C8	3.38	120.47	108.34	5	5
4	A	307	PX4	C1-C2-N1	3.38	126.67	115.82	8	5
4	A	404	PX4	O7-C7-C6	3.38	120.46	108.34	11	1
4	A	335	PX4	O1-P1-O2	3.38	128.15	112.44	13	8
4	A	397	PX4	C7-O7-C23	3.38	125.88	117.80	11	2
4	A	402	PX4	C7-O7-C23	3.38	125.88	117.80	2	3
4	A	341	PX4	C8-C7-C6	3.37	103.92	111.78	3	3
4	A	338	PX4	C12-C11-C10	3.37	100.74	113.13	11	2
4	A	360	PX4	O7-C7-C8	3.37	120.44	108.34	11	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	369	PX4	C1-C2-N1	3.37	126.65	115.82	8	2
4	A	374	PX4	C25-C24-C23	3.37	101.34	113.69	5	1
4	A	386	PX4	C25-C24-C23	3.37	101.34	113.69	7	3
4	A	323	PX4	C5-N1-C3	3.37	100.12	108.98	5	5
4	A	347	PX4	O1-P1-O2	3.37	128.12	112.44	4	6
4	A	351	PX4	O7-C7-C6	3.37	120.43	108.34	9	3
4	A	352	PX4	C31-C30-C29	3.37	97.33	114.37	11	2
4	A	378	PX4	C12-C11-C10	3.37	100.74	113.13	2	1
4	A	398	PX4	O4-P1-O2	3.37	95.58	108.94	1	4
4	A	355	PX4	O7-C23-O8	3.37	115.83	123.70	8	3
4	A	373	PX4	C25-C24-C23	3.37	101.36	113.69	2	4
4	A	377	PX4	C5-N1-C3	3.36	100.14	108.98	10	5
4	A	342	PX4	O7-C7-C6	3.36	120.41	108.34	12	6
4	A	366	PX4	C4-N1-C3	3.36	100.14	108.98	2	5
4	A	357	PX4	O5-C9-O6	3.36	115.22	123.63	1	2
4	A	360	PX4	C25-C24-C23	3.36	101.37	113.69	13	4
4	A	381	PX4	P1-O4-C6	3.36	102.08	121.35	3	7
4	A	351	PX4	O3-P1-O2	3.36	95.62	108.94	8	2
4	A	385	PX4	C3-N1-C2	3.36	96.55	109.91	8	1
4	A	393	PX4	O7-C7-C8	3.36	120.40	108.34	11	3
4	A	409	PX4	C7-O7-C23	3.36	125.83	117.80	8	3
4	A	315	PX4	C4-N1-C3	3.36	100.16	108.98	8	4
4	A	379	PX4	C4-N1-C3	3.36	100.16	108.98	9	3
4	A	383	PX4	C11-C10-C9	3.36	101.40	113.69	1	1
4	A	333	PX4	O7-C7-C6	3.35	120.38	108.34	1	8
4	A	387	PX4	C7-O7-C23	3.35	125.82	117.80	3	9
4	A	400	PX4	O7-C23-C24	3.35	118.74	111.48	14	5
4	A	423	PX4	O1-P1-O2	3.35	128.04	112.44	12	4
4	A	330	PX4	O5-C9-O6	3.35	115.24	123.63	14	6
4	A	330	PX4	C11-C10-C9	3.35	101.41	113.69	8	3
4	A	343	PX4	C26-C25-C24	3.35	125.44	113.13	10	3
4	A	381	PX4	C12-C11-C10	3.35	100.82	113.13	12	3
4	A	401	PX4	C18-C17-C16	3.35	97.44	114.37	1	1
4	A	322	PX4	O7-C7-C6	3.35	120.34	108.34	14	9
4	A	337	PX4	O7-C7-C6	3.35	120.35	108.34	2	5
4	A	409	PX4	O1-P1-O2	3.35	128.01	112.44	13	8
4	A	422	PX4	C7-O7-C23	3.35	125.80	117.80	13	8
4	A	355	PX4	C12-C11-C10	3.34	100.85	113.13	8	1
4	A	415	PX4	C7-O7-C23	3.34	125.80	117.80	12	1
4	A	375	PX4	O1-P1-O2	3.34	127.98	112.44	8	10
4	A	405	PX4	C5-N1-C4	3.34	100.20	108.98	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	306	PX4	O3-P1-O2	3.34	95.71	108.94	8	2
4	A	383	PX4	O5-C9-O6	3.34	115.28	123.63	8	3
4	A	362	PX4	O7-C7-C6	3.33	120.31	108.34	7	5
4	A	395	PX4	C1-C2-N1	3.34	126.53	115.82	4	5
4	A	412	PX4	C5-N1-C3	3.34	117.74	108.98	10	3
4	A	342	PX4	P1-O4-C6	3.33	102.25	121.35	2	8
4	A	364	PX4	P1-O4-C6	3.33	102.25	121.35	5	5
4	A	393	PX4	O3-P1-O2	3.33	95.72	108.94	8	4
4	A	408	PX4	O1-P1-O4	3.33	122.68	107.57	2	5
4	A	430	PX4	C3-N1-C2	3.33	123.16	109.91	12	1
4	A	311	PX4	C26-C25-C24	3.33	125.37	113.13	13	3
4	A	369	PX4	O5-C9-C10	3.33	121.99	111.83	6	4
4	A	398	PX4	O1-P1-O3	3.33	92.47	107.57	12	3
4	A	325	PX4	C7-O7-C23	3.33	109.83	117.80	14	4
4	A	379	PX4	P1-O4-C6	3.33	102.27	121.35	6	10
4	A	306	PX4	O5-C9-C10	3.33	121.98	111.83	8	2
4	A	310	PX4	C5-N1-C4	3.33	100.23	108.98	11	2
4	A	368	PX4	P1-O4-C6	3.33	102.28	121.35	9	8
4	A	396	PX4	C3-N1-C2	3.33	123.14	109.91	5	2
4	A	397	PX4	C34-C33-C32	3.33	97.54	114.37	7	1
4	A	403	PX4	C8-O5-C9	3.33	104.95	117.12	2	1
4	A	408	PX4	O4-P1-O2	3.33	122.12	108.94	8	4
4	A	321	PX4	O5-C9-C10	3.32	121.97	111.83	11	5
4	A	391	PX4	P1-O4-C6	3.32	102.30	121.35	2	8
4	A	312	PX4	P1-O4-C6	3.32	102.31	121.35	1	10
4	A	374	PX4	O1-P1-O2	3.32	127.91	112.44	3	6
4	A	403	PX4	O3-C1-C2	3.32	125.63	109.65	14	3
4	A	430	PX4	O7-C23-O8	3.32	115.94	123.70	3	5
4	A	386	PX4	C11-C10-C9	3.32	101.53	113.69	13	3
4	A	414	PX4	O4-P1-O2	3.32	122.10	108.94	4	2
4	A	318	PX4	O5-C9-C10	3.32	121.95	111.83	3	3
4	A	334	PX4	C5-N1-C4	3.32	100.26	108.98	3	4
4	A	363	PX4	O3-P1-O2	3.32	95.78	108.94	8	5
4	A	338	PX4	C5-N1-C4	3.32	100.26	108.98	13	4
4	A	380	PX4	C33-C32-C31	3.32	97.60	114.37	11	2
4	A	373	PX4	O7-C23-O8	3.31	115.95	123.70	9	7
4	A	329	PX4	C30-C29-C28	3.31	97.62	114.37	3	1
4	A	380	PX4	O4-P1-O2	3.31	122.05	108.94	4	1
4	A	393	PX4	C7-O7-C23	3.31	125.72	117.80	7	4
4	A	351	PX4	O1-P1-O4	3.31	122.56	107.57	8	2
4	A	390	PX4	O1-P1-O4	3.31	122.56	107.57	5	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	423	PX4	P1-O4-C6	3.31	102.39	121.35	14	5
4	A	314	PX4	O7-C7-C6	3.31	120.21	108.34	6	5
4	A	320	PX4	C4-N1-C2	3.31	123.06	109.91	2	4
4	A	321	PX4	C27-C26-C25	3.31	97.65	114.37	7	3
4	A	333	PX4	O7-C23-O8	3.31	115.97	123.70	7	5
4	A	313	PX4	C25-C24-C23	3.31	101.58	113.69	5	2
4	A	317	PX4	O7-C7-C6	3.31	120.20	108.34	9	2
4	A	338	PX4	O5-C9-O6	3.31	115.36	123.63	1	4
4	A	360	PX4	O7-C7-C6	3.31	120.21	108.34	13	3
4	A	410	PX4	C4-N1-C2	3.31	96.77	109.91	14	2
4	A	386	PX4	C3-N1-C2	3.31	96.77	109.91	2	1
4	A	414	PX4	O5-C9-C10	3.31	121.92	111.83	7	5
4	A	348	PX4	C1-C2-N1	3.30	126.43	115.82	3	3
4	A	417	PX4	O7-C23-O8	3.30	115.98	123.70	1	5
4	A	311	PX4	O3-P1-O2	3.30	95.85	108.94	1	2
4	A	321	PX4	O7-C7-C8	3.30	120.19	108.34	5	7
4	A	427	PX4	C34-C33-C32	3.30	97.69	114.37	5	1
4	A	316	PX4	P1-O4-C6	3.30	102.46	121.35	2	9
4	A	349	PX4	C4-N1-C2	3.30	123.01	109.91	12	4
4	A	387	PX4	O1-P1-O2	3.30	127.78	112.44	13	7
4	A	375	PX4	C7-O7-C23	3.29	125.68	117.80	13	5
4	A	396	PX4	O1-P1-O2	3.30	127.77	112.44	5	7
4	A	401	PX4	P1-O4-C6	3.30	102.47	121.35	7	10
4	A	412	PX4	C5-N1-C4	3.30	100.32	108.98	4	3
4	A	330	PX4	C29-C28-C27	3.29	97.72	114.37	3	2
4	A	311	PX4	O5-C9-O6	3.29	115.39	123.63	2	4
4	A	332	PX4	C7-O7-C23	3.29	109.92	117.80	4	4
4	A	387	PX4	C4-N1-C3	3.29	100.33	108.98	14	2
4	A	315	PX4	P1-O4-C6	3.29	102.49	121.35	9	9
4	A	376	PX4	O5-C9-O6	3.29	115.39	123.63	1	4
4	A	327	PX4	O5-C9-O6	3.29	115.40	123.63	10	5
4	A	384	PX4	O7-C23-O8	3.29	116.01	123.70	8	5
4	A	411	PX4	O1-P1-O2	3.29	127.74	112.44	10	9
4	A	411	PX4	C33-C32-C31	3.29	97.75	114.37	9	1
4	A	320	PX4	O8-C23-C24	3.29	110.93	123.78	3	1
4	A	343	PX4	O7-C7-C6	3.29	120.13	108.34	14	5
4	A	393	PX4	C27-C26-C25	3.29	97.75	114.37	14	2
4	A	325	PX4	C4-N1-C2	3.28	96.86	109.91	13	1
4	A	400	PX4	O1-P1-O2	3.28	127.72	112.44	14	7
4	A	372	PX4	C11-C10-C9	3.28	101.67	113.69	10	2
4	A	375	PX4	O7-C7-C6	3.28	120.12	108.34	8	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	377	PX4	O3-C1-C2	3.28	125.44	109.65	3	3
4	A	359	PX4	O3-P1-O2	3.28	95.93	108.94	8	3
4	A	327	PX4	C31-C30-C29	3.28	97.79	114.37	2	1
4	A	311	PX4	P1-O4-C6	3.28	102.57	121.35	14	3
4	A	314	PX4	O1-P1-O2	3.28	127.69	112.44	10	4
4	A	391	PX4	O1-P1-O3	3.28	92.71	107.57	5	4
4	A	332	PX4	O5-C9-O6	3.28	115.43	123.63	2	3
4	A	388	PX4	C28-C27-C26	3.28	97.80	114.37	2	3
4	A	427	PX4	O5-C9-C10	3.28	121.83	111.83	3	1
4	A	336	PX4	O1-P1-O3	3.28	92.72	107.57	7	4
4	A	401	PX4	C7-O7-C23	3.27	125.63	117.80	12	2
4	A	415	PX4	O4-P1-O2	3.28	121.92	108.94	14	3
4	A	409	PX4	P1-O3-C1	3.27	105.67	121.26	3	11
4	A	420	PX4	O7-C23-O8	3.27	116.05	123.70	13	6
4	A	347	PX4	O7-C23-O8	3.27	116.06	123.70	6	6
4	A	372	PX4	C7-O7-C23	3.27	109.97	117.80	6	5
4	A	407	PX4	C4-N1-C3	3.27	100.39	108.98	4	5
4	A	429	PX4	O1-P1-O2	3.27	127.66	112.44	7	7
4	A	316	PX4	C31-C30-C29	3.27	97.84	114.37	4	1
4	A	349	PX4	O7-C7-C6	3.27	120.07	108.34	10	6
4	A	352	PX4	O5-C9-O6	3.27	115.45	123.63	7	4
4	A	379	PX4	C5-N1-C4	3.27	100.39	108.98	14	2
4	A	384	PX4	C26-C25-C24	3.27	101.12	113.13	5	5
4	A	401	PX4	C5-N1-C4	3.27	117.56	108.98	14	4
4	A	392	PX4	O7-C23-O8	3.27	116.07	123.70	11	5
4	A	420	PX4	C5-N1-C2	3.27	122.90	109.91	14	3
4	A	407	PX4	O7-C7-C6	3.27	120.06	108.34	13	9
4	A	411	PX4	O1-P1-O3	3.27	92.76	107.57	6	4
4	A	310	PX4	C5-N1-C3	3.27	100.40	108.98	1	4
4	A	428	PX4	C4-N1-C2	3.27	96.93	109.91	12	2
4	A	336	PX4	O5-C9-O6	3.26	115.46	123.63	2	2
4	A	395	PX4	C34-C33-C32	3.26	97.86	114.37	5	1
4	A	389	PX4	C4-N1-C2	3.26	122.88	109.91	9	3
4	A	426	PX4	O7-C7-C6	3.26	120.05	108.34	9	6
4	A	353	PX4	C28-C27-C26	3.26	97.88	114.37	9	4
4	A	377	PX4	O7-C23-O8	3.26	116.08	123.70	11	1
4	A	368	PX4	O7-C23-C24	3.26	118.53	111.48	10	3
4	A	387	PX4	C29-C28-C27	3.26	97.89	114.37	1	2
4	A	387	PX4	C13-C12-C11	3.26	97.89	114.37	14	2
4	A	426	PX4	C1-C2-N1	3.26	126.28	115.82	11	2
4	A	351	PX4	O5-C9-C10	3.26	121.77	111.83	13	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	379	PX4	C1-C2-N1	3.26	126.28	115.82	6	4
4	A	386	PX4	C4-N1-C3	3.26	117.53	108.98	6	2
4	A	327	PX4	C5-N1-C3	3.26	100.42	108.98	14	3
4	A	331	PX4	C1-C2-N1	3.26	126.27	115.82	9	2
4	A	370	PX4	P1-O4-C6	3.25	102.70	121.35	2	9
4	A	383	PX4	P1-O3-C1	3.26	105.76	121.26	10	10
4	A	402	PX4	O5-C9-C10	3.26	121.76	111.83	6	4
4	A	341	PX4	O1-P1-O2	3.25	127.58	112.44	10	6
4	A	359	PX4	C5-N1-C4	3.25	117.52	108.98	7	3
4	A	377	PX4	C8-O5-C9	3.25	105.22	117.12	5	1
4	A	383	PX4	O7-C23-O8	3.25	116.10	123.70	11	4
4	A	317	PX4	C12-C11-C10	3.25	101.18	113.13	14	1
4	A	402	PX4	C13-C12-C11	3.25	97.93	114.37	9	2
4	A	423	PX4	O5-C9-O6	3.25	115.49	123.63	13	5
4	A	363	PX4	C30-C29-C28	3.25	97.93	114.37	7	2
4	A	384	PX4	C7-O7-C23	3.25	125.57	117.80	10	2
4	A	426	PX4	O1-P1-O2	3.25	127.56	112.44	8	11
4	A	373	PX4	O4-P1-O2	3.25	121.81	108.94	11	2
4	A	393	PX4	O7-C23-O8	3.25	116.11	123.70	3	1
4	A	332	PX4	O1-P1-O2	3.25	127.55	112.44	13	10
4	A	343	PX4	O5-C9-O6	3.25	115.51	123.63	7	4
4	A	357	PX4	C25-C24-C23	3.25	101.80	113.69	12	1
4	A	383	PX4	O5-C9-C10	3.25	121.73	111.83	8	3
4	A	393	PX4	C5-N1-C4	3.24	100.45	108.98	12	5
4	A	337	PX4	C7-O7-C23	3.24	125.56	117.80	8	3
4	A	373	PX4	O7-C7-C6	3.24	119.98	108.34	6	6
4	A	380	PX4	O3-P1-O2	3.24	96.08	108.94	8	7
4	A	366	PX4	O3-P1-O2	3.24	96.09	108.94	12	2
4	A	373	PX4	O5-C9-O6	3.24	115.52	123.63	12	6
4	A	328	PX4	P1-O4-C6	3.24	102.78	121.35	8	10
4	A	337	PX4	C25-C24-C23	3.24	101.82	113.69	9	2
4	A	311	PX4	C4-N1-C3	3.24	100.47	108.98	9	5
4	A	323	PX4	C1-C2-N1	3.24	126.21	115.82	2	3
4	A	342	PX4	C5-N1-C3	3.24	100.47	108.98	9	3
4	A	377	PX4	C4-N1-C2	3.24	122.78	109.91	11	2
4	A	363	PX4	C14-C13-C12	3.24	98.00	114.37	4	4
4	A	384	PX4	O1-P1-O4	3.24	122.25	107.57	7	3
4	A	322	PX4	O7-C7-C8	3.24	119.95	108.34	9	5
4	A	381	PX4	C7-O7-C23	3.24	125.54	117.80	3	5
4	A	401	PX4	C33-C32-C31	3.24	98.01	114.37	6	1
4	A	328	PX4	C1-C2-N1	3.24	126.20	115.82	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	352	PX4	O3-P1-O2	3.23	96.12	108.94	6	5
4	A	370	PX4	O1-P1-O2	3.23	127.49	112.44	11	10
4	A	377	PX4	C5-N1-C4	3.23	117.47	108.98	4	3
4	A	394	PX4	C7-O7-C23	3.23	110.06	117.80	6	3
4	A	409	PX4	C17-C16-C15	3.23	98.02	114.37	6	2
4	A	429	PX4	O3-P1-O2	3.23	96.12	108.94	7	3
4	A	395	PX4	C19-C18-C17	3.23	98.03	114.37	3	2
4	A	415	PX4	O7-C7-C6	3.23	119.94	108.34	2	8
4	A	319	PX4	O4-P1-O2	3.23	121.74	108.94	7	1
4	A	349	PX4	O5-C8-C7	3.23	117.71	108.40	7	9
4	A	385	PX4	O1-P1-O2	3.23	127.47	112.44	8	8
4	A	385	PX4	C11-C10-C9	3.23	101.86	113.69	5	1
4	A	331	PX4	P1-O4-C6	3.23	102.85	121.35	11	8
4	A	374	PX4	C34-C33-C32	3.23	98.05	114.37	6	3
4	A	391	PX4	C25-C24-C23	3.23	101.87	113.69	12	1
4	A	428	PX4	C12-C11-C10	3.23	101.27	113.13	2	2
4	A	409	PX4	C11-C10-C9	3.23	101.88	113.69	1	1
4	A	319	PX4	O5-C9-O6	3.22	115.56	123.63	13	3
4	A	333	PX4	C4-N1-C3	3.22	100.51	108.98	14	3
4	A	328	PX4	O1-P1-O2	3.22	127.44	112.44	14	8
4	A	343	PX4	O7-C23-O8	3.22	116.17	123.70	3	7
4	A	364	PX4	O7-C23-O8	3.22	116.17	123.70	12	6
4	A	368	PX4	O7-C7-C6	3.22	119.91	108.34	5	6
4	A	369	PX4	C16-C15-C14	3.22	98.08	114.37	7	2
4	A	376	PX4	C5-N1-C4	3.22	100.51	108.98	3	4
4	A	422	PX4	C12-C11-C10	3.22	101.28	113.13	10	1
4	A	312	PX4	C1-C2-N1	3.22	126.16	115.82	9	2
4	A	414	PX4	C16-C15-C14	3.22	98.09	114.37	2	2
4	A	417	PX4	C15-C14-C13	3.22	98.09	114.37	14	1
4	A	347	PX4	C12-C11-C10	3.22	101.30	113.13	14	5
4	A	367	PX4	O7-C7-C6	3.22	119.89	108.34	10	3
4	A	391	PX4	C4-N1-C3	3.22	117.43	108.98	5	4
4	A	316	PX4	O1-P1-O2	3.22	127.41	112.44	3	6
4	A	345	PX4	C7-O7-C23	3.22	125.50	117.80	12	4
4	A	371	PX4	O5-C8-C7	3.22	117.67	108.40	4	7
4	A	354	PX4	O3-P1-O2	3.22	96.19	108.94	2	3
4	A	390	PX4	O5-C9-C10	3.21	121.63	111.83	10	6
4	A	391	PX4	C13-C12-C11	3.21	98.12	114.37	3	1
4	A	419	PX4	P1-O4-C6	3.21	102.93	121.35	10	6
4	A	312	PX4	O7-C23-O8	3.21	116.19	123.70	3	4
4	A	353	PX4	C4-N1-C3	3.21	100.54	108.98	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	356	PX4	O7-C7-C6	3.21	119.86	108.34	8	4
4	A	311	PX4	C15-C14-C13	3.21	98.14	114.37	13	1
4	A	334	PX4	O7-C7-C8	3.21	119.86	108.34	14	5
4	A	394	PX4	O4-P1-O2	3.21	121.66	108.94	6	1
4	A	402	PX4	C3-N1-C2	3.21	97.15	109.91	1	3
4	A	327	PX4	C4-N1-C3	3.21	117.40	108.98	8	3
4	A	329	PX4	P1-O4-C6	3.21	102.97	121.35	10	8
4	A	345	PX4	C1-C2-N1	3.21	126.12	115.82	11	4
4	A	349	PX4	C11-C10-C9	3.21	101.94	113.69	8	2
4	A	361	PX4	O1-P1-O2	3.21	127.37	112.44	3	10
4	A	349	PX4	P1-O4-C6	3.21	102.97	121.35	7	10
4	A	363	PX4	C5-N1-C4	3.21	100.55	108.98	1	5
4	A	384	PX4	C5-N1-C3	3.21	100.55	108.98	6	5
4	A	312	PX4	O3-C1-C2	3.21	125.08	109.65	9	3
4	A	316	PX4	O5-C9-C10	3.21	121.61	111.83	12	4
4	A	406	PX4	C4-N1-C3	3.21	100.55	108.98	8	3
4	A	409	PX4	C5-N1-C4	3.21	100.56	108.98	14	2
4	A	424	PX4	C7-O7-C23	3.21	125.47	117.80	7	3
4	A	363	PX4	C8-O5-C9	3.20	105.40	117.12	13	1
4	A	408	PX4	O7-C7-C6	3.20	119.84	108.34	9	7
4	A	309	PX4	C30-C29-C28	3.20	98.18	114.37	8	3
4	A	342	PX4	C1-C2-N1	3.20	126.10	115.82	3	4
4	A	353	PX4	P1-O3-C1	3.20	106.02	121.26	11	8
4	A	385	PX4	O7-C7-C8	3.20	119.83	108.34	5	5
4	A	421	PX4	C27-C26-C25	3.20	98.19	114.37	4	4
4	A	424	PX4	O3-P1-O2	3.20	96.27	108.94	14	2
4	A	384	PX4	C12-C11-C10	3.19	101.39	113.13	6	4
4	A	423	PX4	C26-C25-C24	3.19	101.39	113.13	8	3
4	A	361	PX4	P1-O3-C1	3.19	106.07	121.26	6	8
4	A	374	PX4	O7-C7-C8	3.19	119.79	108.34	8	5
4	A	397	PX4	C11-C10-C9	3.19	102.00	113.69	13	3
4	A	409	PX4	O3-P1-O2	3.19	96.29	108.94	7	1
4	A	424	PX4	O5-C9-O6	3.19	115.65	123.63	10	7
4	A	378	PX4	O7-C7-C6	3.19	119.78	108.34	2	4
4	A	385	PX4	C12-C11-C10	3.19	101.41	113.13	5	1
4	A	375	PX4	P1-O4-C6	3.19	103.09	121.35	14	8
4	A	335	PX4	O7-C7-C6	3.18	119.77	108.34	7	6
4	A	371	PX4	P1-O4-C6	3.18	103.10	121.35	9	4
4	A	427	PX4	C5-N1-C4	3.18	100.61	108.98	13	4
4	A	310	PX4	C12-C11-C10	3.18	101.44	113.13	5	1
4	A	388	PX4	C8-O5-C9	3.18	105.49	117.12	6	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	422	PX4	O7-C23-O8	3.18	116.27	123.70	12	2
4	A	372	PX4	C12-C11-C10	3.18	101.45	113.13	13	4
4	A	393	PX4	P1-O4-C6	3.18	103.15	121.35	9	8
4	A	329	PX4	O5-C9-O6	3.17	115.69	123.63	7	5
4	A	333	PX4	P1-O3-C1	3.17	106.16	121.26	2	8
4	A	383	PX4	C7-O7-C23	3.17	125.39	117.80	10	2
4	A	385	PX4	C27-C26-C25	3.17	98.33	114.37	13	3
4	A	415	PX4	C29-C28-C27	3.17	98.33	114.37	13	2
4	A	312	PX4	C7-O7-C23	3.17	125.38	117.80	12	5
4	A	373	PX4	P1-O4-C6	3.17	103.19	121.35	14	11
4	A	351	PX4	O5-C9-O6	3.17	115.71	123.63	2	5
4	A	365	PX4	O3-P1-O2	3.17	96.38	108.94	5	3
4	A	373	PX4	C12-C11-C10	3.17	101.49	113.13	11	3
4	A	333	PX4	C5-N1-C3	3.16	100.66	108.98	10	3
4	A	344	PX4	O7-C7-C6	3.17	119.70	108.34	14	6
4	A	362	PX4	O3-P1-O2	3.17	96.39	108.94	11	7
4	A	377	PX4	O5-C9-C10	3.17	121.49	111.83	8	2
4	A	345	PX4	O7-C7-C6	3.16	119.69	108.34	9	5
4	A	422	PX4	C1-C2-N1	3.16	125.98	115.82	13	2
4	A	335	PX4	P1-O4-C6	3.16	103.23	121.35	12	11
4	A	346	PX4	C5-N1-C3	3.16	100.67	108.98	14	3
4	A	394	PX4	O5-C9-O6	3.16	115.72	123.63	7	2
4	A	402	PX4	P1-O4-C6	3.16	103.23	121.35	13	8
4	A	339	PX4	O5-C9-C10	3.16	121.47	111.83	1	5
4	A	397	PX4	O7-C7-C8	3.16	119.68	108.34	14	8
4	A	332	PX4	C4-N1-C2	3.16	97.36	109.91	12	1
4	A	324	PX4	O1-P1-O2	3.16	127.12	112.44	8	7
4	A	384	PX4	O5-C9-C10	3.16	121.46	111.83	12	3
4	A	387	PX4	O7-C23-O8	3.16	116.33	123.70	12	2
4	A	393	PX4	O4-P1-O2	3.16	121.44	108.94	5	4
4	A	356	PX4	C26-C25-C24	3.15	101.54	113.13	14	4
4	A	420	PX4	O1-P1-O4	3.15	121.87	107.57	13	8
4	A	395	PX4	O5-C9-C10	3.15	121.45	111.83	4	4
4	A	317	PX4	C8-O5-C9	3.15	105.60	117.12	3	3
4	A	362	PX4	O1-P1-O2	3.15	127.10	112.44	4	2
4	A	421	PX4	O1-P1-O2	3.15	127.10	112.44	8	7
4	A	387	PX4	O7-C23-C24	3.15	118.30	111.48	3	6
4	A	328	PX4	C11-C10-C9	3.15	125.23	113.69	4	2
4	A	419	PX4	O7-C23-O8	3.15	116.34	123.70	5	3
4	A	413	PX4	C5-N1-C4	3.15	100.71	108.98	2	2
4	A	360	PX4	C1-C2-N1	3.14	125.92	115.82	2	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	399	PX4	C11-C10-C9	3.15	102.17	113.69	2	3
4	A	313	PX4	O5-C9-C10	3.14	121.42	111.83	12	5
4	A	314	PX4	C33-C32-C31	3.14	98.48	114.37	8	1
4	A	317	PX4	O1-P1-O2	3.14	127.06	112.44	6	8
4	A	411	PX4	C34-C33-C32	3.14	98.48	114.37	12	2
4	A	344	PX4	C8-O5-C9	3.14	105.64	117.12	14	2
4	A	364	PX4	C4-N1-C3	3.14	100.73	108.98	8	7
4	A	359	PX4	P1-O4-C6	3.14	103.36	121.35	9	8
4	A	372	PX4	O4-P1-O2	3.14	121.38	108.94	3	2
4	A	314	PX4	C20-C19-C18	3.14	98.51	114.37	2	2
4	A	406	PX4	O7-C23-C24	3.14	118.27	111.48	8	3
4	A	309	PX4	C1-C2-N1	3.14	125.89	115.82	4	9
4	A	314	PX4	C5-N1-C4	3.14	100.74	108.98	2	6
4	A	413	PX4	O4-P1-O2	3.14	121.37	108.94	6	5
4	A	418	PX4	O7-C7-C8	3.14	119.59	108.34	12	4
4	A	427	PX4	C25-C24-C23	3.14	102.20	113.69	1	2
4	A	336	PX4	C5-N1-C4	3.14	100.74	108.98	5	2
4	A	310	PX4	O7-C7-C6	3.13	119.59	108.34	8	5
4	A	419	PX4	O1-P1-O2	3.13	127.03	112.44	11	7
4	A	319	PX4	O1-P1-O3	3.13	93.37	107.57	1	2
4	A	374	PX4	C1-C2-N1	3.13	125.88	115.82	9	3
4	A	399	PX4	O5-C9-C10	3.13	121.39	111.83	5	2
4	A	336	PX4	O7-C7-C8	3.13	119.58	108.34	2	3
4	A	366	PX4	C28-C27-C26	3.13	98.54	114.37	11	2
4	A	372	PX4	C4-N1-C3	3.13	100.75	108.98	4	4
4	A	394	PX4	O7-C7-C6	3.13	119.58	108.34	11	4
4	A	396	PX4	O5-C9-O6	3.13	115.80	123.63	4	3
4	A	423	PX4	O1-P1-O3	3.13	93.37	107.57	10	2
4	A	410	PX4	P1-O4-C6	3.13	103.42	121.35	13	6
4	A	427	PX4	O3-P1-O2	3.13	96.53	108.94	5	4
4	A	321	PX4	C5-N1-C4	3.13	100.76	108.98	13	3
4	A	379	PX4	O1-P1-O4	3.13	121.75	107.57	3	3
4	A	314	PX4	O5-C9-C10	3.13	121.37	111.83	14	3
4	A	327	PX4	O1-P1-O2	3.13	126.99	112.44	1	8
4	A	344	PX4	C5-N1-C3	3.13	100.76	108.98	8	3
4	A	425	PX4	O1-P1-O4	3.13	121.74	107.57	2	3
4	A	416	PX4	O5-C9-O6	3.13	115.81	123.63	7	4
4	A	329	PX4	O3-P1-O2	3.12	96.55	108.94	8	3
4	A	336	PX4	O1-P1-O4	3.12	121.73	107.57	12	4
4	A	422	PX4	O7-C7-C8	3.12	119.55	108.34	4	9
4	A	370	PX4	O3-P1-O2	3.12	96.56	108.94	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	382	PX4	O4-P1-O2	3.12	121.31	108.94	7	2
4	A	310	PX4	O7-C23-O8	3.12	116.41	123.70	8	5
4	A	332	PX4	O5-C9-C10	3.12	121.35	111.83	5	3
4	A	386	PX4	P1-O4-C6	3.12	103.48	121.35	1	9
4	A	315	PX4	C1-C2-N1	3.12	125.83	115.82	5	4
4	A	369	PX4	O7-C23-O8	3.12	116.42	123.70	2	3
4	A	394	PX4	O7-C23-O8	3.12	116.42	123.70	7	3
4	A	403	PX4	C32-C31-C30	3.12	98.61	114.37	3	1
4	A	358	PX4	O5-C9-C10	3.12	121.33	111.83	3	5
4	A	376	PX4	O7-C7-C8	3.11	119.52	108.34	12	7
4	A	428	PX4	C15-C14-C13	3.12	98.62	114.37	5	1
4	A	327	PX4	C30-C29-C28	3.11	98.63	114.37	14	4
4	A	364	PX4	O7-C7-C8	3.11	119.51	108.34	5	4
4	A	314	PX4	C18-C17-C16	3.11	98.64	114.37	1	1
4	A	326	PX4	C12-C11-C10	3.11	101.69	113.13	3	4
4	A	424	PX4	P1-O4-C6	3.11	103.51	121.35	13	10
4	A	360	PX4	O1-P1-O3	3.11	93.47	107.57	14	5
4	A	369	PX4	P1-O4-C6	3.11	103.52	121.35	8	7
4	A	375	PX4	C12-C11-C10	3.11	101.71	113.13	1	2
4	A	417	PX4	C3-N1-C2	3.11	97.56	109.91	9	1
4	A	425	PX4	C5-N1-C4	3.11	100.81	108.98	3	6
4	A	429	PX4	C4-N1-C3	3.11	117.14	108.98	12	3
4	A	342	PX4	O5-C9-O6	3.11	131.40	123.63	7	3
4	A	380	PX4	P1-O4-C6	3.11	103.55	121.35	9	11
4	A	403	PX4	C25-C24-C23	3.10	102.32	113.69	5	4
4	A	415	PX4	C8-O5-C9	3.11	105.77	117.12	8	1
4	A	418	PX4	P1-O4-C6	3.11	103.55	121.35	11	12
4	A	428	PX4	O5-C9-O6	3.11	115.86	123.63	11	3
4	A	328	PX4	C5-N1-C4	3.10	117.13	108.98	2	2
4	A	328	PX4	O7-C23-O8	3.10	116.45	123.70	11	1
4	A	330	PX4	C5-N1-C3	3.10	100.82	108.98	13	3
4	A	369	PX4	O5-C9-O6	3.10	115.86	123.63	5	5
4	A	399	PX4	O3-P1-O2	3.10	96.63	108.94	9	1
4	A	311	PX4	C12-C11-C10	3.10	101.73	113.13	4	2
4	A	378	PX4	C26-C25-C24	3.10	101.73	113.13	12	4
4	A	400	PX4	O7-C7-C8	3.10	119.47	108.34	3	5
4	A	418	PX4	O1-P1-O2	3.10	126.88	112.44	4	5
4	A	339	PX4	P1-O4-C6	3.10	103.58	121.35	12	9
4	A	366	PX4	C26-C25-C24	3.10	101.73	113.13	9	3
4	A	326	PX4	C7-O7-C23	3.10	125.21	117.80	3	4
4	A	425	PX4	C30-C29-C28	3.10	98.70	114.37	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	320	PX4	C26-C25-C24	3.10	101.75	113.13	11	2
4	A	327	PX4	P1-O4-C6	3.10	103.61	121.35	5	7
4	A	368	PX4	C11-C10-C9	3.10	102.35	113.69	8	2
4	A	384	PX4	C11-C10-C9	3.10	102.35	113.69	10	2
4	A	408	PX4	O5-C9-C10	3.10	121.28	111.83	1	2
4	A	429	PX4	O7-C23-O8	3.10	116.47	123.70	6	5
4	A	359	PX4	O7-C7-C6	3.10	119.45	108.34	14	8
4	A	430	PX4	C27-C26-C25	3.10	98.72	114.37	3	2
4	A	393	PX4	C1-C2-N1	3.09	125.75	115.82	8	5
4	A	399	PX4	O7-C23-O8	3.09	116.47	123.70	8	4
4	A	402	PX4	C26-C25-C24	3.09	101.76	113.13	11	2
4	A	425	PX4	O1-P1-O2	3.09	126.83	112.44	11	7
4	A	427	PX4	C4-N1-C3	3.09	100.85	108.98	3	3
4	A	427	PX4	C5-N1-C2	3.09	122.21	109.91	11	1
4	A	415	PX4	C5-N1-C4	3.09	100.85	108.98	8	2
4	A	335	PX4	C4-N1-C3	3.09	100.86	108.98	14	5
4	A	343	PX4	C5-N1-C3	3.09	100.86	108.98	4	4
4	A	352	PX4	C5-N1-C3	3.09	100.86	108.98	6	4
4	A	367	PX4	O7-C23-O8	3.09	130.93	123.70	9	4
4	A	385	PX4	O3-P1-O2	3.09	96.69	108.94	12	2
4	A	404	PX4	O3-C1-C2	3.09	124.52	109.65	13	1
4	A	313	PX4	C7-O7-C23	3.09	110.40	117.80	2	6
4	A	423	PX4	O1-P1-O4	3.09	121.56	107.57	10	3
4	A	310	PX4	O7-C7-C8	3.09	119.41	108.34	7	4
4	A	318	PX4	O5-C9-O6	3.09	115.91	123.63	3	2
4	A	371	PX4	O1-P1-O3	3.09	93.58	107.57	3	3
4	A	385	PX4	C8-O5-C9	3.09	128.40	117.12	8	2
4	A	346	PX4	O1-P1-O2	3.09	126.80	112.44	13	6
4	A	340	PX4	C8-O5-C9	3.08	128.39	117.12	9	1
4	A	356	PX4	C1-C2-N1	3.08	125.72	115.82	8	5
4	A	381	PX4	C4-N1-C3	3.08	100.88	108.98	5	1
4	A	410	PX4	O1-P1-O2	3.08	126.79	112.44	7	12
4	A	392	PX4	O5-C9-C10	3.08	121.23	111.83	14	3
4	A	394	PX4	C20-C19-C18	3.08	98.79	114.37	3	4
4	A	343	PX4	C28-C27-C26	3.08	98.80	114.37	4	2
4	A	424	PX4	C5-N1-C3	3.08	117.07	108.98	12	2
4	A	331	PX4	C25-C24-C23	3.08	102.42	113.69	3	2
4	A	350	PX4	O5-C9-O6	3.08	115.93	123.63	13	3
4	A	350	PX4	C7-O7-C23	3.08	125.16	117.80	12	4
4	A	419	PX4	C4-N1-C3	3.08	100.89	108.98	13	2
4	A	318	PX4	C15-C14-C13	3.08	98.82	114.37	3	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	322	PX4	O5-C9-O6	3.08	115.94	123.63	6	4
4	A	335	PX4	O1-P1-O4	3.08	121.51	107.57	10	2
4	A	363	PX4	O5-C9-O6	3.08	115.93	123.63	10	2
4	A	367	PX4	C4-N1-C3	3.08	100.89	108.98	10	4
4	A	393	PX4	O1-P1-O3	3.08	93.62	107.57	14	4
4	A	402	PX4	O5-C9-O6	3.08	115.93	123.63	1	4
4	A	364	PX4	O5-C9-O6	3.07	115.94	123.63	7	4
4	A	362	PX4	C11-C10-C9	3.07	102.44	113.69	10	3
4	A	328	PX4	C5-N1-C3	3.07	100.91	108.98	4	3
4	A	342	PX4	C28-C27-C26	3.07	98.85	114.37	14	2
4	A	378	PX4	C19-C18-C17	3.07	98.84	114.37	4	2
4	A	380	PX4	C12-C11-C10	3.07	101.84	113.13	10	3
4	A	361	PX4	C3-N1-C2	3.07	122.11	109.91	9	3
4	A	407	PX4	C1-C2-N1	3.07	125.68	115.82	13	4
4	A	333	PX4	C1-C2-N1	3.07	125.67	115.82	5	3
4	A	347	PX4	O3-P1-O2	3.07	96.77	108.94	11	2
4	A	381	PX4	C1-C2-N1	3.07	125.67	115.82	2	3
4	A	382	PX4	O1-P1-O3	3.07	93.66	107.57	2	3
4	A	306	PX4	O5-C9-O6	3.07	115.96	123.63	5	3
4	A	315	PX4	O5-C8-C7	3.07	117.23	108.40	13	3
4	A	357	PX4	C1-C2-N1	3.07	125.66	115.82	12	5
4	A	372	PX4	C25-C24-C23	3.07	102.46	113.69	10	2
4	A	421	PX4	C30-C29-C28	3.07	98.87	114.37	13	2
4	A	354	PX4	O7-C7-C6	3.06	119.34	108.34	11	11
4	A	370	PX4	C3-N1-C2	3.06	122.09	109.91	6	3
4	A	330	PX4	C19-C18-C17	3.06	98.89	114.37	8	2
4	A	383	PX4	O1-P1-O2	3.06	126.69	112.44	3	10
4	A	402	PX4	C12-C11-C10	3.06	101.88	113.13	6	3
4	A	336	PX4	C5-N1-C2	3.06	122.08	109.91	7	2
4	A	337	PX4	C8-O5-C9	3.06	105.93	117.12	14	3
4	A	409	PX4	C15-C14-C13	3.06	98.89	114.37	3	1
4	A	411	PX4	O7-C7-C6	3.06	119.32	108.34	1	7
4	A	403	PX4	O7-C7-C8	3.06	119.31	108.34	11	3
4	A	395	PX4	C12-C11-C10	3.06	124.36	113.13	9	1
4	A	311	PX4	C5-N1-C4	3.05	117.00	108.98	10	2
4	A	379	PX4	O5-C9-O6	3.05	115.99	123.63	5	5
4	A	404	PX4	O7-C7-C8	3.05	119.30	108.34	4	3
4	A	413	PX4	O7-C7-C6	3.05	119.30	108.34	4	4
4	A	425	PX4	O7-C23-O8	3.05	116.57	123.70	2	3
4	A	314	PX4	C5-N1-C3	3.05	116.98	108.98	8	2
4	A	316	PX4	O5-C9-O6	3.05	116.00	123.63	12	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	325	PX4	O7-C7-C8	3.05	119.29	108.34	9	2
4	A	418	PX4	C8-O5-C9	3.05	105.97	117.12	5	2
4	A	353	PX4	C31-C30-C29	3.05	98.97	114.37	11	1
4	A	327	PX4	O8-C23-C24	3.05	111.87	123.78	1	2
4	A	371	PX4	O1-P1-O2	3.05	126.62	112.44	4	8
4	A	322	PX4	P1-O4-C6	3.04	103.90	121.35	5	10
4	A	397	PX4	C4-N1-C3	3.05	100.98	108.98	6	2
4	A	330	PX4	O7-C7-C6	3.04	119.26	108.34	10	2
4	A	368	PX4	O5-C9-O6	3.04	116.01	123.63	4	5
4	A	403	PX4	C4-N1-C3	3.04	100.98	108.98	3	4
4	A	425	PX4	C26-C25-C24	3.04	124.31	113.13	4	2
4	A	343	PX4	O5-C9-C10	3.04	121.11	111.83	9	4
4	A	355	PX4	O1-P1-O2	3.04	126.59	112.44	8	9
4	A	430	PX4	C8-O5-C9	3.04	106.00	117.12	2	2
4	A	324	PX4	C5-N1-C3	3.04	116.96	108.98	1	2
4	A	336	PX4	C7-O7-C23	3.04	125.07	117.80	10	2
4	A	378	PX4	C4-N1-C3	3.04	100.99	108.98	12	2
4	A	418	PX4	C1-C2-N1	3.04	125.58	115.82	10	4
4	A	401	PX4	C5-N1-C2	3.04	121.99	109.91	11	2
4	A	341	PX4	O7-C7-C6	3.04	119.24	108.34	9	4
4	A	341	PX4	C1-C2-N1	3.04	125.57	115.82	12	3
4	A	350	PX4	O1-P1-O4	3.04	121.34	107.57	10	3
4	A	356	PX4	O3-P1-O2	3.04	96.89	108.94	3	2
4	A	399	PX4	C33-C32-C31	3.04	99.01	114.37	5	1
4	A	413	PX4	O7-C23-O8	3.04	116.60	123.70	12	4
4	A	316	PX4	C27-C26-C25	3.04	99.02	114.37	1	1
4	A	371	PX4	C27-C26-C25	3.04	99.02	114.37	5	3
4	A	317	PX4	O5-C9-C10	3.03	121.09	111.83	3	7
4	A	326	PX4	C5-N1-C3	3.03	116.94	108.98	13	3
4	A	399	PX4	O7-C7-C8	3.03	119.22	108.34	6	3
4	A	357	PX4	O5-C9-C10	3.03	121.08	111.83	12	4
4	A	405	PX4	C29-C28-C27	3.03	99.05	114.37	6	2
4	A	420	PX4	C11-C10-C9	3.03	102.59	113.69	11	3
4	A	326	PX4	C4-N1-C3	3.03	101.03	108.98	3	3
4	A	329	PX4	O7-C7-C6	3.03	119.20	108.34	6	3
4	A	363	PX4	C5-N1-C3	3.03	116.92	108.98	2	4
4	A	378	PX4	C13-C12-C11	3.03	99.07	114.37	13	2
4	A	380	PX4	C17-C16-C15	3.03	99.07	114.37	8	5
4	A	399	PX4	C1-C2-N1	3.03	125.53	115.82	10	6
4	A	430	PX4	O3-P1-O2	3.03	96.94	108.94	3	4
4	A	346	PX4	C26-C25-C24	3.02	102.02	113.13	4	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	P1-O4-C6	3.03	104.02	121.35	2	7
4	A	353	PX4	C29-C28-C27	3.02	99.08	114.37	11	2
4	A	367	PX4	O1-P1-O2	3.02	126.51	112.44	8	9
4	A	374	PX4	C8-O5-C9	3.02	106.07	117.12	13	2
4	A	380	PX4	O1-P1-O4	3.02	121.27	107.57	11	5
4	A	400	PX4	C8-O5-C9	3.02	106.07	117.12	9	3
4	A	405	PX4	C3-N1-C2	3.02	121.93	109.91	13	1
4	A	319	PX4	C26-C25-C24	3.02	102.03	113.13	2	1
4	A	333	PX4	O1-P1-O2	3.02	126.50	112.44	10	7
4	A	378	PX4	C1-C2-N1	3.02	125.52	115.82	10	2
4	A	326	PX4	O7-C7-C6	3.02	119.17	108.34	12	2
4	A	329	PX4	O1-P1-O4	3.02	121.25	107.57	4	1
4	A	318	PX4	C28-C27-C26	3.02	99.11	114.37	8	1
4	A	351	PX4	C4-N1-C3	3.02	101.05	108.98	11	3
4	A	356	PX4	C5-N1-C4	3.02	116.91	108.98	13	2
4	A	398	PX4	O7-C7-C6	3.02	119.18	108.34	7	2
4	A	397	PX4	C12-C11-C10	3.02	102.04	113.13	9	3
4	A	412	PX4	O5-C9-O6	3.02	131.18	123.63	11	1
4	A	307	PX4	O1-P1-O2	3.02	126.47	112.44	2	6
4	A	333	PX4	O7-C7-C8	3.02	119.17	108.34	1	3
4	A	368	PX4	O7-C23-O8	3.02	116.65	123.70	6	5
4	A	380	PX4	O7-C7-C6	3.02	119.17	108.34	1	3
4	A	416	PX4	O7-C7-C8	3.02	119.17	108.34	3	5
4	A	363	PX4	O7-C7-C6	3.02	119.16	108.34	8	4
4	A	338	PX4	C11-C10-C9	3.01	124.74	113.69	12	4
4	A	417	PX4	C29-C28-C27	3.01	99.13	114.37	11	3
4	A	333	PX4	C30-C29-C28	3.01	99.15	114.37	14	3
4	A	365	PX4	O3-C1-C2	3.01	124.14	109.65	11	2
4	A	372	PX4	O5-C9-C10	3.01	121.01	111.83	10	4
4	A	308	PX4	C34-C33-C32	3.01	99.16	114.37	2	3
4	A	394	PX4	O1-P1-O2	3.01	126.44	112.44	11	8
4	A	417	PX4	P1-O4-C6	3.01	104.11	121.35	5	10
4	A	328	PX4	O5-C9-C10	3.01	121.01	111.83	13	7
4	A	347	PX4	C18-C17-C16	3.01	99.16	114.37	12	2
4	A	354	PX4	C29-C28-C27	3.01	99.17	114.37	13	2
4	A	395	PX4	O7-C23-O8	3.01	116.67	123.70	1	3
4	A	423	PX4	O5-C9-C10	3.01	121.01	111.83	3	4
4	A	403	PX4	O7-C23-O8	3.01	130.74	123.70	10	3
4	A	407	PX4	O5-C9-C10	3.01	121.00	111.83	6	3
4	A	418	PX4	C25-C24-C23	3.01	102.68	113.69	8	3
4	A	428	PX4	C20-C19-C18	3.01	99.17	114.37	13	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	316	PX4	C5-N1-C4	3.01	101.08	108.98	3	3
4	A	333	PX4	C33-C32-C31	3.01	99.18	114.37	12	1
4	A	323	PX4	P1-O4-C6	3.00	104.14	121.35	1	9
4	A	395	PX4	C33-C32-C31	3.00	99.18	114.37	4	1
4	A	315	PX4	C5-N1-C4	3.00	101.09	108.98	14	4
4	A	321	PX4	O4-P1-O2	3.00	120.83	108.94	14	4
4	A	326	PX4	O1-P1-O2	3.00	126.41	112.44	9	8
4	A	389	PX4	C25-C24-C23	3.00	124.70	113.69	2	4
4	A	339	PX4	C1-C2-N1	3.00	125.45	115.82	11	3
4	A	357	PX4	C5-N1-C3	3.00	101.09	108.98	1	2
4	A	396	PX4	C7-O7-C23	3.00	124.98	117.80	7	2
4	A	417	PX4	C17-C16-C15	3.00	99.20	114.37	6	2
4	A	428	PX4	C3-N1-C2	3.00	97.98	109.91	14	3
4	A	358	PX4	C3-N1-C2	3.00	97.98	109.91	8	1
4	A	375	PX4	O7-C23-O8	3.00	116.69	123.70	7	4
4	A	394	PX4	C26-C25-C24	3.00	102.11	113.13	6	3
4	A	364	PX4	C5-N1-C3	3.00	101.10	108.98	5	3
4	A	311	PX4	O7-C7-C6	3.00	119.09	108.34	13	5
4	A	334	PX4	P1-O4-C6	2.99	104.19	121.35	2	9
4	A	338	PX4	O5-C9-C10	3.00	120.97	111.83	8	3
4	A	351	PX4	C11-C10-C9	3.00	102.72	113.69	8	5
4	A	430	PX4	O1-P1-O2	3.00	126.38	112.44	8	8
4	A	372	PX4	O3-P1-O2	2.99	97.07	108.94	13	2
4	A	380	PX4	C11-C10-C9	2.99	102.73	113.69	8	3
4	A	374	PX4	C4-N1-C2	2.99	121.80	109.91	11	1
4	A	386	PX4	C12-C11-C10	2.99	102.14	113.13	7	4
4	A	394	PX4	C4-N1-C3	2.99	101.12	108.98	3	3
4	A	331	PX4	C32-C31-C30	2.99	99.26	114.37	8	1
4	A	371	PX4	O7-C7-C8	2.99	119.07	108.34	6	5
4	A	404	PX4	C1-C2-N1	2.99	125.42	115.82	7	4
4	A	387	PX4	C5-N1-C4	2.99	101.13	108.98	14	1
4	A	407	PX4	O4-P1-O2	2.99	120.78	108.94	13	3
4	A	411	PX4	C25-C24-C23	2.99	102.74	113.69	5	2
4	A	355	PX4	O7-C7-C6	2.99	119.06	108.34	11	4
4	A	366	PX4	C5-N1-C3	2.99	101.13	108.98	5	4
4	A	421	PX4	C32-C31-C30	2.99	99.27	114.37	7	1
4	A	424	PX4	O1-P1-O3	2.99	94.03	107.57	4	2
4	A	331	PX4	C5-N1-C3	2.99	116.82	108.98	5	3
4	A	337	PX4	O1-P1-O2	2.98	126.33	112.44	13	4
4	A	341	PX4	O5-C9-C10	2.98	120.94	111.83	1	5
4	A	406	PX4	O7-C7-C6	2.99	119.05	108.34	11	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	403	PX4	C5-N1-C4	2.98	101.14	108.98	4	4
4	A	306	PX4	C1-C2-N1	2.98	125.39	115.82	12	2
4	A	366	PX4	C18-C17-C16	2.98	99.30	114.37	9	1
4	A	378	PX4	C11-C10-C9	2.98	102.76	113.69	8	1
4	A	308	PX4	C30-C29-C28	2.98	99.30	114.37	2	1
4	A	341	PX4	C4-N1-C3	2.98	116.80	108.98	1	3
4	A	395	PX4	O7-C7-C8	2.98	119.03	108.34	14	6
4	A	388	PX4	O5-C9-C10	2.98	120.91	111.83	14	5
4	A	396	PX4	C4-N1-C3	2.98	101.15	108.98	5	1
4	A	419	PX4	O7-C7-C8	2.98	119.03	108.34	12	7
4	A	335	PX4	C8-O5-C9	2.98	106.24	117.12	10	2
4	A	318	PX4	C8-O5-C9	2.98	106.24	117.12	11	2
4	A	351	PX4	C1-C2-N1	2.97	125.37	115.82	11	3
4	A	322	PX4	O5-C9-C10	2.97	120.90	111.83	6	4
4	A	334	PX4	C1-C2-N1	2.97	125.36	115.82	4	2
4	A	361	PX4	C30-C29-C28	2.97	99.34	114.37	7	1
4	A	345	PX4	C12-C11-C10	2.97	124.05	113.13	7	3
4	A	353	PX4	O7-C7-C8	2.97	119.00	108.34	3	3
4	A	385	PX4	O5-C9-C10	2.97	120.89	111.83	13	4
4	A	401	PX4	C12-C11-C10	2.97	102.21	113.13	3	1
4	A	413	PX4	O3-P1-O2	2.97	97.17	108.94	13	5
4	A	325	PX4	C11-C10-C9	2.97	102.82	113.69	1	4
4	A	425	PX4	C29-C28-C27	2.97	99.37	114.37	3	1
4	A	427	PX4	O3-C1-C2	2.97	123.93	109.65	6	2
4	A	370	PX4	C14-C13-C12	2.96	99.38	114.37	7	4
4	A	372	PX4	O1-P1-O2	2.97	126.24	112.44	10	7
4	A	328	PX4	C26-C25-C24	2.96	102.24	113.13	9	3
4	A	329	PX4	O7-C7-C8	2.96	118.97	108.34	12	8
4	A	391	PX4	C12-C11-C10	2.96	102.24	113.13	10	3
4	A	408	PX4	P1-O4-C6	2.96	104.37	121.35	5	7
4	A	410	PX4	O4-P1-O2	2.96	120.68	108.94	2	2
4	A	332	PX4	O7-C7-C6	2.96	118.97	108.34	4	4
4	A	383	PX4	C16-C15-C14	2.96	99.40	114.37	9	2
4	A	390	PX4	C12-C11-C10	2.96	102.25	113.13	4	1
4	A	427	PX4	C7-O7-C23	2.96	110.71	117.80	10	4
4	A	331	PX4	C28-C27-C26	2.96	99.41	114.37	3	1
4	A	409	PX4	C1-C2-N1	2.96	125.32	115.82	2	3
4	A	328	PX4	O7-C7-C8	2.96	118.96	108.34	1	7
4	A	354	PX4	C25-C24-C23	2.96	102.86	113.69	7	3
4	A	363	PX4	C12-C11-C10	2.96	102.26	113.13	11	3
4	A	406	PX4	C11-C10-C9	2.96	102.86	113.69	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	424	PX4	C14-C13-C12	2.96	99.41	114.37	8	1
4	A	313	PX4	C12-C11-C10	2.96	102.26	113.13	11	1
4	A	327	PX4	C28-C27-C26	2.96	99.42	114.37	9	1
4	A	365	PX4	O1-P1-O3	2.96	94.16	107.57	6	2
4	A	375	PX4	O5-C9-C10	2.96	120.85	111.83	11	4
4	A	422	PX4	P1-O4-C6	2.96	104.41	121.35	5	7
4	A	316	PX4	C26-C25-C24	2.95	102.27	113.13	4	2
4	A	390	PX4	O3-P1-O2	2.95	97.23	108.94	1	2
4	A	356	PX4	C5-N1-C2	2.95	121.64	109.91	2	1
4	A	379	PX4	C19-C18-C17	2.95	99.45	114.37	7	2
4	A	395	PX4	C25-C24-C23	2.95	102.88	113.69	6	3
4	A	334	PX4	O7-C7-C6	2.95	118.93	108.34	6	3
4	A	402	PX4	C16-C15-C14	2.95	99.46	114.37	6	1
4	A	404	PX4	C19-C18-C17	2.95	99.46	114.37	3	1
4	A	406	PX4	O5-C9-C10	2.95	120.83	111.83	12	5
4	A	426	PX4	C12-C11-C10	2.95	102.29	113.13	8	1
4	A	340	PX4	C1-C2-N1	2.95	125.29	115.82	11	3
4	A	410	PX4	O7-C7-C6	2.95	118.92	108.34	9	2
4	A	336	PX4	C15-C14-C13	2.95	99.47	114.37	9	2
4	A	346	PX4	O3-P1-O2	2.95	97.25	108.94	12	1
4	A	364	PX4	C27-C26-C25	2.95	99.47	114.37	7	2
4	A	309	PX4	C5-N1-C3	2.95	116.71	108.98	2	2
4	A	320	PX4	C8-O5-C9	2.94	106.36	117.12	6	4
4	A	367	PX4	C11-C10-C9	2.95	102.90	113.69	3	4
4	A	372	PX4	O7-C23-O8	2.94	116.82	123.70	4	3
4	A	389	PX4	O5-C9-C10	2.94	120.81	111.83	4	5
4	A	392	PX4	O1-P1-O2	2.94	126.14	112.44	13	12
4	A	429	PX4	C25-C24-C23	2.94	102.91	113.69	12	1
4	A	351	PX4	C12-C11-C10	2.94	102.31	113.13	4	5
4	A	322	PX4	C5-N1-C3	2.94	101.25	108.98	9	4
4	A	417	PX4	O1-P1-O2	2.94	126.14	112.44	12	6
4	A	371	PX4	C16-C15-C14	2.94	99.50	114.37	1	3
4	A	377	PX4	C12-C11-C10	2.94	102.32	113.13	6	3
4	A	405	PX4	C19-C18-C17	2.94	99.50	114.37	6	2
4	A	423	PX4	O7-C7-C8	2.94	118.90	108.34	11	2
4	A	320	PX4	C3-N1-C2	2.94	98.22	109.91	5	1
4	A	344	PX4	O7-C7-C8	2.94	118.89	108.34	12	4
4	A	395	PX4	C4-N1-C3	2.94	101.25	108.98	8	1
4	A	402	PX4	P1-O3-C1	2.94	107.27	121.26	8	9
4	A	411	PX4	C12-C11-C10	2.94	102.33	113.13	6	1
4	A	413	PX4	C25-C24-C23	2.94	102.92	113.69	11	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	365	PX4	C5-N1-C2	2.94	98.23	109.91	13	1
4	A	366	PX4	C30-C29-C28	2.94	99.51	114.37	11	1
4	A	386	PX4	C33-C32-C31	2.94	99.51	114.37	3	5
4	A	326	PX4	C30-C29-C28	2.94	99.53	114.37	2	1
4	A	388	PX4	C5-N1-C2	2.94	121.58	109.91	7	1
4	A	398	PX4	C29-C28-C27	2.94	99.53	114.37	1	2
4	A	409	PX4	C18-C17-C16	2.94	99.53	114.37	3	1
4	A	416	PX4	C4-N1-C2	2.94	121.58	109.91	14	4
4	A	418	PX4	O7-C7-C6	2.94	118.88	108.34	8	3
4	A	341	PX4	C34-C33-C32	2.93	99.54	114.37	1	1
4	A	345	PX4	O7-C7-C8	2.93	118.87	108.34	13	3
4	A	371	PX4	O7-C7-C6	2.93	118.87	108.34	9	4
4	A	375	PX4	C5-N1-C3	2.93	116.68	108.98	7	3
4	A	385	PX4	C32-C31-C30	2.93	99.54	114.37	2	2
4	A	329	PX4	C26-C25-C24	2.93	102.36	113.13	9	3
4	A	345	PX4	C8-O5-C9	2.93	106.40	117.12	11	1
4	A	429	PX4	C1-C2-N1	2.93	125.23	115.82	12	5
4	A	347	PX4	O5-C9-O6	2.93	116.30	123.63	11	4
4	A	375	PX4	O1-P1-O3	2.93	94.28	107.57	4	2
4	A	430	PX4	C25-C24-C23	2.93	102.95	113.69	7	1
4	A	375	PX4	O4-P1-O2	2.93	120.55	108.94	4	5
4	A	420	PX4	O7-C7-C6	2.93	118.85	108.34	1	6
4	A	316	PX4	O1-P1-O3	2.93	94.30	107.57	14	3
4	A	350	PX4	C1-C2-N1	2.93	125.22	115.82	2	4
4	A	353	PX4	C3-N1-C2	2.93	121.55	109.91	8	2
4	A	356	PX4	C4-N1-C2	2.93	98.28	109.91	2	1
4	A	316	PX4	O7-C23-C24	2.93	117.81	111.48	2	6
4	A	396	PX4	C26-C25-C24	2.93	102.38	113.13	1	1
4	A	342	PX4	C29-C28-C27	2.92	99.58	114.37	10	2
4	A	366	PX4	C12-C11-C10	2.92	102.38	113.13	10	2
4	A	361	PX4	C5-N1-C4	2.92	116.65	108.98	14	3
4	A	308	PX4	C7-O7-C23	2.92	124.79	117.80	13	1
4	A	319	PX4	C12-C11-C10	2.92	123.86	113.13	13	1
4	A	334	PX4	C14-C13-C12	2.92	99.59	114.37	11	3
4	A	316	PX4	O3-P1-O2	2.92	97.36	108.94	3	3
4	A	320	PX4	C11-C10-C9	2.92	102.99	113.69	6	2
4	A	366	PX4	C25-C24-C23	2.92	102.99	113.69	8	1
4	A	388	PX4	C5-N1-C4	2.92	101.30	108.98	5	4
4	A	400	PX4	O7-C23-O8	2.92	116.88	123.70	14	5
4	A	422	PX4	O1-P1-O2	2.92	126.03	112.44	7	8
4	A	312	PX4	C26-C25-C24	2.92	123.84	113.13	8	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	335	PX4	C27-C26-C25	2.92	99.63	114.37	7	2
4	A	354	PX4	C26-C25-C24	2.92	102.41	113.13	4	2
4	A	359	PX4	C12-C11-C10	2.92	102.41	113.13	11	1
4	A	372	PX4	C1-C2-N1	2.92	125.18	115.82	5	1
4	A	370	PX4	O1-P1-O4	2.92	120.78	107.57	1	3
4	A	376	PX4	O4-P1-O2	2.92	120.49	108.94	2	3
4	A	384	PX4	O3-P1-O2	2.92	97.38	108.94	3	2
4	A	413	PX4	C3-N1-C2	2.92	98.32	109.91	6	1
4	A	419	PX4	O1-P1-O3	2.92	94.35	107.57	2	2
4	A	311	PX4	O1-P1-O3	2.91	94.36	107.57	5	3
4	A	314	PX4	C15-C14-C13	2.91	99.64	114.37	12	1
4	A	331	PX4	O5-C9-C10	2.91	120.72	111.83	7	4
4	A	317	PX4	P1-O4-C6	2.91	104.67	121.35	1	8
4	A	321	PX4	C7-O7-C23	2.91	124.76	117.80	4	4
4	A	354	PX4	O5-C9-C10	2.91	120.71	111.83	11	4
4	A	369	PX4	O1-P1-O4	2.91	120.77	107.57	13	3
4	A	409	PX4	O7-C7-C6	2.91	118.79	108.34	3	6
4	A	415	PX4	C12-C11-C10	2.91	123.82	113.13	13	2
4	A	354	PX4	C8-O5-C9	2.91	106.49	117.12	1	3
4	A	379	PX4	O7-C7-C6	2.91	118.77	108.34	9	4
4	A	428	PX4	C8-O5-C9	2.91	106.49	117.12	4	2
4	A	314	PX4	O5-C9-O6	2.91	116.36	123.63	3	5
4	A	348	PX4	O1-P1-O2	2.91	125.97	112.44	1	6
4	A	408	PX4	O5-C9-O6	2.91	116.36	123.63	8	7
4	A	415	PX4	O5-C9-C10	2.91	120.70	111.83	13	2
4	A	309	PX4	P1-O4-C6	2.90	104.71	121.35	9	2
4	A	315	PX4	O5-C9-O6	2.90	116.36	123.63	9	5
4	A	399	PX4	C20-C19-C18	2.90	99.69	114.37	13	2
4	A	408	PX4	C4-N1-C3	2.91	101.34	108.98	9	3
4	A	315	PX4	C8-O5-C9	2.90	106.51	117.12	8	1
4	A	318	PX4	O3-C1-C2	2.90	123.62	109.65	10	1
4	A	346	PX4	C11-C10-C9	2.90	103.05	113.69	11	2
4	A	363	PX4	O4-P1-O2	2.90	120.44	108.94	1	4
4	A	312	PX4	O7-C7-C6	2.90	118.75	108.34	5	3
4	A	333	PX4	O3-P1-O2	2.90	97.44	108.94	9	4
4	A	350	PX4	C34-C33-C32	2.90	99.70	114.37	3	1
4	A	368	PX4	O3-C1-C2	2.90	123.61	109.65	9	2
4	A	371	PX4	C25-C24-C23	2.90	103.06	113.69	8	3
4	A	422	PX4	C8-O5-C9	2.90	106.51	117.12	6	3
4	A	333	PX4	C31-C30-C29	2.90	99.71	114.37	9	3
4	A	340	PX4	C5-N1-C2	2.90	98.38	109.91	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	349	PX4	C4-N1-C3	2.90	101.36	108.98	4	2
4	A	350	PX4	O1-P1-O2	2.90	125.93	112.44	5	8
4	A	309	PX4	C15-C14-C13	2.90	99.72	114.37	10	1
4	A	317	PX4	O7-C23-O8	2.90	130.48	123.70	2	3
4	A	334	PX4	C15-C14-C13	2.90	99.72	114.37	8	2
4	A	337	PX4	O5-C9-C10	2.90	120.67	111.83	5	1
4	A	341	PX4	C5-N1-C3	2.90	101.36	108.98	5	3
4	A	343	PX4	O6-C9-C10	2.90	112.45	123.78	9	2
4	A	353	PX4	C26-C25-C24	2.90	102.48	113.13	7	1
4	A	355	PX4	O7-C23-C24	2.90	117.75	111.48	10	6
4	A	368	PX4	C25-C24-C23	2.90	103.08	113.69	13	2
4	A	385	PX4	C17-C16-C15	2.90	99.72	114.37	2	2
4	A	385	PX4	C26-C25-C24	2.90	102.48	113.13	2	2
4	A	403	PX4	O5-C9-O6	2.90	116.38	123.63	6	4
4	A	421	PX4	C14-C13-C12	2.90	99.72	114.37	14	1
4	A	388	PX4	C17-C16-C15	2.90	99.72	114.37	5	2
4	A	407	PX4	C34-C33-C32	2.90	99.72	114.37	8	1
4	A	347	PX4	C15-C14-C13	2.90	99.73	114.37	7	2
4	A	411	PX4	O5-C9-C10	2.90	120.67	111.83	13	5
4	A	349	PX4	O3-P1-O2	2.90	120.41	108.94	3	3
4	A	378	PX4	C31-C30-C29	2.90	99.73	114.37	9	3
4	A	404	PX4	O5-C9-C10	2.90	120.66	111.83	2	4
4	A	404	PX4	C4-N1-C2	2.90	121.42	109.91	9	2
4	A	328	PX4	O7-C7-C6	2.89	118.72	108.34	5	5
4	A	340	PX4	C30-C29-C28	2.89	99.75	114.37	14	1
4	A	344	PX4	C28-C27-C26	2.89	99.75	114.37	13	1
4	A	383	PX4	C17-C16-C15	2.89	99.75	114.37	6	1
4	A	307	PX4	C28-C27-C26	2.89	99.76	114.37	4	1
4	A	310	PX4	C26-C25-C24	2.89	102.51	113.13	3	2
4	A	336	PX4	C26-C25-C24	2.89	102.50	113.13	12	1
4	A	322	PX4	C32-C31-C30	2.89	99.76	114.37	6	1
4	A	323	PX4	O1-P1-O2	2.89	125.88	112.44	9	7
4	A	338	PX4	C4-N1-C3	2.89	101.39	108.98	13	2
4	A	396	PX4	O7-C7-C6	2.89	118.71	108.34	11	4
4	A	420	PX4	C31-C30-C29	2.89	99.76	114.37	9	1
4	A	341	PX4	C14-C13-C12	2.89	99.77	114.37	6	1
4	A	308	PX4	O5-C9-C10	2.89	120.64	111.83	6	4
4	A	315	PX4	O3-C1-C2	2.89	123.54	109.65	13	2
4	A	318	PX4	C31-C30-C29	2.89	99.78	114.37	6	3
4	A	334	PX4	O1-P1-O3	2.89	94.48	107.57	4	1
4	A	336	PX4	C4-N1-C3	2.89	101.39	108.98	13	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	405	PX4	O5-C9-C10	2.89	120.64	111.83	4	6
4	A	332	PX4	C26-C25-C24	2.88	102.53	113.13	12	3
4	A	427	PX4	C12-C11-C10	2.89	102.53	113.13	8	3
4	A	367	PX4	C27-C26-C25	2.88	99.79	114.37	2	2
4	A	393	PX4	C20-C19-C18	2.88	99.80	114.37	7	1
4	A	376	PX4	C34-C33-C32	2.88	99.81	114.37	2	2
4	A	349	PX4	C12-C11-C10	2.88	102.56	113.13	1	3
4	A	360	PX4	O5-C9-C10	2.88	120.60	111.83	11	2
4	A	364	PX4	C18-C17-C16	2.88	99.83	114.37	10	1
4	A	374	PX4	O1-P1-O4	2.88	120.60	107.57	8	2
4	A	397	PX4	C18-C17-C16	2.88	99.83	114.37	2	1
4	A	330	PX4	O1-P1-O2	2.87	125.81	112.44	12	6
4	A	405	PX4	O3-C1-C2	2.87	123.48	109.65	14	1
4	A	356	PX4	O5-C9-C10	2.87	120.59	111.83	10	3
4	A	358	PX4	C4-N1-C3	2.87	101.43	108.98	12	4
4	A	309	PX4	C18-C17-C16	2.87	99.86	114.37	11	3
4	A	333	PX4	O1-P1-O4	2.87	120.57	107.57	3	4
4	A	343	PX4	C13-C12-C11	2.87	99.86	114.37	4	2
4	A	352	PX4	O5-C9-C10	2.87	120.58	111.83	6	6
4	A	313	PX4	C5-N1-C4	2.87	101.45	108.98	7	2
4	A	322	PX4	C25-C24-C23	2.87	124.20	113.69	13	1
4	A	351	PX4	O1-P1-O2	2.87	125.78	112.44	4	6
4	A	395	PX4	C5-N1-C4	2.87	116.50	108.98	1	2
4	A	420	PX4	C19-C18-C17	2.86	99.89	114.37	4	2
4	A	365	PX4	O5-C8-C7	2.86	116.65	108.40	3	8
4	A	366	PX4	O5-C9-C10	2.86	120.57	111.83	10	3
4	A	383	PX4	C5-N1-C3	2.86	101.46	108.98	7	3
4	A	315	PX4	C26-C25-C24	2.86	102.61	113.13	2	1
4	A	321	PX4	C5-N1-C3	2.86	101.46	108.98	4	3
4	A	324	PX4	O3-C1-C2	2.86	123.41	109.65	11	3
4	A	338	PX4	C7-O7-C23	2.86	124.64	117.80	2	8
4	A	345	PX4	C3-N1-C2	2.86	98.54	109.91	2	2
4	A	359	PX4	C15-C14-C13	2.86	99.90	114.37	14	2
4	A	306	PX4	O1-P1-O4	2.86	120.53	107.57	8	1
4	A	323	PX4	C7-O7-C23	2.86	124.64	117.80	8	2
4	A	340	PX4	C5-N1-C3	2.86	101.47	108.98	1	3
4	A	430	PX4	C12-C11-C10	2.86	102.62	113.13	5	1
4	A	401	PX4	O5-C9-O6	2.86	116.48	123.63	13	5
4	A	317	PX4	C5-N1-C3	2.86	116.48	108.98	13	2
4	A	414	PX4	C15-C14-C13	2.86	99.92	114.37	1	3
4	A	418	PX4	O3-P1-O2	2.86	97.61	108.94	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	343	PX4	C4-N1-C2	2.86	98.56	109.91	5	1
4	A	317	PX4	C3-N1-C2	2.85	98.56	109.91	14	1
4	A	353	PX4	C8-O5-C9	2.85	106.69	117.12	9	4
4	A	392	PX4	C3-N1-C2	2.85	121.26	109.91	1	2
4	A	412	PX4	C12-C11-C10	2.85	102.64	113.13	5	3
4	A	428	PX4	O7-C7-C8	2.85	118.58	108.34	6	5
4	A	310	PX4	C11-C10-C9	2.85	103.25	113.69	14	4
4	A	319	PX4	C20-C19-C18	2.85	99.95	114.37	12	1
4	A	321	PX4	C3-N1-C2	2.85	121.24	109.91	13	2
4	A	359	PX4	C11-C10-C9	2.85	103.25	113.69	9	1
4	A	383	PX4	O1-P1-O3	2.85	94.65	107.57	3	4
4	A	374	PX4	C7-O7-C23	2.85	124.61	117.80	12	4
4	A	426	PX4	O7-C23-O8	2.85	117.05	123.70	7	6
4	A	380	PX4	O8-C23-C24	2.85	112.65	123.78	10	2
4	A	334	PX4	C5-N1-C3	2.84	116.45	108.98	14	2
4	A	361	PX4	O5-C9-C10	2.84	120.50	111.83	6	4
4	A	372	PX4	P1-O4-C6	2.84	105.06	121.35	11	9
4	A	391	PX4	C18-C17-C16	2.84	100.00	114.37	12	2
4	A	402	PX4	C27-C26-C25	2.84	100.00	114.37	2	2
4	A	340	PX4	C3-N1-C2	2.84	121.20	109.91	1	2
4	A	370	PX4	C30-C29-C28	2.84	100.01	114.37	3	2
4	A	371	PX4	O3-P1-O2	2.84	97.68	108.94	3	1
4	A	378	PX4	O1-P1-O4	2.84	94.69	107.57	14	2
4	A	401	PX4	O1-P1-O2	2.84	125.66	112.44	10	5
4	A	402	PX4	O1-P1-O3	2.84	94.69	107.57	6	2
4	A	316	PX4	O7-C23-O8	2.84	117.07	123.70	7	3
4	A	329	PX4	C3-N1-C2	2.84	121.19	109.91	5	2
4	A	333	PX4	C5-N1-C4	2.84	116.43	108.98	8	5
4	A	337	PX4	C12-C11-C10	2.84	102.70	113.13	4	2
4	A	340	PX4	O7-C23-O8	2.84	117.07	123.70	11	7
4	A	349	PX4	C19-C18-C17	2.84	100.02	114.37	4	3
4	A	361	PX4	O1-P1-O4	2.84	120.43	107.57	10	3
4	A	306	PX4	C26-C25-C24	2.84	102.71	113.13	12	3
4	A	328	PX4	C29-C28-C27	2.84	100.03	114.37	12	2
4	A	336	PX4	C18-C17-C16	2.84	100.03	114.37	11	2
4	A	388	PX4	C32-C31-C30	2.84	100.03	114.37	8	2
4	A	399	PX4	C15-C14-C13	2.84	100.03	114.37	4	2
4	A	419	PX4	O3-C1-C2	2.83	123.29	109.65	10	1
4	A	332	PX4	C5-N1-C4	2.83	101.53	108.98	4	2
4	A	364	PX4	C14-C13-C12	2.83	100.05	114.37	5	2
4	A	325	PX4	C1-C2-N1	2.83	124.91	115.82	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	C27-C26-C25	2.83	100.06	114.37	5	2
4	A	353	PX4	C33-C32-C31	2.83	100.06	114.37	14	1
4	A	365	PX4	C14-C13-C12	2.83	100.05	114.37	2	3
4	A	372	PX4	C4-N1-C2	2.83	121.17	109.91	11	1
4	A	395	PX4	O4-P1-O2	2.83	97.71	108.94	5	1
4	A	313	PX4	C1-C2-N1	2.83	124.90	115.82	8	4
4	A	422	PX4	C3-N1-C2	2.83	121.16	109.91	5	1
4	A	322	PX4	O5-C8-C7	2.83	116.55	108.40	6	4
4	A	338	PX4	C25-C24-C23	2.83	103.33	113.69	3	3
4	A	343	PX4	O1-P1-O2	2.83	125.60	112.44	4	6
4	A	365	PX4	O7-C7-C8	2.83	118.49	108.34	13	2
4	A	402	PX4	O4-P1-O2	2.83	120.14	108.94	4	2
4	A	320	PX4	C4-N1-C3	2.83	101.55	108.98	10	3
4	A	357	PX4	O8-C23-C24	2.83	112.73	123.78	5	2
4	A	380	PX4	C5-N1-C4	2.83	101.55	108.98	10	3
4	A	327	PX4	O7-C7-C6	2.82	118.48	108.34	2	5
4	A	399	PX4	O1-P1-O4	2.83	120.37	107.57	10	2
4	A	380	PX4	C4-N1-C3	2.82	116.39	108.98	11	3
4	A	319	PX4	O7-C7-C8	2.82	118.47	108.34	6	6
4	A	307	PX4	C31-C30-C29	2.82	100.10	114.37	5	4
4	A	371	PX4	C1-C2-N1	2.82	124.88	115.82	2	2
4	A	382	PX4	C32-C31-C30	2.82	100.10	114.37	5	1
4	A	428	PX4	C11-C10-C9	2.82	103.35	113.69	9	1
4	A	430	PX4	C11-C10-C9	2.82	103.36	113.69	12	2
4	A	320	PX4	O1-P1-O3	2.82	94.79	107.57	8	2
4	A	377	PX4	O7-C7-C6	2.82	118.46	108.34	2	2
4	A	410	PX4	C19-C18-C17	2.82	100.12	114.37	10	2
4	A	414	PX4	O7-C7-C8	2.82	118.45	108.34	2	2
4	A	422	PX4	C31-C30-C29	2.82	100.12	114.37	2	2
4	A	352	PX4	O1-P1-O4	2.82	120.34	107.57	5	1
4	A	380	PX4	O5-C9-O6	2.82	116.58	123.63	12	5
4	A	407	PX4	C33-C32-C31	2.82	100.13	114.37	7	1
4	A	423	PX4	C4-N1-C3	2.82	101.58	108.98	2	3
4	A	318	PX4	C7-O7-C23	2.82	124.53	117.80	11	6
4	A	363	PX4	O1-P1-O3	2.82	94.80	107.57	6	3
4	A	377	PX4	O7-C7-C8	2.81	118.44	108.34	5	6
4	A	385	PX4	C1-C2-N1	2.81	124.86	115.82	7	3
4	A	406	PX4	O1-P1-O3	2.82	94.81	107.57	5	2
4	A	314	PX4	O3-C1-C2	2.81	123.19	109.65	5	1
4	A	342	PX4	O1-P1-O4	2.81	120.32	107.57	8	2
4	A	347	PX4	O1-P1-O3	2.81	94.81	107.57	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	331	PX4	C5-N1-C4	2.81	101.59	108.98	14	3
4	A	391	PX4	C17-C16-C15	2.81	100.15	114.37	13	1
4	A	417	PX4	C20-C19-C18	2.81	100.15	114.37	5	2
4	A	307	PX4	O3-P1-O2	2.81	97.80	108.94	9	1
4	A	365	PX4	O4-P1-O2	2.81	120.08	108.94	10	2
4	A	317	PX4	C11-C10-C9	2.81	103.40	113.69	13	1
4	A	371	PX4	C31-C30-C29	2.81	100.17	114.37	5	1
4	A	389	PX4	C1-C2-N1	2.81	124.84	115.82	12	2
4	A	397	PX4	C5-N1-C2	2.81	121.08	109.91	8	3
4	A	398	PX4	C18-C17-C16	2.81	100.16	114.37	2	3
4	A	339	PX4	C31-C30-C29	2.81	100.17	114.37	10	3
4	A	404	PX4	C30-C29-C28	2.81	100.17	114.37	1	2
4	A	377	PX4	O5-C9-O6	2.81	116.61	123.63	6	2
4	A	409	PX4	C4-N1-C3	2.81	101.60	108.98	11	2
4	A	361	PX4	C8-O5-C9	2.81	106.86	117.12	8	2
4	A	368	PX4	O5-C9-C10	2.81	120.39	111.83	9	1
4	A	425	PX4	O7-C7-C6	2.81	118.41	108.34	1	4
4	A	357	PX4	C5-N1-C4	2.80	116.34	108.98	2	2
4	A	368	PX4	C17-C16-C15	2.80	100.20	114.37	7	1
4	A	373	PX4	C11-C10-C9	2.80	103.42	113.69	3	2
4	A	410	PX4	C33-C32-C31	2.80	100.19	114.37	7	1
4	A	357	PX4	C12-C11-C10	2.80	102.83	113.13	10	3
4	A	376	PX4	O7-C7-C6	2.80	118.40	108.34	3	3
4	A	381	PX4	O5-C9-O6	2.80	116.62	123.63	7	2
4	A	348	PX4	C14-C13-C12	2.80	100.21	114.37	5	2
4	A	353	PX4	C14-C13-C12	2.80	100.21	114.37	7	1
4	A	372	PX4	C5-N1-C2	2.80	121.04	109.91	4	2
4	A	414	PX4	C1-C2-N1	2.80	124.81	115.82	14	3
4	A	316	PX4	O3-C1-C2	2.80	123.12	109.65	3	1
4	A	342	PX4	O1-P1-O3	2.80	94.88	107.57	8	1
4	A	387	PX4	C25-C24-C23	2.80	103.43	113.69	10	2
4	A	370	PX4	O7-C7-C6	2.80	118.38	108.34	11	4
4	A	379	PX4	C8-O5-C9	2.80	106.89	117.12	9	1
4	A	403	PX4	O3-P1-O2	2.80	97.84	108.94	9	1
4	A	344	PX4	C27-C26-C25	2.80	100.22	114.37	10	2
4	A	398	PX4	C4-N1-C2	2.80	121.03	109.91	1	2
4	A	419	PX4	C5-N1-C3	2.80	116.33	108.98	8	1
4	A	340	PX4	C5-N1-C4	2.80	101.63	108.98	6	5
4	A	362	PX4	C8-O5-C9	2.80	106.90	117.12	3	2
4	A	366	PX4	C32-C31-C30	2.80	100.23	114.37	1	1
4	A	386	PX4	C15-C14-C13	2.80	100.23	114.37	5	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	403	PX4	C16-C15-C14	2.80	100.23	114.37	5	2
4	A	340	PX4	C31-C30-C29	2.80	100.24	114.37	14	2
4	A	397	PX4	C5-N1-C3	2.79	116.31	108.98	3	1
4	A	406	PX4	C8-O5-C9	2.79	106.91	117.12	6	1
4	A	307	PX4	C12-C11-C10	2.79	102.87	113.13	10	3
4	A	330	PX4	C25-C24-C23	2.79	103.46	113.69	6	1
4	A	328	PX4	C4-N1-C3	2.79	101.64	108.98	2	3
4	A	338	PX4	O1-P1-O2	2.79	125.44	112.44	1	7
4	A	355	PX4	O5-C9-C10	2.79	120.35	111.83	5	2
4	A	399	PX4	C27-C26-C25	2.79	100.25	114.37	3	2
4	A	380	PX4	C8-O5-C9	2.79	106.92	117.12	6	3
4	A	381	PX4	C14-C13-C12	2.79	100.26	114.37	7	1
4	A	404	PX4	O1-P1-O2	2.79	125.43	112.44	3	4
4	A	415	PX4	O1-P1-O3	2.79	94.91	107.57	14	5
4	A	321	PX4	O1-P1-O4	2.79	120.22	107.57	1	5
4	A	348	PX4	O5-C9-C10	2.79	120.34	111.83	7	6
4	A	381	PX4	O7-C23-O8	2.79	117.18	123.70	5	4
4	A	370	PX4	C13-C12-C11	2.79	100.28	114.37	1	4
4	A	384	PX4	C13-C12-C11	2.79	100.27	114.37	4	1
4	A	425	PX4	C1-C2-N1	2.79	124.77	115.82	8	2
4	A	326	PX4	C31-C30-C29	2.79	100.28	114.37	4	1
4	A	330	PX4	C1-C2-N1	2.79	124.77	115.82	8	4
4	A	340	PX4	O1-P1-O2	2.79	125.41	112.44	1	6
4	A	377	PX4	O1-P1-O4	2.79	120.20	107.57	9	2
4	A	385	PX4	O7-C23-O8	2.79	117.19	123.70	1	2
4	A	387	PX4	O7-C7-C6	2.79	118.34	108.34	5	4
4	A	358	PX4	C19-C18-C17	2.79	100.28	114.37	7	1
4	A	392	PX4	C4-N1-C2	2.79	120.99	109.91	9	3
4	A	416	PX4	C25-C24-C23	2.79	123.90	113.69	14	3
4	A	341	PX4	O3-P1-O2	2.78	97.90	108.94	11	4
4	A	322	PX4	C1-C2-N1	2.78	124.76	115.82	6	1
4	A	346	PX4	O1-P1-O4	2.78	94.95	107.57	6	1
4	A	352	PX4	C4-N1-C3	2.78	101.67	108.98	3	3
4	A	412	PX4	C4-N1-C3	2.78	116.29	108.98	3	2
4	A	413	PX4	O5-C9-O6	2.78	116.67	123.63	7	4
4	A	417	PX4	O7-C7-C8	2.78	118.33	108.34	11	5
4	A	358	PX4	O3-P1-O2	2.78	97.91	108.94	8	2
4	A	388	PX4	C16-C15-C14	2.78	100.31	114.37	4	3
4	A	389	PX4	O7-C7-C8	2.78	118.32	108.34	13	3
4	A	402	PX4	C15-C14-C13	2.78	100.30	114.37	14	2
4	A	419	PX4	C17-C16-C15	2.78	100.31	114.37	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	318	PX4	C1-C2-N1	2.78	124.75	115.82	1	2
4	A	309	PX4	C4-N1-C3	2.78	101.68	108.98	13	2
4	A	340	PX4	C11-C10-C9	2.78	103.52	113.69	14	2
4	A	358	PX4	C7-O7-C23	2.78	124.44	117.80	1	3
4	A	306	PX4	O4-P1-O2	2.78	119.94	108.94	7	1
4	A	327	PX4	C3-N1-C2	2.78	120.95	109.91	3	1
4	A	375	PX4	O3-C1-C2	2.78	123.02	109.65	13	1
4	A	311	PX4	O1-P1-O2	2.78	125.36	112.44	8	3
4	A	326	PX4	O1-P1-O4	2.78	120.15	107.57	11	2
4	A	327	PX4	C18-C17-C16	2.77	100.34	114.37	14	1
4	A	359	PX4	C5-N1-C3	2.77	101.69	108.98	9	4
4	A	362	PX4	O7-C23-O8	2.77	117.22	123.70	4	1
4	A	367	PX4	C34-C33-C32	2.77	100.34	114.37	11	2
4	A	416	PX4	C5-N1-C3	2.78	116.27	108.98	4	7
4	A	342	PX4	O3-P1-O2	2.77	97.94	108.94	9	2
4	A	346	PX4	O5-C9-C10	2.77	120.29	111.83	3	2
4	A	332	PX4	C4-N1-C3	2.77	101.70	108.98	10	3
4	A	365	PX4	C8-C7-C6	2.77	105.33	111.78	8	9
4	A	369	PX4	C8-O5-C9	2.77	106.99	117.12	7	2
4	A	322	PX4	C12-C11-C10	2.77	123.30	113.13	7	3
4	A	335	PX4	C12-C11-C10	2.77	102.96	113.13	2	3
4	A	352	PX4	O1-P1-O3	2.77	95.02	107.57	4	1
4	A	368	PX4	O4-P1-O2	2.77	119.91	108.94	9	1
4	A	394	PX4	C3-N1-C2	2.77	120.92	109.91	8	1
4	A	373	PX4	O3-C1-C2	2.77	122.97	109.65	4	1
4	A	330	PX4	C26-C25-C24	2.77	102.97	113.13	6	2
4	A	352	PX4	O6-C9-C10	2.77	112.96	123.78	3	2
4	A	415	PX4	C11-C10-C9	2.77	103.56	113.69	14	1
4	A	385	PX4	O5-C9-O6	2.76	116.71	123.63	4	3
4	A	401	PX4	O7-C23-O8	2.76	117.24	123.70	8	1
4	A	335	PX4	C5-N1-C3	2.76	116.23	108.98	5	3
4	A	307	PX4	C11-C10-C9	2.76	103.57	113.69	14	3
4	A	312	PX4	C25-C24-C23	2.76	103.58	113.69	5	3
4	A	351	PX4	C5-N1-C4	2.76	101.72	108.98	8	2
4	A	369	PX4	C11-C10-C9	2.76	123.82	113.69	4	2
4	A	404	PX4	C25-C24-C23	2.76	123.82	113.69	14	3
4	A	348	PX4	C5-N1-C4	2.76	101.72	108.98	10	2
4	A	365	PX4	C4-N1-C3	2.76	116.22	108.98	8	1
4	A	414	PX4	C30-C29-C28	2.76	100.42	114.37	8	2
4	A	316	PX4	O4-P1-O2	2.76	119.87	108.94	14	3
4	A	406	PX4	C12-C11-C10	2.76	102.99	113.13	6	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	329	PX4	O5-C9-C10	2.76	120.24	111.83	9	7
4	A	391	PX4	O7-C23-O8	2.76	117.26	123.70	7	2
4	A	399	PX4	C7-O7-C23	2.76	111.20	117.80	8	3
4	A	319	PX4	O7-C23-O8	2.76	117.26	123.70	13	5
4	A	366	PX4	O8-C23-C24	2.76	113.00	123.78	13	2
4	A	420	PX4	C16-C15-C14	2.76	100.44	114.37	11	1
4	A	423	PX4	C19-C18-C17	2.76	100.44	114.37	11	3
4	A	360	PX4	C11-C10-C9	2.75	103.61	113.69	2	1
4	A	385	PX4	O1-P1-O4	2.75	120.04	107.57	4	2
4	A	404	PX4	C5-N1-C2	2.75	120.85	109.91	10	1
4	A	318	PX4	C5-N1-C3	2.75	116.20	108.98	10	4
4	A	325	PX4	O4-P1-O2	2.75	119.84	108.94	11	3
4	A	351	PX4	O3-C1-C2	2.75	122.88	109.65	6	2
4	A	397	PX4	C25-C24-C23	2.75	103.62	113.69	9	2
4	A	350	PX4	O8-C23-C24	2.75	113.03	123.78	7	2
4	A	395	PX4	O3-P1-O2	2.75	98.04	108.94	9	2
4	A	339	PX4	C4-N1-C2	2.75	98.99	109.91	10	4
4	A	315	PX4	O5-C9-C10	2.75	120.21	111.83	11	5
4	A	382	PX4	O1-P1-O4	2.75	120.02	107.57	6	4
4	A	401	PX4	C8-O5-C9	2.75	107.08	117.12	8	5
4	A	359	PX4	C1-C2-N1	2.75	124.63	115.82	4	4
4	A	360	PX4	O3-P1-O2	2.75	98.05	108.94	6	1
4	A	365	PX4	O7-C7-C6	2.74	118.19	108.34	12	2
4	A	371	PX4	O5-C9-O6	2.74	116.76	123.63	10	2
4	A	399	PX4	C14-C13-C12	2.75	100.49	114.37	7	3
4	A	428	PX4	O3-C1-C2	2.75	122.86	109.65	9	1
4	A	357	PX4	O7-C7-C6	2.74	118.18	108.34	11	3
4	A	377	PX4	C11-C10-C9	2.74	103.64	113.69	8	3
4	A	348	PX4	O7-C7-C8	2.74	118.18	108.34	3	2
4	A	390	PX4	C5-N1-C3	2.74	101.77	108.98	2	3
4	A	400	PX4	C7-O7-C23	2.74	124.36	117.80	4	4
4	A	335	PX4	C28-C27-C26	2.74	100.52	114.37	4	2
4	A	361	PX4	C19-C18-C17	2.74	100.52	114.37	9	1
4	A	367	PX4	C7-O7-C23	2.74	124.35	117.80	3	4
4	A	389	PX4	C26-C25-C24	2.74	103.06	113.13	4	2
4	A	427	PX4	C5-N1-C3	2.74	101.78	108.98	11	4
4	A	378	PX4	C4-N1-C2	2.74	120.80	109.91	8	2
4	A	400	PX4	C1-C2-N1	2.74	124.61	115.82	5	3
4	A	327	PX4	C12-C11-C10	2.74	103.07	113.13	5	2
4	A	339	PX4	C11-C10-C9	2.74	103.66	113.69	14	2
4	A	412	PX4	O1-P1-O3	2.74	95.16	107.57	8	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	417	PX4	O1-P1-O4	2.74	119.97	107.57	14	2
4	A	309	PX4	C28-C27-C26	2.74	100.54	114.37	13	3
4	A	357	PX4	C26-C25-C24	2.74	103.08	113.13	6	2
4	A	344	PX4	O3-C1-C2	2.73	122.81	109.65	11	4
4	A	346	PX4	C4-N1-C2	2.74	99.04	109.91	12	3
4	A	356	PX4	C4-N1-C3	2.73	101.80	108.98	9	3
4	A	371	PX4	C32-C31-C30	2.73	100.55	114.37	2	2
4	A	406	PX4	C28-C27-C26	2.73	100.56	114.37	6	3
4	A	428	PX4	O4-P1-O2	2.73	119.77	108.94	5	2
4	A	337	PX4	C29-C28-C27	2.73	100.56	114.37	5	1
4	A	410	PX4	C3-N1-C2	2.73	120.77	109.91	13	2
4	A	428	PX4	O1-P1-O2	2.73	125.15	112.44	5	7
4	A	334	PX4	C27-C26-C25	2.73	100.57	114.37	14	2
4	A	334	PX4	O3-P1-O2	2.73	98.11	108.94	11	2
4	A	353	PX4	O4-P1-O2	2.73	119.75	108.94	2	3
4	A	362	PX4	C14-C13-C12	2.73	100.57	114.37	13	2
4	A	366	PX4	C1-C2-N1	2.73	124.58	115.82	2	4
4	A	383	PX4	C1-C2-N1	2.73	124.58	115.82	9	2
4	A	310	PX4	O1-P1-O4	2.73	119.92	107.57	11	4
4	A	376	PX4	O6-C9-C10	2.73	113.12	123.78	11	4
4	A	377	PX4	C1-C2-N1	2.73	124.57	115.82	3	2
4	A	406	PX4	C19-C18-C17	2.73	100.58	114.37	12	1
4	A	312	PX4	C30-C29-C28	2.73	100.59	114.37	4	1
4	A	342	PX4	C12-C11-C10	2.73	103.11	113.13	1	3
4	A	337	PX4	C5-N1-C2	2.72	120.74	109.91	2	2
4	A	316	PX4	C1-C2-N1	2.72	124.56	115.82	4	6
4	A	324	PX4	C34-C33-C32	2.72	100.61	114.37	11	1
4	A	371	PX4	C33-C32-C31	2.72	100.61	114.37	7	2
4	A	375	PX4	C14-C13-C12	2.72	100.61	114.37	8	1
4	A	381	PX4	C26-C25-C24	2.72	103.13	113.13	1	2
4	A	392	PX4	C12-C11-C10	2.72	103.13	113.13	7	1
4	A	421	PX4	C1-C2-N1	2.72	124.56	115.82	9	2
4	A	347	PX4	O1-P1-O4	2.72	119.89	107.57	5	2
4	A	374	PX4	O1-P1-O3	2.72	95.24	107.57	3	3
4	A	381	PX4	C8-O5-C9	2.72	127.06	117.12	2	1
4	A	307	PX4	C20-C19-C18	2.72	100.63	114.37	2	2
4	A	337	PX4	C5-N1-C4	2.72	101.84	108.98	7	2
4	A	383	PX4	C4-N1-C3	2.72	101.84	108.98	4	1
4	A	414	PX4	C7-O7-C23	2.72	124.30	117.80	11	3
4	A	416	PX4	C1-C2-N1	2.72	124.54	115.82	14	3
4	A	344	PX4	C4-N1-C3	2.71	101.85	108.98	6	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	410	PX4	C1-C2-N1	2.71	124.53	115.82	7	6
4	A	315	PX4	C25-C24-C23	2.71	103.75	113.69	9	2
4	A	385	PX4	O7-C7-C6	2.71	118.08	108.34	3	3
4	A	392	PX4	C11-C10-C9	2.71	103.75	113.69	4	2
4	A	399	PX4	C19-C18-C17	2.71	100.65	114.37	3	2
4	A	403	PX4	C14-C13-C12	2.71	100.65	114.37	11	3
4	A	423	PX4	C3-N1-C2	2.71	120.70	109.91	9	2
4	A	307	PX4	C15-C14-C13	2.71	100.66	114.37	1	1
4	A	315	PX4	C12-C11-C10	2.71	103.16	113.13	2	3
4	A	330	PX4	P1-O4-C6	2.71	105.81	121.35	7	6
4	A	342	PX4	C4-N1-C3	2.71	101.85	108.98	12	2
4	A	349	PX4	C27-C26-C25	2.71	100.66	114.37	14	2
4	A	419	PX4	C8-O5-C9	2.71	107.21	117.12	5	2
4	A	428	PX4	C26-C25-C24	2.71	103.17	113.13	13	2
4	A	391	PX4	C27-C26-C25	2.71	100.67	114.37	2	1
4	A	416	PX4	P1-O4-C6	2.71	105.82	121.35	9	4
4	A	430	PX4	C5-N1-C4	2.71	101.86	108.98	5	3
4	A	358	PX4	C29-C28-C27	2.71	100.68	114.37	8	3
4	A	376	PX4	C19-C18-C17	2.71	100.68	114.37	4	1
4	A	393	PX4	C17-C16-C15	2.71	100.68	114.37	13	1
4	A	312	PX4	O5-C9-O6	2.71	116.86	123.63	2	2
4	A	349	PX4	C34-C33-C32	2.71	100.69	114.37	5	2
4	A	356	PX4	O7-C23-O8	2.71	117.38	123.70	10	1
4	A	413	PX4	C31-C30-C29	2.71	100.68	114.37	9	1
4	A	425	PX4	C14-C13-C12	2.71	100.69	114.37	8	1
4	A	393	PX4	C4-N1-C2	2.71	120.66	109.91	12	2
4	A	420	PX4	C20-C19-C18	2.71	100.69	114.37	6	2
4	A	344	PX4	C33-C32-C31	2.70	100.70	114.37	8	1
4	A	351	PX4	C5-N1-C2	2.70	99.16	109.91	1	4
4	A	316	PX4	C11-C10-C9	2.70	123.60	113.69	5	1
4	A	334	PX4	C29-C28-C27	2.70	100.70	114.37	12	3
4	A	388	PX4	C1-C2-N1	2.70	124.50	115.82	6	4
4	A	409	PX4	C25-C24-C23	2.70	103.79	113.69	6	2
4	A	359	PX4	O5-C9-C10	2.70	120.07	111.83	6	4
4	A	362	PX4	P1-O4-C6	2.70	105.87	121.35	4	5
4	A	342	PX4	C25-C24-C23	2.70	103.81	113.69	11	3
4	A	356	PX4	O8-C23-C24	2.70	113.22	123.78	7	1
4	A	396	PX4	C18-C17-C16	2.70	100.72	114.37	8	2
4	A	375	PX4	O6-C9-C10	2.70	113.23	123.78	12	1
4	A	403	PX4	C11-C10-C9	2.70	103.80	113.69	3	1
4	A	356	PX4	C29-C28-C27	2.70	100.73	114.37	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	C27-C26-C25	2.70	100.73	114.37	6	2
4	A	326	PX4	C19-C18-C17	2.70	100.74	114.37	4	2
4	A	330	PX4	O7-C7-C8	2.70	118.02	108.34	1	6
4	A	330	PX4	O1-P1-O4	2.70	119.78	107.57	3	3
4	A	364	PX4	C20-C19-C18	2.70	100.74	114.37	11	1
4	A	401	PX4	C16-C15-C14	2.70	100.74	114.37	13	1
4	A	369	PX4	C12-C11-C10	2.69	103.22	113.13	5	4
4	A	339	PX4	C7-O7-C23	2.69	111.35	117.80	2	2
4	A	393	PX4	C18-C17-C16	2.69	100.75	114.37	6	1
4	A	324	PX4	C32-C31-C30	2.69	100.76	114.37	11	1
4	A	397	PX4	C13-C12-C11	2.69	100.75	114.37	14	2
4	A	380	PX4	C13-C12-C11	2.69	100.76	114.37	6	1
4	A	399	PX4	C3-N1-C2	2.69	99.21	109.91	12	3
4	A	412	PX4	O5-C9-C10	2.69	120.05	111.83	7	2
4	A	326	PX4	C5-N1-C4	2.69	101.91	108.98	1	3
4	A	398	PX4	O6-C9-C10	2.69	113.25	123.78	2	1
4	A	407	PX4	O1-P1-O3	2.69	95.37	107.57	10	1
4	A	334	PX4	C8-O5-C9	2.69	107.28	117.12	12	2
4	A	348	PX4	C25-C24-C23	2.69	103.84	113.69	5	1
4	A	425	PX4	O3-C1-C2	2.69	122.60	109.65	1	3
4	A	327	PX4	C8-O5-C9	2.69	107.29	117.12	12	1
4	A	353	PX4	C5-N1-C4	2.69	101.91	108.98	10	2
4	A	354	PX4	C5-N1-C2	2.69	120.60	109.91	9	3
4	A	380	PX4	C5-N1-C3	2.69	101.92	108.98	12	3
4	A	337	PX4	C26-C25-C24	2.69	103.25	113.13	6	1
4	A	359	PX4	O1-P1-O4	2.69	119.75	107.57	11	3
4	A	384	PX4	C25-C24-C23	2.69	103.85	113.69	9	1
4	A	379	PX4	C26-C25-C24	2.69	103.26	113.13	1	2
4	A	390	PX4	C8-O5-C9	2.69	107.30	117.12	5	2
4	A	396	PX4	O3-P1-O2	2.69	98.28	108.94	11	3
4	A	428	PX4	C7-O7-C23	2.69	124.23	117.80	8	5
4	A	326	PX4	O6-C9-C10	2.69	113.28	123.78	7	2
4	A	350	PX4	O5-C9-C10	2.69	120.02	111.83	11	3
4	A	308	PX4	C20-C19-C18	2.68	100.80	114.37	9	1
4	A	374	PX4	C30-C29-C28	2.68	100.80	114.37	3	1
4	A	392	PX4	C20-C19-C18	2.68	100.80	114.37	14	2
4	A	321	PX4	C12-C11-C10	2.68	103.27	113.13	4	1
4	A	404	PX4	C34-C33-C32	2.68	100.81	114.37	11	1
4	A	419	PX4	O5-C9-C10	2.68	120.01	111.83	3	3
4	A	420	PX4	C4-N1-C3	2.68	116.02	108.98	7	3
4	A	321	PX4	C4-N1-C3	2.68	101.94	108.98	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	356	PX4	O4-P1-O2	2.68	119.56	108.94	14	3
4	A	373	PX4	C4-N1-C3	2.68	116.02	108.98	10	1
4	A	385	PX4	C19-C18-C17	2.68	100.81	114.37	12	1
4	A	418	PX4	C17-C16-C15	2.68	100.82	114.37	12	1
4	A	317	PX4	O4-P1-O2	2.68	119.55	108.94	3	1
4	A	338	PX4	C4-N1-C2	2.68	120.56	109.91	13	2
4	A	379	PX4	C5-N1-C3	2.68	116.01	108.98	14	3
4	A	409	PX4	O8-C23-C24	2.68	113.31	123.78	4	1
4	A	411	PX4	O4-P1-O2	2.68	119.55	108.94	14	5
4	A	346	PX4	C1-C2-N1	2.68	124.42	115.82	9	4
4	A	349	PX4	C26-C25-C24	2.68	103.29	113.13	9	2
4	A	322	PX4	C29-C28-C27	2.68	100.84	114.37	6	2
4	A	322	PX4	C8-O5-C9	2.68	107.33	117.12	14	2
4	A	370	PX4	C5-N1-C3	2.68	101.94	108.98	6	3
4	A	323	PX4	C4-N1-C3	2.68	101.95	108.98	11	4
4	A	373	PX4	C20-C19-C18	2.68	100.84	114.37	14	3
4	A	388	PX4	C25-C24-C23	2.68	103.89	113.69	5	1
4	A	422	PX4	O1-P1-O3	2.68	95.44	107.57	4	3
4	A	356	PX4	C13-C12-C11	2.68	100.84	114.37	5	2
4	A	394	PX4	C11-C10-C9	2.68	123.50	113.69	14	2
4	A	324	PX4	C29-C28-C27	2.67	100.86	114.37	14	3
4	A	351	PX4	C31-C30-C29	2.67	100.85	114.37	4	2
4	A	371	PX4	O6-C9-C10	2.67	134.24	123.78	14	2
4	A	416	PX4	O1-P1-O4	2.67	119.69	107.57	13	2
4	A	417	PX4	C27-C26-C25	2.67	100.85	114.37	14	2
4	A	323	PX4	C28-C27-C26	2.67	100.87	114.37	3	2
4	A	360	PX4	C5-N1-C2	2.67	120.53	109.91	12	3
4	A	389	PX4	O4-P1-O2	2.67	119.53	108.94	3	1
4	A	407	PX4	C29-C28-C27	2.67	100.86	114.37	11	2
4	A	373	PX4	C17-C16-C15	2.67	100.87	114.37	3	1
4	A	421	PX4	C4-N1-C3	2.67	101.96	108.98	2	1
4	A	337	PX4	C34-C33-C32	2.67	100.87	114.37	5	3
4	A	391	PX4	C33-C32-C31	2.67	100.87	114.37	7	2
4	A	400	PX4	O5-C9-C10	2.67	119.98	111.83	11	2
4	A	421	PX4	C5-N1-C3	2.67	101.96	108.98	7	2
4	A	398	PX4	C17-C16-C15	2.67	100.88	114.37	2	2
4	A	328	PX4	C16-C15-C14	2.67	100.88	114.37	5	2
4	A	417	PX4	O5-C9-C10	2.67	119.97	111.83	7	3
4	A	372	PX4	O1-P1-O3	2.67	95.48	107.57	3	2
4	A	375	PX4	C11-C10-C9	2.67	103.92	113.69	1	3
4	A	423	PX4	C12-C11-C10	2.67	122.93	113.13	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	O5-C9-O6	2.67	116.96	123.63	4	1
4	A	320	PX4	C15-C14-C13	2.66	100.90	114.37	2	2
4	A	340	PX4	O5-C9-C10	2.67	119.96	111.83	12	3
4	A	406	PX4	C33-C32-C31	2.67	100.90	114.37	11	2
4	A	410	PX4	C8-O5-C9	2.67	126.86	117.12	11	2
4	A	337	PX4	O3-C1-C2	2.66	122.47	109.65	8	1
4	A	358	PX4	O7-C7-C6	2.66	117.90	108.34	10	7
4	A	380	PX4	O6-C9-C10	2.66	113.37	123.78	10	2
4	A	308	PX4	C33-C32-C31	2.66	100.92	114.37	8	1
4	A	310	PX4	C1-C2-N1	2.66	124.36	115.82	8	3
4	A	324	PX4	C11-C10-C9	2.66	103.94	113.69	2	1
4	A	331	PX4	O3-P1-O2	2.66	98.39	108.94	7	4
4	A	340	PX4	C15-C14-C13	2.66	100.93	114.37	13	1
4	A	397	PX4	O7-C7-C6	2.66	117.88	108.34	8	2
4	A	374	PX4	C33-C32-C31	2.66	100.93	114.37	6	2
4	A	420	PX4	O6-C9-C10	2.66	113.39	123.78	13	2
4	A	318	PX4	C14-C13-C12	2.66	100.94	114.37	8	1
4	A	345	PX4	O7-C23-C24	2.66	117.23	111.48	7	3
4	A	355	PX4	C8-O5-C9	2.66	126.83	117.12	10	1
4	A	314	PX4	C26-C25-C24	2.65	103.37	113.13	7	3
4	A	315	PX4	O1-P1-O4	2.66	119.60	107.57	9	1
4	A	344	PX4	C25-C24-C23	2.66	123.42	113.69	4	1
4	A	346	PX4	O4-P1-O2	2.66	98.41	108.94	7	1
4	A	382	PX4	C15-C14-C13	2.66	100.94	114.37	2	2
4	A	308	PX4	C13-C12-C11	2.65	100.96	114.37	8	2
4	A	325	PX4	C4-N1-C3	2.65	102.01	108.98	9	2
4	A	377	PX4	O1-P1-O2	2.65	124.79	112.44	7	5
4	A	391	PX4	C19-C18-C17	2.65	100.96	114.37	12	2
4	A	429	PX4	C5-N1-C2	2.65	99.36	109.91	13	1
4	A	345	PX4	O8-C23-C24	2.65	113.41	123.78	2	1
4	A	307	PX4	C13-C12-C11	2.65	100.97	114.37	10	2
4	A	309	PX4	O4-P1-O2	2.65	119.44	108.94	14	7
4	A	390	PX4	C30-C29-C28	2.65	100.97	114.37	12	1
4	A	399	PX4	C4-N1-C3	2.65	115.94	108.98	1	3
4	A	325	PX4	C20-C19-C18	2.65	100.98	114.37	5	2
4	A	329	PX4	C5-N1-C4	2.65	102.02	108.98	4	3
4	A	360	PX4	C8-O5-C9	2.65	107.43	117.12	13	1
4	A	409	PX4	O3-C1-C2	2.65	122.41	109.65	11	3
4	A	419	PX4	C30-C29-C28	2.65	100.97	114.37	12	1
4	A	426	PX4	C19-C18-C17	2.65	100.98	114.37	10	1
4	A	430	PX4	C13-C12-C11	2.65	100.97	114.37	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	314	PX4	C12-C11-C10	2.65	103.40	113.13	11	2
4	A	323	PX4	C11-C10-C9	2.65	103.99	113.69	9	2
4	A	365	PX4	O8-C23-C24	2.64	113.44	123.78	13	1
4	A	348	PX4	C31-C30-C29	2.64	101.00	114.37	1	2
4	A	350	PX4	O4-P1-O2	2.64	119.42	108.94	7	6
4	A	364	PX4	C31-C30-C29	2.64	101.00	114.37	6	1
4	A	320	PX4	C16-C15-C14	2.64	101.01	114.37	12	4
4	A	336	PX4	O7-C23-O8	2.64	117.53	123.70	2	1
4	A	354	PX4	O1-P1-O3	2.64	95.59	107.57	4	3
4	A	366	PX4	C8-O5-C9	2.64	107.46	117.12	13	1
4	A	373	PX4	C5-N1-C3	2.64	115.92	108.98	11	1
4	A	414	PX4	C25-C24-C23	2.64	123.38	113.69	7	1
4	A	357	PX4	C5-N1-C2	2.64	99.41	109.91	5	3
4	A	307	PX4	O5-C9-C10	2.64	119.89	111.83	7	4
4	A	310	PX4	C3-N1-C2	2.64	120.41	109.91	1	1
4	A	353	PX4	O5-C9-C10	2.64	119.89	111.83	6	6
4	A	358	PX4	C27-C26-C25	2.64	101.02	114.37	2	1
4	A	320	PX4	C18-C17-C16	2.64	101.03	114.37	10	3
4	A	323	PX4	C8-O5-C9	2.64	107.47	117.12	1	2
4	A	393	PX4	O5-C9-O6	2.64	117.03	123.63	4	5
4	A	426	PX4	O3-P1-O2	2.64	98.48	108.94	8	2
4	A	333	PX4	C14-C13-C12	2.64	101.04	114.37	9	2
4	A	324	PX4	C5-N1-C4	2.64	102.05	108.98	10	2
4	A	329	PX4	O6-C9-C10	2.64	113.47	123.78	5	1
4	A	365	PX4	O5-C9-C10	2.64	119.87	111.83	3	1
4	A	369	PX4	C3-N1-C2	2.64	120.39	109.91	12	3
4	A	370	PX4	O7-C7-C8	2.64	117.80	108.34	8	2
4	A	388	PX4	C15-C14-C13	2.64	101.04	114.37	14	2
4	A	335	PX4	C15-C14-C13	2.63	101.05	114.37	1	3
4	A	364	PX4	C4-N1-C2	2.63	120.38	109.91	13	2
4	A	347	PX4	C27-C26-C25	2.63	127.68	114.37	5	1
4	A	349	PX4	O7-C23-O8	2.63	117.55	123.70	9	5
4	A	356	PX4	C34-C33-C32	2.63	101.06	114.37	12	2
4	A	406	PX4	C5-N1-C3	2.63	102.06	108.98	13	1
4	A	413	PX4	O5-C9-C10	2.63	119.86	111.83	2	4
4	A	312	PX4	C28-C27-C26	2.63	101.06	114.37	1	3
4	A	335	PX4	C31-C30-C29	2.63	101.07	114.37	6	1
4	A	338	PX4	C31-C30-C29	2.63	101.07	114.37	8	1
4	A	365	PX4	C20-C19-C18	2.63	101.07	114.37	13	1
4	A	371	PX4	C8-O5-C9	2.63	107.50	117.12	5	2
4	A	415	PX4	O3-C1-C2	2.63	122.31	109.65	5	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	379	PX4	C20-C19-C18	2.63	101.08	114.37	2	1
4	A	392	PX4	C33-C32-C31	2.63	101.07	114.37	9	1
4	A	408	PX4	C27-C26-C25	2.63	101.07	114.37	5	5
4	A	308	PX4	O7-C7-C6	2.63	117.78	108.34	5	2
4	A	308	PX4	C32-C31-C30	2.63	101.08	114.37	13	2
4	A	336	PX4	C33-C32-C31	2.63	101.08	114.37	4	1
4	A	392	PX4	C7-O7-C23	2.63	111.51	117.80	14	2
4	A	320	PX4	C13-C12-C11	2.63	101.10	114.37	1	2
4	A	352	PX4	C34-C33-C32	2.63	101.09	114.37	8	2
4	A	406	PX4	O3-C1-C2	2.63	122.29	109.65	3	1
4	A	351	PX4	C32-C31-C30	2.63	101.10	114.37	13	1
4	A	343	PX4	C32-C31-C30	2.62	101.11	114.37	2	3
4	A	398	PX4	C25-C24-C23	2.62	104.08	113.69	2	2
4	A	405	PX4	O5-C9-O6	2.62	117.06	123.63	1	2
4	A	418	PX4	C4-N1-C2	2.62	120.34	109.91	9	1
4	A	350	PX4	O1-P1-O3	2.62	95.68	107.57	13	2
4	A	380	PX4	O3-C1-C2	2.62	122.26	109.65	1	1
4	A	413	PX4	C12-C11-C10	2.62	103.49	113.13	4	3
4	A	364	PX4	O3-C1-C2	2.62	122.26	109.65	11	1
4	A	420	PX4	C5-N1-C4	2.62	102.09	108.98	1	6
4	A	316	PX4	C29-C28-C27	2.62	101.13	114.37	9	1
4	A	320	PX4	O4-P1-O2	2.62	119.32	108.94	2	3
4	A	334	PX4	C17-C16-C15	2.62	101.12	114.37	14	1
4	A	335	PX4	C5-N1-C2	2.62	120.33	109.91	3	1
4	A	387	PX4	C26-C25-C24	2.62	103.50	113.13	9	3
4	A	405	PX4	C30-C29-C28	2.62	101.13	114.37	13	1
4	A	411	PX4	O1-P1-O4	2.62	119.44	107.57	1	4
4	A	307	PX4	C8-O5-C9	2.62	107.55	117.12	5	2
4	A	412	PX4	C25-C24-C23	2.62	104.10	113.69	7	3
4	A	390	PX4	O7-C7-C6	2.62	117.73	108.34	10	2
4	A	403	PX4	C34-C33-C32	2.62	101.14	114.37	1	1
4	A	418	PX4	C30-C29-C28	2.62	101.14	114.37	5	1
4	A	363	PX4	C32-C31-C30	2.62	101.15	114.37	12	2
4	A	403	PX4	O4-P1-O2	2.62	119.30	108.94	8	1
4	A	329	PX4	C32-C31-C30	2.61	127.58	114.37	11	1
4	A	403	PX4	C3-N1-C2	2.61	99.52	109.91	12	1
4	A	351	PX4	C34-C33-C32	2.61	101.16	114.37	14	1
4	A	408	PX4	C19-C18-C17	2.61	101.16	114.37	7	2
4	A	343	PX4	O3-C1-C2	2.61	122.21	109.65	10	3
4	A	367	PX4	C5-N1-C4	2.61	115.83	108.98	5	2
4	A	407	PX4	C16-C15-C14	2.61	101.17	114.37	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PX4	C4-N1-C3	2.61	102.12	108.98	13	3
4	A	421	PX4	O6-C9-C10	2.61	113.57	123.78	9	1
4	A	314	PX4	C1-C2-N1	2.61	124.20	115.82	1	4
4	A	381	PX4	O4-P1-O2	2.61	119.28	108.94	6	2
4	A	400	PX4	O5-C9-O6	2.61	117.10	123.63	11	4
4	A	318	PX4	C27-C26-C25	2.61	101.18	114.37	14	1
4	A	316	PX4	C7-O7-C23	2.61	124.04	117.80	11	2
4	A	336	PX4	C3-N1-C2	2.61	120.28	109.91	10	1
4	A	318	PX4	C4-N1-C3	2.61	102.13	108.98	10	2
4	A	319	PX4	C4-N1-C3	2.61	102.13	108.98	5	4
4	A	320	PX4	C12-C11-C10	2.61	103.55	113.13	13	2
4	A	354	PX4	C4-N1-C3	2.61	102.13	108.98	13	4
4	A	355	PX4	C4-N1-C2	2.61	99.54	109.91	10	3
4	A	386	PX4	C7-O7-C23	2.61	111.56	117.80	12	2
4	A	323	PX4	C30-C29-C28	2.61	101.20	114.37	5	1
4	A	363	PX4	C13-C12-C11	2.61	101.20	114.37	2	2
4	A	372	PX4	O7-C7-C6	2.61	117.69	108.34	1	5
4	A	375	PX4	C5-N1-C4	2.61	102.13	108.98	14	1
4	A	378	PX4	C8-O5-C9	2.61	107.60	117.12	3	2
4	A	384	PX4	O7-C7-C6	2.61	117.69	108.34	1	2
4	A	326	PX4	O4-P1-O2	2.60	119.25	108.94	11	3
4	A	346	PX4	O3-C1-C2	2.60	122.18	109.65	9	1
4	A	374	PX4	C11-C10-C9	2.60	104.15	113.69	1	2
4	A	340	PX4	C29-C28-C27	2.60	101.21	114.37	6	2
4	A	376	PX4	C32-C31-C30	2.60	101.21	114.37	11	2
4	A	412	PX4	O4-P1-O2	2.60	98.62	108.94	4	6
4	A	340	PX4	O8-C23-C24	2.60	113.61	123.78	12	2
4	A	386	PX4	C26-C25-C24	2.60	103.57	113.13	5	1
4	A	414	PX4	C5-N1-C3	2.60	102.14	108.98	6	2
4	A	419	PX4	O4-P1-O2	2.60	98.62	108.94	12	2
4	A	344	PX4	C26-C25-C24	2.60	103.57	113.13	14	2
4	A	351	PX4	C25-C24-C23	2.60	104.16	113.69	14	1
4	A	323	PX4	C14-C13-C12	2.60	101.24	114.37	9	3
4	A	345	PX4	C11-C10-C9	2.60	104.17	113.69	10	2
4	A	354	PX4	O3-C1-C2	2.60	122.16	109.65	2	2
4	A	359	PX4	C36-C35-C34	2.60	95.81	113.36	14	1
4	A	410	PX4	C28-C27-C26	2.60	101.23	114.37	3	2
4	A	327	PX4	C33-C32-C31	2.60	101.24	114.37	13	1
4	A	337	PX4	C33-C32-C31	2.60	101.24	114.37	8	2
4	A	370	PX4	C31-C30-C29	2.60	101.24	114.37	7	1
4	A	374	PX4	C4-N1-C3	2.60	102.15	108.98	5	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	405	PX4	C12-C11-C10	2.60	103.58	113.13	6	3
4	A	410	PX4	O7-C7-C8	2.60	117.66	108.34	9	3
4	A	426	PX4	C28-C27-C26	2.60	101.24	114.37	1	2
4	A	326	PX4	O1-P1-O3	2.60	95.80	107.57	6	1
4	A	426	PX4	C17-C16-C15	2.60	101.25	114.37	2	1
4	A	430	PX4	C29-C28-C27	2.60	101.24	114.37	1	1
4	A	418	PX4	O5-C9-C10	2.60	119.75	111.83	7	1
4	A	311	PX4	C20-C19-C18	2.59	101.26	114.37	8	2
4	A	318	PX4	O1-P1-O4	2.59	119.32	107.57	4	1
4	A	327	PX4	C20-C19-C18	2.59	101.26	114.37	5	3
4	A	343	PX4	C1-C2-N1	2.59	124.14	115.82	2	1
4	A	367	PX4	C3-N1-C2	2.59	99.60	109.91	13	1
4	A	387	PX4	O6-C9-C10	2.59	113.64	123.78	9	1
4	A	353	PX4	C12-C11-C10	2.59	103.60	113.13	10	3
4	A	312	PX4	O5-C9-C10	2.59	119.74	111.83	13	3
4	A	320	PX4	O7-C23-O8	2.59	117.64	123.70	6	2
4	A	380	PX4	C7-O7-C23	2.59	111.59	117.80	5	3
4	A	384	PX4	C4-N1-C3	2.59	102.17	108.98	12	2
4	A	393	PX4	O3-C1-C2	2.59	122.11	109.65	12	1
4	A	313	PX4	C17-C16-C15	2.59	101.28	114.37	7	1
4	A	335	PX4	O5-C9-O6	2.59	117.15	123.63	13	3
4	A	375	PX4	O7-C7-C8	2.59	117.63	108.34	7	7
4	A	319	PX4	C28-C27-C26	2.59	101.29	114.37	9	2
4	A	378	PX4	C33-C32-C31	2.59	101.29	114.37	1	2
4	A	379	PX4	O3-C1-C2	2.59	122.10	109.65	5	3
4	A	427	PX4	C16-C15-C14	2.59	101.28	114.37	1	3
4	A	308	PX4	C18-C17-C16	2.59	101.30	114.37	9	1
4	A	332	PX4	C27-C26-C25	2.59	101.29	114.37	12	1
4	A	344	PX4	C3-N1-C2	2.59	99.63	109.91	1	2
4	A	407	PX4	C15-C14-C13	2.59	101.29	114.37	13	1
4	A	428	PX4	C1-C2-N1	2.59	124.13	115.82	5	4
4	A	328	PX4	C18-C17-C16	2.59	101.30	114.37	5	2
4	A	420	PX4	O7-C7-C8	2.59	117.62	108.34	1	1
4	A	306	PX4	C16-C15-C14	2.58	101.31	114.37	7	1
4	A	309	PX4	O1-P1-O3	2.58	95.86	107.57	11	4
4	A	327	PX4	C14-C13-C12	2.58	101.31	114.37	12	1
4	A	369	PX4	C30-C29-C28	2.58	101.30	114.37	12	2
4	A	382	PX4	C14-C13-C12	2.58	101.31	114.37	3	1
4	A	398	PX4	C3-N1-C2	2.58	120.18	109.91	6	1
4	A	394	PX4	O3-C1-C2	2.58	122.08	109.65	4	1
4	A	376	PX4	C16-C15-C14	2.58	101.31	114.37	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C8-O5-C9	2.58	107.68	117.12	13	2
4	A	421	PX4	C25-C24-C23	2.58	104.23	113.69	4	2
4	A	328	PX4	C20-C19-C18	2.58	101.32	114.37	13	1
4	A	397	PX4	O1-P1-O4	2.58	119.27	107.57	14	1
4	A	348	PX4	C30-C29-C28	2.58	101.33	114.37	14	1
4	A	416	PX4	O4-P1-O2	2.58	119.16	108.94	10	4
4	A	376	PX4	C12-C11-C10	2.58	103.65	113.13	10	1
4	A	309	PX4	C25-C24-C23	2.58	104.25	113.69	5	1
4	A	316	PX4	C5-N1-C3	2.58	115.75	108.98	5	1
4	A	351	PX4	C18-C17-C16	2.58	101.34	114.37	11	1
4	A	367	PX4	C12-C11-C10	2.58	103.66	113.13	9	1
4	A	391	PX4	C1-C2-N1	2.58	124.10	115.82	13	3
4	A	368	PX4	C8-O5-C9	2.58	107.70	117.12	6	5
4	A	328	PX4	C4-N1-C2	2.58	120.15	109.91	12	2
4	A	336	PX4	O5-C9-C10	2.58	119.69	111.83	9	6
4	A	371	PX4	C14-C13-C12	2.58	101.35	114.37	12	1
4	A	397	PX4	C17-C16-C15	2.58	101.35	114.37	6	1
4	A	402	PX4	C19-C18-C17	2.58	101.35	114.37	13	1
4	A	348	PX4	C12-C11-C10	2.57	103.67	113.13	2	3
4	A	325	PX4	C13-C12-C11	2.57	101.37	114.37	12	2
4	A	343	PX4	O4-P1-O2	2.57	119.13	108.94	2	2
4	A	362	PX4	C1-C2-N1	2.57	124.08	115.82	12	1
4	A	406	PX4	C5-N1-C4	2.57	102.22	108.98	12	2
4	A	428	PX4	C5-N1-C4	2.57	115.74	108.98	1	2
4	A	360	PX4	C12-C11-C10	2.57	103.68	113.13	5	1
4	A	382	PX4	C5-N1-C4	2.57	102.22	108.98	4	2
4	A	316	PX4	C34-C33-C32	2.57	101.38	114.37	14	1
4	A	329	PX4	C14-C13-C12	2.57	101.37	114.37	2	2
4	A	341	PX4	O4-P1-O2	2.57	98.75	108.94	7	1
4	A	342	PX4	O3-C1-C2	2.57	122.01	109.65	8	2
4	A	358	PX4	C15-C14-C13	2.57	101.38	114.37	10	1
4	A	374	PX4	C20-C19-C18	2.57	101.37	114.37	6	1
4	A	363	PX4	C5-N1-C2	2.57	99.70	109.91	3	1
4	A	402	PX4	C32-C31-C30	2.57	101.38	114.37	9	1
4	A	405	PX4	O7-C23-O8	2.57	117.70	123.70	9	4
4	A	337	PX4	O1-P1-O3	2.57	119.20	107.57	8	2
4	A	361	PX4	C11-C10-C9	2.57	104.29	113.69	14	2
4	A	362	PX4	C30-C29-C28	2.57	101.39	114.37	6	1
4	A	364	PX4	O4-P1-O2	2.57	119.11	108.94	13	3
4	A	386	PX4	C5-N1-C4	2.57	102.23	108.98	7	3
4	A	414	PX4	C33-C32-C31	2.57	101.38	114.37	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	393	PX4	C25-C24-C23	2.57	104.29	113.69	14	1
4	A	365	PX4	O1-P1-O4	2.57	119.20	107.57	13	4
4	A	423	PX4	O4-P1-O2	2.57	119.11	108.94	1	3
4	A	409	PX4	C13-C12-C11	2.57	101.40	114.37	10	1
4	A	317	PX4	C25-C24-C23	2.56	123.09	113.69	7	2
4	A	354	PX4	C12-C11-C10	2.56	103.71	113.13	2	2
4	A	388	PX4	O4-P1-O2	2.56	119.10	108.94	10	1
4	A	391	PX4	C26-C25-C24	2.56	103.71	113.13	12	1
4	A	366	PX4	C34-C33-C32	2.56	101.41	114.37	6	2
4	A	389	PX4	C7-O7-C23	2.56	123.93	117.80	10	3
4	A	394	PX4	O5-C9-C10	2.56	119.65	111.83	4	4
4	A	423	PX4	C28-C27-C26	2.56	101.42	114.37	9	2
4	A	341	PX4	O7-C23-O8	2.56	117.72	123.70	5	1
4	A	372	PX4	C27-C26-C25	2.56	101.42	114.37	13	1
4	A	378	PX4	C14-C13-C12	2.56	101.42	114.37	1	1
4	A	381	PX4	C29-C28-C27	2.56	101.43	114.37	8	2
4	A	385	PX4	O3-C1-C2	2.56	121.97	109.65	12	2
4	A	392	PX4	C28-C27-C26	2.56	101.43	114.37	14	2
4	A	394	PX4	C31-C30-C29	2.56	101.42	114.37	9	1
4	A	404	PX4	C31-C30-C29	2.56	101.43	114.37	5	1
4	A	427	PX4	O6-C9-C10	2.56	113.78	123.78	12	1
4	A	320	PX4	O1-P1-O4	2.56	119.16	107.57	8	1
4	A	338	PX4	C18-C17-C16	2.56	101.44	114.37	14	4
4	A	390	PX4	C16-C15-C14	2.56	101.44	114.37	3	2
4	A	306	PX4	C20-C19-C18	2.55	101.45	114.37	1	1
4	A	361	PX4	C4-N1-C2	2.56	120.07	109.91	6	2
4	A	371	PX4	C5-N1-C4	2.56	102.26	108.98	7	2
4	A	374	PX4	C5-N1-C4	2.55	102.27	108.98	13	2
4	A	395	PX4	C31-C30-C29	2.56	101.45	114.37	7	3
4	A	416	PX4	C14-C13-C12	2.56	101.45	114.37	5	3
4	A	366	PX4	C5-N1-C4	2.55	102.27	108.98	7	2
4	A	367	PX4	C25-C24-C23	2.55	104.33	113.69	9	2
4	A	324	PX4	C3-N1-C2	2.55	120.06	109.91	2	1
4	A	328	PX4	C30-C29-C28	2.55	101.46	114.37	3	2
4	A	330	PX4	O4-P1-O2	2.55	98.81	108.94	8	3
4	A	375	PX4	C28-C27-C26	2.55	101.46	114.37	8	2
4	A	387	PX4	C4-N1-C2	2.55	120.06	109.91	9	1
4	A	427	PX4	O1-P1-O4	2.55	119.14	107.57	7	2
4	A	321	PX4	C1-C2-N1	2.55	124.01	115.82	11	4
4	A	331	PX4	O1-P1-O4	2.55	119.13	107.57	14	1
4	A	335	PX4	C11-C10-C9	2.55	104.34	113.69	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	C4-N1-C3	2.55	102.27	108.98	10	1
4	A	348	PX4	C4-N1-C2	2.55	120.06	109.91	10	1
4	A	401	PX4	O7-C7-C8	2.55	117.50	108.34	8	3
4	A	416	PX4	C20-C19-C18	2.55	101.47	114.37	10	4
4	A	323	PX4	C27-C26-C25	2.55	101.49	114.37	8	3
4	A	334	PX4	C33-C32-C31	2.55	101.48	114.37	5	1
4	A	428	PX4	C30-C29-C28	2.55	101.48	114.37	3	1
4	A	372	PX4	O3-C1-C2	2.55	121.91	109.65	4	1
4	A	403	PX4	O1-P1-O4	2.55	119.11	107.57	6	2
4	A	411	PX4	C28-C27-C26	2.55	101.49	114.37	6	2
4	A	319	PX4	O7-C7-C6	2.55	117.48	108.34	3	2
4	A	312	PX4	C12-C11-C10	2.55	103.77	113.13	4	2
4	A	322	PX4	O1-P1-O3	2.55	119.11	107.57	3	3
4	A	331	PX4	C18-C17-C16	2.55	101.50	114.37	9	1
4	A	336	PX4	C27-C26-C25	2.55	101.50	114.37	8	3
4	A	359	PX4	C4-N1-C3	2.55	102.29	108.98	3	3
4	A	384	PX4	C18-C17-C16	2.55	101.50	114.37	14	2
4	A	407	PX4	C26-C25-C24	2.55	122.48	113.13	6	2
4	A	420	PX4	C1-C2-N1	2.55	124.00	115.82	11	4
4	A	376	PX4	C26-C25-C24	2.54	103.78	113.13	2	2
4	A	400	PX4	C15-C14-C13	2.54	101.51	114.37	6	1
4	A	426	PX4	C25-C24-C23	2.54	104.37	113.69	12	1
4	A	347	PX4	C8-O5-C9	2.54	107.83	117.12	13	2
4	A	366	PX4	C3-N1-C2	2.54	120.02	109.91	14	1
4	A	391	PX4	C32-C31-C30	2.54	101.52	114.37	2	2
4	A	327	PX4	O4-P1-O2	2.54	119.00	108.94	5	1
4	A	334	PX4	O4-P1-O2	2.54	119.00	108.94	10	5
4	A	373	PX4	C5-N1-C4	2.54	102.31	108.98	5	1
4	A	389	PX4	C5-N1-C2	2.54	99.82	109.91	2	1
4	A	396	PX4	C8-O5-C9	2.54	107.84	117.12	2	1
4	A	396	PX4	C34-C33-C32	2.54	101.54	114.37	1	2
4	A	421	PX4	O3-C1-C2	2.54	121.86	109.65	10	1
4	A	332	PX4	C19-C18-C17	2.54	101.54	114.37	2	1
4	A	340	PX4	C7-O7-C23	2.54	123.86	117.80	9	1
4	A	342	PX4	C16-C15-C14	2.54	101.55	114.37	3	2
4	A	341	PX4	C8-O5-C9	2.53	107.86	117.12	12	1
4	A	352	PX4	C5-N1-C2	2.54	99.83	109.91	6	1
4	A	360	PX4	O6-C9-C10	2.54	113.87	123.78	13	1
4	A	388	PX4	O3-C1-C2	2.54	121.85	109.65	1	3
4	A	393	PX4	C5-N1-C3	2.54	102.32	108.98	7	2
4	A	405	PX4	O1-P1-O2	2.54	124.24	112.44	9	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	409	PX4	C20-C19-C18	2.54	101.55	114.37	2	1
4	A	407	PX4	C18-C17-C16	2.53	101.56	114.37	9	2
4	A	411	PX4	C14-C13-C12	2.53	101.56	114.37	8	2
4	A	343	PX4	C17-C16-C15	2.53	101.56	114.37	14	1
4	A	407	PX4	C32-C31-C30	2.53	101.56	114.37	4	3
4	A	415	PX4	C5-N1-C2	2.53	99.84	109.91	11	1
4	A	352	PX4	C4-N1-C2	2.53	99.84	109.91	14	1
4	A	358	PX4	C34-C33-C32	2.53	101.57	114.37	7	1
4	A	307	PX4	C34-C33-C32	2.53	101.58	114.37	1	2
4	A	326	PX4	C4-N1-C2	2.53	119.97	109.91	3	1
4	A	399	PX4	C18-C17-C16	2.53	101.57	114.37	11	1
4	A	393	PX4	C12-C11-C10	2.53	103.83	113.13	9	5
4	A	410	PX4	C18-C17-C16	2.53	101.57	114.37	4	1
4	A	361	PX4	C18-C17-C16	2.53	101.58	114.37	1	2
4	A	412	PX4	C18-C17-C16	2.53	101.58	114.37	14	1
4	A	417	PX4	C18-C17-C16	2.53	101.58	114.37	14	2
4	A	382	PX4	C12-C11-C10	2.53	103.83	113.13	5	1
4	A	331	PX4	O7-C7-C6	2.53	117.41	108.34	5	3
4	A	356	PX4	C33-C32-C31	2.53	101.59	114.37	6	1
4	A	339	PX4	C17-C16-C15	2.53	127.14	114.37	12	2
4	A	342	PX4	C5-N1-C4	2.53	115.61	108.98	6	3
4	A	378	PX4	O3-C1-C2	2.53	121.81	109.65	14	3
4	A	370	PX4	O4-P1-O2	2.53	118.94	108.94	3	1
4	A	383	PX4	C20-C19-C18	2.53	101.60	114.37	8	3
4	A	358	PX4	C4-N1-C2	2.52	119.94	109.91	3	1
4	A	366	PX4	O1-P1-O3	2.52	96.12	107.57	12	2
4	A	346	PX4	C33-C32-C31	2.52	101.61	114.37	5	2
4	A	349	PX4	O6-C9-C10	2.52	113.91	123.78	14	1
4	A	406	PX4	C16-C15-C14	2.52	101.61	114.37	7	2
4	A	428	PX4	O1-P1-O4	2.52	119.01	107.57	6	2
4	A	357	PX4	C30-C29-C28	2.52	101.62	114.37	1	1
4	A	367	PX4	C5-N1-C2	2.52	99.88	109.91	2	1
4	A	320	PX4	O5-C9-C10	2.52	119.52	111.83	13	4
4	A	362	PX4	C27-C26-C25	2.52	101.62	114.37	5	1
4	A	363	PX4	C27-C26-C25	2.52	101.62	114.37	8	1
4	A	401	PX4	O3-C1-C2	2.52	121.79	109.65	7	1
4	A	409	PX4	C30-C29-C28	2.52	101.62	114.37	7	1
4	A	421	PX4	C16-C15-C14	2.52	101.62	114.37	11	2
4	A	428	PX4	C27-C26-C25	2.52	101.62	114.37	1	1
4	A	375	PX4	C27-C26-C25	2.52	101.62	114.37	3	1
4	A	415	PX4	C17-C16-C15	2.52	101.63	114.37	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	C3-N1-C2	2.52	119.92	109.91	3	2
4	A	344	PX4	O4-P1-O2	2.52	118.92	108.94	4	1
4	A	403	PX4	C20-C19-C18	2.52	101.64	114.37	2	1
4	A	413	PX4	C33-C32-C31	2.52	101.64	114.37	7	2
4	A	357	PX4	C11-C10-C9	2.52	104.47	113.69	8	1
4	A	385	PX4	C16-C15-C14	2.52	101.65	114.37	8	1
4	A	391	PX4	O7-C7-C6	2.52	117.37	108.34	2	2
4	A	392	PX4	C25-C24-C23	2.52	122.92	113.69	2	2
4	A	327	PX4	C5-N1-C2	2.52	119.91	109.91	10	2
4	A	336	PX4	C8-O5-C9	2.51	107.93	117.12	3	1
4	A	337	PX4	O5-C9-O6	2.51	117.34	123.63	7	7
4	A	392	PX4	C32-C31-C30	2.51	101.66	114.37	6	1
4	A	320	PX4	C33-C32-C31	2.51	101.67	114.37	7	1
4	A	380	PX4	C27-C26-C25	2.51	101.67	114.37	10	4
4	A	394	PX4	O7-C7-C8	2.51	117.36	108.34	13	2
4	A	346	PX4	O8-C23-C24	2.51	113.96	123.78	2	2
4	A	328	PX4	C25-C24-C23	2.51	104.51	113.69	9	1
4	A	383	PX4	O1-P1-O4	2.51	118.93	107.57	12	5
4	A	422	PX4	C5-N1-C4	2.51	102.39	108.98	9	2
4	A	318	PX4	C5-N1-C4	2.51	102.39	108.98	2	2
4	A	317	PX4	C26-C25-C24	2.50	103.92	113.13	5	1
4	A	319	PX4	C1-C2-N1	2.50	123.86	115.82	8	1
4	A	330	PX4	C12-C11-C10	2.50	103.92	113.13	10	1
4	A	339	PX4	O7-C7-C8	2.50	117.33	108.34	3	2
4	A	347	PX4	C5-N1-C3	2.51	102.39	108.98	4	3
4	A	363	PX4	C4-N1-C2	2.51	119.87	109.91	3	1
4	A	396	PX4	C25-C24-C23	2.51	104.51	113.69	1	2
4	A	339	PX4	O7-C7-C6	2.50	117.33	108.34	13	3
4	A	363	PX4	C26-C25-C24	2.50	103.92	113.13	7	3
4	A	384	PX4	C30-C29-C28	2.50	101.71	114.37	1	2
4	A	324	PX4	C8-O5-C9	2.50	107.97	117.12	1	1
4	A	312	PX4	C31-C30-C29	2.50	101.72	114.37	14	3
4	A	312	PX4	C20-C19-C18	2.50	101.72	114.37	12	1
4	A	323	PX4	O3-P1-O2	2.50	99.02	108.94	12	2
4	A	351	PX4	C14-C13-C12	2.50	101.72	114.37	8	2
4	A	339	PX4	C33-C32-C31	2.50	101.73	114.37	6	1
4	A	349	PX4	O4-P1-O2	2.50	118.84	108.94	10	1
4	A	397	PX4	O3-C1-C2	2.50	121.68	109.65	5	3
4	A	410	PX4	C5-N1-C4	2.50	102.41	108.98	6	3
4	A	352	PX4	C16-C15-C14	2.50	101.73	114.37	13	1
4	A	308	PX4	C1-C2-N1	2.50	123.84	115.82	13	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	326	PX4	C11-C10-C9	2.50	122.85	113.69	13	3
4	A	353	PX4	C1-C2-N1	2.50	123.84	115.82	4	1
4	A	366	PX4	O7-C7-C6	2.50	117.31	108.34	9	2
4	A	378	PX4	O7-C7-C8	2.50	117.31	108.34	11	5
4	A	398	PX4	C4-N1-C3	2.50	102.41	108.98	7	3
4	A	414	PX4	C3-N1-C2	2.50	119.84	109.91	14	3
4	A	428	PX4	C17-C16-C15	2.50	101.73	114.37	5	2
4	A	336	PX4	C5-N1-C3	2.50	102.42	108.98	9	3
4	A	379	PX4	C27-C26-C25	2.50	101.74	114.37	10	1
4	A	400	PX4	C19-C18-C17	2.50	101.75	114.37	11	3
4	A	419	PX4	C12-C11-C10	2.50	103.95	113.13	13	3
4	A	429	PX4	C14-C13-C12	2.50	101.75	114.37	12	1
4	A	344	PX4	C5-N1-C2	2.50	119.83	109.91	2	1
4	A	347	PX4	C19-C18-C17	2.50	101.75	114.37	13	1
4	A	353	PX4	O8-C23-C24	2.50	114.02	123.78	7	2
4	A	417	PX4	C5-N1-C2	2.50	119.83	109.91	14	2
4	A	361	PX4	C14-C13-C12	2.49	101.76	114.37	1	2
4	A	387	PX4	C15-C14-C13	2.49	101.76	114.37	1	2
4	A	412	PX4	C1-C2-N1	2.49	123.83	115.82	11	2
4	A	317	PX4	C1-C2-N1	2.49	123.82	115.82	4	4
4	A	331	PX4	C4-N1-C2	2.49	100.00	109.91	5	4
4	A	338	PX4	O1-P1-O3	2.49	96.27	107.57	9	1
4	A	345	PX4	C5-N1-C2	2.49	119.82	109.91	8	2
4	A	389	PX4	O5-C9-O6	2.49	117.39	123.63	14	4
4	A	418	PX4	O5-C9-O6	2.49	117.39	123.63	2	5
4	A	427	PX4	C13-C12-C11	2.49	101.76	114.37	13	1
4	A	430	PX4	C5-N1-C3	2.49	102.43	108.98	2	2
4	A	307	PX4	C25-C24-C23	2.49	104.56	113.69	13	2
4	A	312	PX4	C4-N1-C2	2.49	119.81	109.91	8	1
4	A	329	PX4	O4-P1-O2	2.49	118.81	108.94	8	2
4	A	365	PX4	C13-C12-C11	2.49	101.77	114.37	2	2
4	A	365	PX4	C25-C24-C23	2.49	104.56	113.69	10	2
4	A	402	PX4	O8-C23-C24	2.49	114.03	123.78	8	1
4	A	420	PX4	C25-C24-C23	2.49	104.56	113.69	3	3
4	A	313	PX4	C5-N1-C2	2.49	119.81	109.91	2	3
4	A	334	PX4	O1-P1-O4	2.49	96.28	107.57	3	1
4	A	369	PX4	C29-C28-C27	2.49	101.78	114.37	6	2
4	A	416	PX4	C31-C30-C29	2.49	101.78	114.37	8	2
4	A	420	PX4	O4-P1-O2	2.49	99.06	108.94	13	1
4	A	428	PX4	C28-C27-C26	2.49	101.78	114.37	10	1
4	A	338	PX4	O8-C23-C24	2.49	114.06	123.78	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	331	PX4	C14-C13-C12	2.49	101.80	114.37	6	1
4	A	354	PX4	C14-C13-C12	2.49	101.80	114.37	3	3
4	A	407	PX4	C8-O5-C9	2.49	126.21	117.12	6	2
4	A	359	PX4	C4-N1-C2	2.49	119.79	109.91	2	1
4	A	340	PX4	O3-P1-O2	2.48	99.09	108.94	4	1
4	A	318	PX4	C12-C11-C10	2.48	104.01	113.13	5	2
4	A	354	PX4	C30-C29-C28	2.48	101.82	114.37	7	2
4	A	357	PX4	C29-C28-C27	2.48	101.82	114.37	2	3
4	A	391	PX4	O5-C9-O6	2.48	117.42	123.63	9	2
4	A	376	PX4	C4-N1-C3	2.48	115.50	108.98	3	1
4	A	391	PX4	C34-C33-C32	2.48	101.82	114.37	11	3
4	A	405	PX4	C31-C30-C29	2.48	101.82	114.37	9	1
4	A	367	PX4	C8-O5-C9	2.48	108.05	117.12	11	1
4	A	413	PX4	C28-C27-C26	2.48	101.82	114.37	6	1
4	A	360	PX4	C14-C13-C12	2.48	101.84	114.37	4	2
4	A	377	PX4	C25-C24-C23	2.48	104.61	113.69	10	4
4	A	412	PX4	C30-C29-C28	2.48	101.83	114.37	5	4
4	A	320	PX4	C14-C13-C12	2.48	101.84	114.37	8	1
4	A	347	PX4	C32-C31-C30	2.48	101.85	114.37	14	2
4	A	384	PX4	C5-N1-C2	2.48	119.76	109.91	5	3
4	A	395	PX4	C4-N1-C2	2.48	119.76	109.91	14	1
4	A	345	PX4	C34-C33-C32	2.48	101.85	114.37	7	2
4	A	360	PX4	O4-P1-O2	2.48	118.75	108.94	11	4
4	A	354	PX4	C1-C2-N1	2.48	123.77	115.82	8	5
4	A	356	PX4	C31-C30-C29	2.48	101.85	114.37	2	2
4	A	412	PX4	C3-N1-C2	2.48	119.75	109.91	1	3
4	A	426	PX4	C26-C25-C24	2.48	104.03	113.13	10	1
4	A	367	PX4	O7-C7-C8	2.48	117.22	108.34	8	2
4	A	311	PX4	C30-C29-C28	2.47	101.86	114.37	10	1
4	A	391	PX4	C14-C13-C12	2.47	101.86	114.37	7	2
4	A	394	PX4	C8-O5-C9	2.47	108.08	117.12	6	2
4	A	406	PX4	C4-N1-C2	2.47	119.74	109.91	3	2
4	A	382	PX4	C5-N1-C2	2.47	119.74	109.91	9	1
4	A	389	PX4	C12-C11-C10	2.47	104.04	113.13	7	2
4	A	427	PX4	C8-O5-C9	2.47	126.16	117.12	8	5
4	A	326	PX4	C14-C13-C12	2.47	101.88	114.37	11	2
4	A	336	PX4	C1-C2-N1	2.47	123.75	115.82	9	2
4	A	368	PX4	C1-C2-N1	2.47	123.75	115.82	13	2
4	A	345	PX4	C5-N1-C4	2.47	102.49	108.98	14	2
4	A	311	PX4	C5-N1-C2	2.47	119.72	109.91	4	1
4	A	351	PX4	O4-P1-O2	2.47	118.72	108.94	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	377	PX4	C7-O7-C23	2.47	111.89	117.80	3	5
4	A	379	PX4	C29-C28-C27	2.47	101.89	114.37	11	2
4	A	410	PX4	C26-C25-C24	2.47	104.06	113.13	8	2
4	A	410	PX4	C14-C13-C12	2.47	101.88	114.37	9	2
4	A	420	PX4	C12-C11-C10	2.47	104.05	113.13	12	2
4	A	318	PX4	C25-C24-C23	2.47	122.73	113.69	7	3
4	A	337	PX4	C27-C26-C25	2.47	101.90	114.37	11	3
4	A	343	PX4	C11-C10-C9	2.47	104.66	113.69	5	2
4	A	310	PX4	C25-C24-C23	2.46	104.66	113.69	9	1
4	A	346	PX4	C5-N1-C4	2.47	102.50	108.98	11	2
4	A	346	PX4	C16-C15-C14	2.46	101.91	114.37	8	2
4	A	352	PX4	C28-C27-C26	2.46	101.91	114.37	13	2
4	A	372	PX4	C13-C12-C11	2.47	101.91	114.37	6	3
4	A	424	PX4	C25-C24-C23	2.47	104.66	113.69	5	2
4	A	424	PX4	C3-N1-C2	2.46	119.71	109.91	9	1
4	A	325	PX4	C14-C13-C12	2.46	101.92	114.37	8	1
4	A	342	PX4	C5-N1-C2	2.46	100.12	109.91	14	3
4	A	352	PX4	O4-P1-O2	2.46	118.70	108.94	4	2
4	A	365	PX4	C34-C33-C32	2.46	101.92	114.37	10	1
4	A	395	PX4	C26-C25-C24	2.46	104.08	113.13	4	1
4	A	406	PX4	O1-P1-O4	2.46	118.73	107.57	12	2
4	A	410	PX4	C25-C24-C23	2.46	122.72	113.69	3	3
4	A	419	PX4	O3-P1-O2	2.46	99.18	108.94	3	1
4	A	331	PX4	C7-O7-C23	2.46	123.68	117.80	2	3
4	A	372	PX4	O8-C23-C24	2.46	114.16	123.78	1	2
4	A	382	PX4	C25-C24-C23	2.46	104.69	113.69	11	2
4	A	404	PX4	C5-N1-C3	2.46	115.43	108.98	2	3
4	A	422	PX4	C5-N1-C3	2.46	115.43	108.98	7	2
4	A	429	PX4	C13-C12-C11	2.46	101.94	114.37	3	1
4	A	310	PX4	O3-P1-O2	2.46	99.20	108.94	14	1
4	A	334	PX4	O5-C9-O6	2.46	117.48	123.63	14	2
4	A	312	PX4	C14-C13-C12	2.46	101.96	114.37	11	1
4	A	342	PX4	C32-C31-C30	2.46	101.95	114.37	9	1
4	A	363	PX4	C33-C32-C31	2.46	101.95	114.37	3	1
4	A	371	PX4	O4-P1-O2	2.46	99.20	108.94	2	3
4	A	394	PX4	C34-C33-C32	2.45	101.96	114.37	13	1
4	A	395	PX4	C5-N1-C3	2.46	102.53	108.98	8	1
4	A	401	PX4	C11-C10-C9	2.46	104.70	113.69	7	5
4	A	407	PX4	C25-C24-C23	2.46	104.70	113.69	1	1
4	A	410	PX4	C11-C10-C9	2.46	104.70	113.69	1	2
4	A	411	PX4	O3-C1-C2	2.46	121.47	109.65	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	345	PX4	C13-C12-C11	2.45	101.96	114.37	6	4
4	A	420	PX4	C28-C27-C26	2.46	101.95	114.37	10	2
4	A	324	PX4	C28-C27-C26	2.45	101.97	114.37	1	3
4	A	330	PX4	C34-C33-C32	2.45	101.97	114.37	10	1
4	A	352	PX4	C15-C14-C13	2.45	101.96	114.37	7	1
4	A	389	PX4	C18-C17-C16	2.45	101.97	114.37	6	1
4	A	415	PX4	C25-C24-C23	2.45	104.70	113.69	11	1
4	A	339	PX4	C25-C24-C23	2.45	104.71	113.69	2	5
4	A	347	PX4	O3-C1-C2	2.45	121.45	109.65	7	2
4	A	381	PX4	C4-N1-C2	2.45	100.17	109.91	11	3
4	A	385	PX4	C25-C24-C23	2.45	104.71	113.69	13	2
4	A	309	PX4	C31-C30-C29	2.45	101.99	114.37	9	2
4	A	317	PX4	C29-C28-C27	2.45	101.98	114.37	2	4
4	A	322	PX4	C17-C16-C15	2.45	101.99	114.37	2	5
4	A	330	PX4	C8-O5-C9	2.45	108.17	117.12	1	1
4	A	324	PX4	O5-C9-O6	2.45	117.50	123.63	9	1
4	A	335	PX4	C29-C28-C27	2.45	101.99	114.37	5	1
4	A	352	PX4	C11-C10-C9	2.45	122.67	113.69	9	1
4	A	354	PX4	C31-C30-C29	2.45	101.98	114.37	14	3
4	A	400	PX4	C33-C32-C31	2.45	101.98	114.37	3	1
4	A	363	PX4	O5-C9-C10	2.45	119.30	111.83	9	6
4	A	375	PX4	C16-C15-C14	2.45	101.99	114.37	6	2
4	A	383	PX4	O3-C1-C2	2.45	121.43	109.65	13	1
4	A	388	PX4	C31-C30-C29	2.45	102.00	114.37	14	2
4	A	310	PX4	C29-C28-C27	2.45	102.00	114.37	10	1
4	A	324	PX4	O3-P1-O2	2.45	99.24	108.94	4	2
4	A	329	PX4	C31-C30-C29	2.45	102.01	114.37	10	3
4	A	356	PX4	O5-C9-O6	2.45	117.51	123.63	4	2
4	A	387	PX4	C30-C29-C28	2.45	102.00	114.37	13	1
4	A	376	PX4	C25-C24-C23	2.44	104.73	113.69	1	2
4	A	378	PX4	C20-C19-C18	2.44	102.02	114.37	11	2
4	A	397	PX4	C14-C13-C12	2.44	102.01	114.37	14	1
4	A	309	PX4	O7-C7-C8	2.44	117.11	108.34	3	1
4	A	355	PX4	C34-C33-C32	2.44	102.02	114.37	2	1
4	A	368	PX4	C5-N1-C4	2.44	102.56	108.98	12	3
4	A	307	PX4	C17-C16-C15	2.44	102.03	114.37	12	2
4	A	348	PX4	C32-C31-C30	2.44	102.03	114.37	12	1
4	A	310	PX4	C32-C31-C30	2.44	102.03	114.37	9	3
4	A	321	PX4	C33-C32-C31	2.44	102.03	114.37	6	1
4	A	333	PX4	C27-C26-C25	2.44	102.03	114.37	8	1
4	A	336	PX4	O4-P1-O2	2.44	118.61	108.94	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	390	PX4	C5-N1-C2	2.44	119.61	109.91	3	2
4	A	314	PX4	C34-C33-C32	2.44	102.04	114.37	14	1
4	A	363	PX4	C31-C30-C29	2.44	102.03	114.37	14	2
4	A	370	PX4	C27-C26-C25	2.44	102.03	114.37	9	1
4	A	372	PX4	C34-C33-C32	2.44	102.03	114.37	10	2
4	A	425	PX4	O6-C9-C10	2.44	114.23	123.78	9	2
4	A	421	PX4	C36-C35-C34	2.44	96.89	113.36	6	2
4	A	312	PX4	C4-N1-C3	2.44	102.57	108.98	2	1
4	A	313	PX4	C32-C31-C30	2.44	102.05	114.37	3	2
4	A	317	PX4	C7-O7-C23	2.44	123.63	117.80	6	1
4	A	343	PX4	O1-P1-O4	2.44	118.62	107.57	12	1
4	A	348	PX4	C5-N1-C2	2.44	119.60	109.91	8	3
4	A	350	PX4	C11-C10-C9	2.44	104.76	113.69	6	2
4	A	319	PX4	C25-C24-C23	2.44	104.77	113.69	13	3
4	A	330	PX4	O1-P1-O3	2.44	96.52	107.57	3	3
4	A	372	PX4	O1-P1-O4	2.44	118.61	107.57	6	1
4	A	377	PX4	C31-C30-C29	2.44	102.05	114.37	8	1
4	A	414	PX4	O5-C9-O6	2.44	117.53	123.63	9	3
4	A	410	PX4	C16-C15-C14	2.44	102.05	114.37	12	1
4	A	415	PX4	C31-C30-C29	2.44	102.05	114.37	10	2
4	A	423	PX4	O3-C1-C2	2.44	121.38	109.65	3	2
4	A	347	PX4	C13-C12-C11	2.44	102.06	114.37	4	2
4	A	362	PX4	C3-N1-C2	2.44	119.59	109.91	7	1
4	A	388	PX4	O1-P1-O4	2.43	118.60	107.57	1	2
4	A	341	PX4	C18-C17-C16	2.43	102.07	114.37	14	1
4	A	336	PX4	O3-C1-C2	2.43	121.35	109.65	4	1
4	A	354	PX4	C16-C15-C14	2.43	102.07	114.37	12	1
4	A	410	PX4	C29-C28-C27	2.43	102.06	114.37	4	3
4	A	356	PX4	C28-C27-C26	2.43	102.07	114.37	5	1
4	A	378	PX4	O8-C23-C24	2.43	114.27	123.78	4	1
4	A	384	PX4	C5-N1-C4	2.43	102.59	108.98	1	3
4	A	320	PX4	C27-C26-C25	2.43	102.09	114.37	5	2
4	A	345	PX4	C19-C18-C17	2.43	102.08	114.37	12	2
4	A	389	PX4	C15-C14-C13	2.43	102.08	114.37	1	2
4	A	393	PX4	C3-N1-C2	2.43	119.56	109.91	9	2
4	A	398	PX4	O7-C7-C8	2.43	117.06	108.34	7	4
4	A	400	PX4	O4-P1-O2	2.43	99.31	108.94	12	1
4	A	323	PX4	O8-C23-C24	2.43	114.29	123.78	4	2
4	A	347	PX4	C14-C13-C12	2.43	102.09	114.37	7	2
4	A	430	PX4	C30-C29-C28	2.43	102.09	114.37	6	2
4	A	350	PX4	C29-C28-C27	2.43	102.10	114.37	11	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	C29-C28-C27	2.43	102.10	114.37	1	1
4	A	415	PX4	C32-C31-C30	2.43	102.10	114.37	9	1
4	A	352	PX4	C14-C13-C12	2.42	102.11	114.37	12	1
4	A	364	PX4	O8-C23-C24	2.43	114.30	123.78	11	1
4	A	373	PX4	C13-C12-C11	2.43	102.11	114.37	7	2
4	A	422	PX4	C15-C14-C13	2.43	102.11	114.37	6	2
4	A	426	PX4	C4-N1-C3	2.43	102.60	108.98	10	2
4	A	323	PX4	C12-C11-C10	2.42	104.22	113.13	6	1
4	A	352	PX4	C32-C31-C30	2.42	102.12	114.37	12	1
4	A	391	PX4	C30-C29-C28	2.42	102.12	114.37	5	1
4	A	400	PX4	C16-C15-C14	2.42	102.12	114.37	7	2
4	A	318	PX4	O4-P1-O2	2.42	118.53	108.94	11	1
4	A	355	PX4	O5-C9-O6	2.42	117.57	123.63	8	3
4	A	375	PX4	C5-N1-C2	2.42	119.53	109.91	12	2
4	A	387	PX4	O1-P1-O4	2.42	118.54	107.57	12	1
4	A	329	PX4	C5-N1-C3	2.42	102.62	108.98	2	1
4	A	381	PX4	O8-C23-C24	2.42	114.32	123.78	3	1
4	A	382	PX4	C4-N1-C2	2.42	119.53	109.91	2	2
4	A	309	PX4	C34-C33-C32	2.42	102.15	114.37	6	2
4	A	315	PX4	C30-C29-C28	2.42	102.14	114.37	10	1
4	A	403	PX4	C33-C32-C31	2.42	102.15	114.37	8	2
4	A	425	PX4	C34-C33-C32	2.42	102.14	114.37	7	2
4	A	316	PX4	C5-N1-C2	2.42	119.51	109.91	11	2
4	A	328	PX4	C34-C33-C32	2.42	102.16	114.37	2	2
4	A	385	PX4	C34-C33-C32	2.42	102.16	114.37	6	3
4	A	413	PX4	C8-O5-C9	2.42	125.95	117.12	4	3
4	A	423	PX4	C18-C17-C16	2.42	102.16	114.37	10	1
4	A	424	PX4	C33-C32-C31	2.42	102.16	114.37	13	1
4	A	347	PX4	C34-C33-C32	2.41	102.17	114.37	4	3
4	A	308	PX4	C16-C15-C14	2.41	102.17	114.37	3	2
4	A	309	PX4	C27-C26-C25	2.41	102.17	114.37	14	1
4	A	360	PX4	C26-C25-C24	2.41	104.26	113.13	13	1
4	A	362	PX4	C20-C19-C18	2.41	102.17	114.37	6	2
4	A	364	PX4	C25-C24-C23	2.41	104.85	113.69	2	3
4	A	405	PX4	O7-C7-C8	2.41	117.00	108.34	11	3
4	A	411	PX4	O7-C23-O8	2.41	118.07	123.70	7	2
4	A	413	PX4	O3-C1-C2	2.41	121.26	109.65	12	1
4	A	423	PX4	C30-C29-C28	2.41	102.17	114.37	4	1
4	A	359	PX4	C27-C26-C25	2.41	102.18	114.37	14	2
4	A	389	PX4	C32-C31-C30	2.41	102.18	114.37	3	1
4	A	390	PX4	O1-P1-O3	2.41	96.64	107.57	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	306	PX4	C5-N1-C4	2.41	102.65	108.98	7	2
4	A	313	PX4	C13-C12-C11	2.41	102.20	114.37	14	1
4	A	314	PX4	O7-C7-C8	2.41	116.98	108.34	4	6
4	A	338	PX4	C19-C18-C17	2.41	102.19	114.37	8	1
4	A	348	PX4	C27-C26-C25	2.41	102.19	114.37	9	2
4	A	408	PX4	C17-C16-C15	2.41	102.18	114.37	4	1
4	A	353	PX4	C25-C24-C23	2.41	104.87	113.69	11	2
4	A	386	PX4	C18-C17-C16	2.41	102.19	114.37	8	1
4	A	389	PX4	C33-C32-C31	2.41	102.19	114.37	1	1
4	A	389	PX4	C11-C10-C9	2.41	104.86	113.69	7	1
4	A	421	PX4	C8-O5-C9	2.41	108.31	117.12	10	1
4	A	322	PX4	C14-C13-C12	2.41	102.20	114.37	10	1
4	A	326	PX4	C1-C2-N1	2.41	123.55	115.82	2	3
4	A	372	PX4	C16-C15-C14	2.41	102.20	114.37	6	3
4	A	384	PX4	C15-C14-C13	2.41	102.20	114.37	14	1
4	A	337	PX4	C32-C31-C30	2.41	102.20	114.37	12	1
4	A	403	PX4	C31-C30-C29	2.41	102.20	114.37	10	1
4	A	317	PX4	C34-C33-C32	2.40	102.22	114.37	9	1
4	A	325	PX4	O5-C9-O6	2.40	117.61	123.63	11	2
4	A	343	PX4	O1-P1-O3	2.40	96.67	107.57	2	1
4	A	354	PX4	C11-C10-C9	2.40	104.89	113.69	12	1
4	A	366	PX4	O4-P1-O2	2.40	118.46	108.94	8	4
4	A	368	PX4	C14-C13-C12	2.40	102.21	114.37	7	1
4	A	386	PX4	O1-P1-O4	2.40	118.46	107.57	10	1
4	A	409	PX4	C29-C28-C27	2.40	102.21	114.37	8	1
4	A	415	PX4	C20-C19-C18	2.41	102.21	114.37	5	1
4	A	369	PX4	C32-C31-C30	2.40	102.22	114.37	5	3
4	A	306	PX4	C29-C28-C27	2.40	102.23	114.37	8	1
4	A	308	PX4	C25-C24-C23	2.40	104.90	113.69	11	3
4	A	321	PX4	C14-C13-C12	2.40	102.24	114.37	8	2
4	A	397	PX4	C15-C14-C13	2.40	102.23	114.37	2	3
4	A	306	PX4	C25-C24-C23	2.40	122.48	113.69	11	1
4	A	369	PX4	C13-C12-C11	2.40	102.24	114.37	11	1
4	A	372	PX4	O5-C9-O6	2.40	129.63	123.63	8	2
4	A	372	PX4	C20-C19-C18	2.40	102.25	114.37	10	1
4	A	382	PX4	C18-C17-C16	2.40	102.24	114.37	7	2
4	A	362	PX4	C13-C12-C11	2.40	102.25	114.37	7	2
4	A	377	PX4	C28-C27-C26	2.40	102.25	114.37	4	1
4	A	385	PX4	C29-C28-C27	2.40	102.25	114.37	9	1
4	A	394	PX4	C5-N1-C3	2.40	102.68	108.98	6	5
4	A	399	PX4	C17-C16-C15	2.40	102.25	114.37	14	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	317	PX4	C32-C31-C30	2.40	102.26	114.37	7	1
4	A	309	PX4	O5-C9-O6	2.40	117.64	123.63	11	4
4	A	344	PX4	O5-C9-C10	2.40	119.14	111.83	11	2
4	A	389	PX4	O7-C7-C6	2.40	116.94	108.34	7	1
4	A	413	PX4	C16-C15-C14	2.40	102.25	114.37	6	1
4	A	309	PX4	C26-C25-C24	2.39	104.33	113.13	5	3
4	A	317	PX4	C14-C13-C12	2.40	102.26	114.37	13	1
4	A	430	PX4	C26-C25-C24	2.40	104.32	113.13	6	1
4	A	347	PX4	C7-O7-C23	2.39	123.53	117.80	2	1
4	A	342	PX4	O6-C9-C10	2.39	114.42	123.78	2	1
4	A	343	PX4	C15-C14-C13	2.39	102.27	114.37	2	1
4	A	359	PX4	C16-C15-C14	2.39	102.27	114.37	4	1
4	A	365	PX4	C7-O7-C23	2.39	123.53	117.80	6	2
4	A	366	PX4	C13-C12-C11	2.39	102.27	114.37	3	2
4	A	381	PX4	O3-C1-C2	2.39	121.17	109.65	5	1
4	A	385	PX4	C15-C14-C13	2.39	102.27	114.37	6	1
4	A	391	PX4	C4-N1-C2	2.39	119.42	109.91	13	1
4	A	412	PX4	C8-O5-C9	2.39	125.87	117.12	12	3
4	A	412	PX4	O3-P1-O2	2.39	99.45	108.94	12	1
4	A	307	PX4	C5-N1-C3	2.39	102.69	108.98	9	3
4	A	350	PX4	C26-C25-C24	2.39	104.34	113.13	4	2
4	A	343	PX4	C5-N1-C2	2.39	119.41	109.91	13	1
4	A	352	PX4	O7-C23-O8	2.39	118.11	123.70	10	3
4	A	368	PX4	C31-C30-C29	2.39	102.28	114.37	5	2
4	A	413	PX4	C32-C31-C30	2.39	102.28	114.37	7	1
4	A	425	PX4	C5-N1-C2	2.39	119.42	109.91	10	3
4	A	328	PX4	O4-P1-O2	2.39	99.47	108.94	10	2
4	A	347	PX4	C16-C15-C14	2.39	102.29	114.37	7	2
4	A	414	PX4	C14-C13-C12	2.39	102.29	114.37	6	1
4	A	430	PX4	C28-C27-C26	2.39	102.29	114.37	4	2
4	A	367	PX4	C4-N1-C2	2.39	119.40	109.91	10	2
4	A	368	PX4	C3-N1-C2	2.39	119.40	109.91	14	1
4	A	382	PX4	C8-O5-C9	2.39	108.39	117.12	3	4
4	A	369	PX4	C4-N1-C2	2.39	100.43	109.91	13	1
4	A	378	PX4	C30-C29-C28	2.39	102.31	114.37	8	2
4	A	390	PX4	C5-N1-C4	2.39	102.71	108.98	3	1
4	A	390	PX4	C25-C24-C23	2.39	104.95	113.69	4	2
4	A	420	PX4	C15-C14-C13	2.38	102.31	114.37	7	2
4	A	393	PX4	C29-C28-C27	2.38	102.32	114.37	2	2
4	A	395	PX4	C18-C17-C16	2.38	102.32	114.37	12	1
4	A	419	PX4	O5-C9-O6	2.38	117.67	123.63	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	421	PX4	C31-C30-C29	2.38	102.32	114.37	14	2
4	A	411	PX4	C18-C17-C16	2.38	102.32	114.37	14	2
4	A	320	PX4	O7-C7-C6	2.38	116.89	108.34	7	4
4	A	319	PX4	C31-C30-C29	2.38	102.34	114.37	6	1
4	A	345	PX4	C31-C30-C29	2.38	102.34	114.37	5	1
4	A	352	PX4	C27-C26-C25	2.38	102.33	114.37	4	1
4	A	356	PX4	C16-C15-C14	2.38	102.33	114.37	11	1
4	A	387	PX4	C33-C32-C31	2.38	102.33	114.37	11	2
4	A	370	PX4	C26-C25-C24	2.38	104.38	113.13	2	2
4	A	412	PX4	C26-C25-C24	2.38	104.38	113.13	2	3
4	A	315	PX4	C3-N1-C2	2.38	119.36	109.91	12	2
4	A	319	PX4	C15-C14-C13	2.38	102.35	114.37	10	2
4	A	326	PX4	C26-C25-C24	2.38	104.39	113.13	13	2
4	A	330	PX4	C5-N1-C2	2.38	100.46	109.91	2	2
4	A	356	PX4	C5-N1-C3	2.38	115.22	108.98	3	1
4	A	359	PX4	C18-C17-C16	2.38	102.34	114.37	14	2
4	A	424	PX4	C11-C10-C9	2.38	122.41	113.69	11	1
4	A	324	PX4	O8-C23-C24	2.38	114.49	123.78	5	1
4	A	344	PX4	C12-C11-C10	2.38	104.40	113.13	9	1
4	A	348	PX4	O6-C9-C10	2.38	114.49	123.78	13	3
4	A	369	PX4	O7-C7-C6	2.38	116.87	108.34	8	2
4	A	408	PX4	C32-C31-C30	2.38	102.35	114.37	7	2
4	A	413	PX4	O6-C9-C10	2.38	114.48	123.78	11	1
4	A	423	PX4	C1-C2-N1	2.38	123.45	115.82	12	2
4	A	426	PX4	C11-C10-C9	2.38	104.98	113.69	7	2
4	A	426	PX4	O1-P1-O4	2.38	118.34	107.57	8	1
4	A	332	PX4	C20-C19-C18	2.37	102.37	114.37	8	1
4	A	422	PX4	C13-C12-C11	2.37	102.37	114.37	3	1
4	A	424	PX4	C1-C2-N1	2.38	123.44	115.82	10	2
4	A	398	PX4	C15-C14-C13	2.37	102.37	114.37	1	1
4	A	316	PX4	C14-C13-C12	2.37	102.38	114.37	10	1
4	A	325	PX4	C15-C14-C13	2.37	102.38	114.37	2	1
4	A	326	PX4	C17-C16-C15	2.37	102.38	114.37	8	1
4	A	335	PX4	C34-C33-C32	2.37	102.38	114.37	13	1
4	A	345	PX4	C17-C16-C15	2.37	102.38	114.37	7	2
4	A	358	PX4	C5-N1-C4	2.37	102.75	108.98	12	1
4	A	383	PX4	C13-C12-C11	2.37	102.38	114.37	13	1
4	A	388	PX4	C3-N1-C2	2.37	100.48	109.91	8	1
4	A	322	PX4	C11-C10-C9	2.37	122.38	113.69	2	2
4	A	337	PX4	C18-C17-C16	2.37	102.39	114.37	2	1
4	A	352	PX4	O7-C7-C6	2.37	116.85	108.34	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	362	PX4	C26-C25-C24	2.37	104.42	113.13	13	1
4	A	394	PX4	C18-C17-C16	2.37	102.39	114.37	11	1
4	A	413	PX4	C13-C12-C11	2.37	102.39	114.37	3	1
4	A	390	PX4	C1-C2-N1	2.37	123.42	115.82	8	1
4	A	403	PX4	C26-C25-C24	2.37	104.42	113.13	7	2
4	A	382	PX4	C30-C29-C28	2.37	102.40	114.37	11	1
4	A	416	PX4	C17-C16-C15	2.37	102.39	114.37	4	2
4	A	314	PX4	C16-C15-C14	2.37	102.40	114.37	9	2
4	A	340	PX4	O3-C1-C2	2.37	121.04	109.65	6	1
4	A	347	PX4	C1-C2-N1	2.37	123.42	115.82	1	2
4	A	381	PX4	C17-C16-C15	2.37	102.41	114.37	12	2
4	A	382	PX4	O3-C1-C2	2.37	121.04	109.65	12	3
4	A	384	PX4	C28-C27-C26	2.37	102.40	114.37	5	2
4	A	408	PX4	C20-C19-C18	2.37	102.41	114.37	9	1
4	A	413	PX4	C26-C25-C24	2.37	104.43	113.13	6	3
4	A	415	PX4	C26-C25-C24	2.37	104.43	113.13	4	1
4	A	415	PX4	C14-C13-C12	2.37	102.40	114.37	13	1
4	A	306	PX4	C18-C17-C16	2.36	102.41	114.37	13	1
4	A	321	PX4	C18-C17-C16	2.37	102.41	114.37	1	1
4	A	367	PX4	C20-C19-C18	2.37	102.41	114.37	7	2
4	A	358	PX4	C1-C2-N1	2.36	123.41	115.82	6	1
4	A	315	PX4	C29-C28-C27	2.36	102.42	114.37	12	3
4	A	344	PX4	O3-P1-O2	2.36	99.57	108.94	2	3
4	A	381	PX4	C18-C17-C16	2.36	102.42	114.37	2	2
4	A	401	PX4	C1-C2-N1	2.36	123.41	115.82	8	2
4	A	428	PX4	C19-C18-C17	2.36	102.42	114.37	14	1
4	A	346	PX4	C28-C27-C26	2.36	102.43	114.37	1	1
4	A	373	PX4	C3-N1-C2	2.36	100.52	109.91	2	1
4	A	390	PX4	C20-C19-C18	2.36	102.43	114.37	6	2
4	A	425	PX4	O8-C23-C24	2.36	114.55	123.78	7	1
4	A	316	PX4	C18-C17-C16	2.36	102.44	114.37	2	1
4	A	339	PX4	C28-C27-C26	2.36	102.44	114.37	12	1
4	A	353	PX4	O7-C7-C6	2.36	116.81	108.34	7	3
4	A	362	PX4	C29-C28-C27	2.36	102.44	114.37	12	2
4	A	404	PX4	C12-C11-C10	2.36	104.46	113.13	9	1
4	A	406	PX4	C17-C16-C15	2.36	102.44	114.37	11	2
4	A	417	PX4	C13-C12-C11	2.36	102.44	114.37	9	3
4	A	329	PX4	C5-N1-C2	2.36	100.54	109.91	9	1
4	A	340	PX4	C28-C27-C26	2.36	102.45	114.37	3	2
4	A	359	PX4	C25-C24-C23	2.36	105.05	113.69	11	2
4	A	331	PX4	O5-C9-O6	2.36	117.73	123.63	7	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	343	PX4	C8-O5-C9	2.36	125.73	117.12	7	1
4	A	357	PX4	O1-P1-O4	2.36	118.25	107.57	11	2
4	A	348	PX4	O8-C23-C24	2.36	114.57	123.78	7	1
4	A	366	PX4	O5-C9-O6	2.36	117.73	123.63	7	2
4	A	381	PX4	C3-N1-C2	2.36	119.28	109.91	5	2
4	A	389	PX4	C17-C16-C15	2.36	102.46	114.37	11	1
4	A	422	PX4	O3-C1-C2	2.36	120.99	109.65	5	1
4	A	427	PX4	C32-C31-C30	2.36	102.45	114.37	5	1
4	A	405	PX4	C11-C10-C9	2.36	105.06	113.69	5	2
4	A	313	PX4	C27-C26-C25	2.35	102.47	114.37	12	2
4	A	313	PX4	C15-C14-C13	2.35	102.47	114.37	6	1
4	A	329	PX4	C35-C34-C33	2.35	94.61	115.25	11	1
4	A	356	PX4	C12-C11-C10	2.35	104.48	113.13	12	2
4	A	409	PX4	C5-N1-C3	2.35	115.16	108.98	12	2
4	A	417	PX4	C11-C10-C9	2.35	105.07	113.69	14	2
4	A	342	PX4	C33-C32-C31	2.35	102.47	114.37	3	2
4	A	343	PX4	C25-C24-C23	2.35	122.32	113.69	1	1
4	A	428	PX4	C4-N1-C3	2.35	102.79	108.98	10	3
4	A	309	PX4	O3-C1-C2	2.35	120.96	109.65	5	1
4	A	336	PX4	C19-C18-C17	2.35	102.48	114.37	2	2
4	A	346	PX4	C22-C21-C20	2.35	97.48	113.36	14	1
4	A	353	PX4	C15-C14-C13	2.35	102.49	114.37	7	3
4	A	359	PX4	C3-N1-C2	2.35	119.26	109.91	11	2
4	A	392	PX4	O3-P1-O2	2.35	118.25	108.94	8	2
4	A	396	PX4	O1-P1-O3	2.35	96.91	107.57	13	1
4	A	307	PX4	C4-N1-C3	2.35	102.81	108.98	12	2
4	A	312	PX4	C13-C12-C11	2.35	102.49	114.37	2	2
4	A	318	PX4	O3-P1-O2	2.35	99.63	108.94	5	1
4	A	353	PX4	C19-C18-C17	2.35	102.50	114.37	6	2
4	A	426	PX4	C4-N1-C2	2.35	100.57	109.91	12	1
4	A	306	PX4	C11-C10-C9	2.35	105.10	113.69	11	1
4	A	338	PX4	C8-O5-C9	2.35	108.54	117.12	6	2
4	A	413	PX4	C27-C26-C25	2.35	102.50	114.37	4	1
4	A	420	PX4	C32-C31-C30	2.35	102.50	114.37	4	2
4	A	429	PX4	C18-C17-C16	2.35	102.50	114.37	6	2
4	A	332	PX4	C5-N1-C2	2.35	100.59	109.91	5	1
4	A	418	PX4	C26-C25-C24	2.35	104.51	113.13	5	1
4	A	333	PX4	C17-C16-C15	2.34	102.52	114.37	10	2
4	A	423	PX4	C34-C33-C32	2.35	102.51	114.37	5	2
4	A	311	PX4	C22-C21-C20	2.34	97.54	113.36	5	2
4	A	365	PX4	C29-C28-C27	2.34	102.52	114.37	14	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	372	PX4	C17-C16-C15	2.34	102.52	114.37	5	2
4	A	386	PX4	O4-P1-O2	2.34	118.22	108.94	1	3
4	A	421	PX4	C28-C27-C26	2.34	102.52	114.37	13	2
4	A	341	PX4	C25-C24-C23	2.34	105.11	113.69	1	1
4	A	393	PX4	C11-C10-C9	2.34	105.11	113.69	11	1
4	A	426	PX4	C8-O5-C9	2.34	108.55	117.12	8	2
4	A	342	PX4	C31-C30-C29	2.34	102.53	114.37	14	1
4	A	313	PX4	O5-C9-O6	2.34	117.77	123.63	1	3
4	A	346	PX4	C32-C31-C30	2.34	102.53	114.37	4	2
4	A	373	PX4	C18-C17-C16	2.34	102.53	114.37	14	1
4	A	377	PX4	C14-C13-C12	2.34	102.53	114.37	9	1
4	A	396	PX4	C14-C13-C12	2.34	102.53	114.37	5	1
4	A	416	PX4	C16-C15-C14	2.34	102.53	114.37	2	1
4	A	422	PX4	C4-N1-C2	2.34	100.60	109.91	6	1
4	A	348	PX4	O3-P1-O2	2.34	99.66	108.94	6	4
4	A	377	PX4	C16-C15-C14	2.34	102.55	114.37	4	1
4	A	400	PX4	O3-C1-C2	2.34	120.91	109.65	14	1
4	A	384	PX4	C31-C30-C29	2.34	102.55	114.37	11	1
4	A	394	PX4	C1-C2-N1	2.34	123.33	115.82	10	2
4	A	398	PX4	C19-C18-C17	2.34	102.55	114.37	4	1
4	A	409	PX4	C4-N1-C2	2.34	100.61	109.91	13	2
4	A	307	PX4	C18-C17-C16	2.34	102.56	114.37	10	1
4	A	308	PX4	C4-N1-C2	2.34	119.20	109.91	6	4
4	A	336	PX4	C32-C31-C30	2.34	102.55	114.37	3	2
4	A	411	PX4	C30-C29-C28	2.34	102.55	114.37	3	1
4	A	338	PX4	C32-C31-C30	2.34	102.56	114.37	10	1
4	A	350	PX4	C5-N1-C2	2.34	100.62	109.91	6	2
4	A	313	PX4	C14-C13-C12	2.33	102.57	114.37	8	1
4	A	320	PX4	C32-C31-C30	2.34	102.56	114.37	3	2
4	A	336	PX4	C28-C27-C26	2.34	102.56	114.37	12	2
4	A	346	PX4	C5-N1-C2	2.33	119.19	109.91	4	2
4	A	351	PX4	O7-C23-O8	2.33	129.16	123.70	4	1
4	A	401	PX4	O8-C23-C24	2.34	114.65	123.78	6	2
4	A	331	PX4	C27-C26-C25	2.33	102.57	114.37	4	2
4	A	401	PX4	O7-C7-C6	2.33	116.72	108.34	1	3
4	A	401	PX4	C34-C33-C32	2.33	102.57	114.37	5	2
4	A	349	PX4	O5-C9-C10	2.33	118.95	111.83	4	2
4	A	362	PX4	C5-N1-C2	2.33	100.64	109.91	6	1
4	A	368	PX4	C16-C15-C14	2.33	102.58	114.37	8	1
4	A	388	PX4	C26-C25-C24	2.33	121.70	113.13	13	2
4	A	396	PX4	C12-C11-C10	2.33	104.56	113.13	9	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	322	PX4	C28-C27-C26	2.33	102.58	114.37	2	2
4	A	335	PX4	C13-C12-C11	2.33	102.58	114.37	10	1
4	A	354	PX4	O6-C9-C10	2.33	114.66	123.78	13	1
4	A	313	PX4	C26-C25-C24	2.33	104.56	113.13	5	2
4	A	408	PX4	C34-C33-C32	2.33	102.59	114.37	4	1
4	A	426	PX4	O6-C9-C10	2.33	114.67	123.78	3	2
4	A	328	PX4	C5-N1-C2	2.33	119.17	109.91	3	1
4	A	410	PX4	C36-C35-C34	2.33	97.64	113.36	4	1
4	A	417	PX4	C5-N1-C3	2.33	115.09	108.98	3	3
4	A	423	PX4	C5-N1-C2	2.33	119.17	109.91	5	1
4	A	323	PX4	O1-P1-O4	2.33	118.11	107.57	8	2
4	A	326	PX4	C8-O5-C9	2.33	108.61	117.12	13	1
4	A	400	PX4	O1-P1-O4	2.33	118.12	107.57	3	3
4	A	377	PX4	C3-N1-C2	2.33	119.16	109.91	13	2
4	A	389	PX4	C31-C30-C29	2.33	102.61	114.37	9	2
4	A	411	PX4	C17-C16-C15	2.33	102.60	114.37	10	1
4	A	324	PX4	C19-C18-C17	2.33	102.61	114.37	12	2
4	A	334	PX4	C11-C10-C9	2.33	105.17	113.69	3	1
4	A	338	PX4	C15-C14-C13	2.33	102.61	114.37	8	2
4	A	356	PX4	C14-C13-C12	2.33	102.61	114.37	2	1
4	A	404	PX4	C28-C27-C26	2.33	102.61	114.37	14	1
4	A	406	PX4	C7-O7-C23	2.33	123.36	117.80	5	2
4	A	329	PX4	C27-C26-C25	2.32	126.11	114.37	13	1
4	A	342	PX4	C14-C13-C12	2.32	102.62	114.37	2	1
4	A	355	PX4	C27-C26-C25	2.32	102.62	114.37	3	2
4	A	362	PX4	C28-C27-C26	2.32	102.62	114.37	6	1
4	A	375	PX4	C4-N1-C2	2.32	119.15	109.91	3	1
4	A	410	PX4	C12-C11-C10	2.32	104.59	113.13	1	2
4	A	412	PX4	C36-C35-C34	2.32	97.67	113.36	5	1
4	A	323	PX4	C4-N1-C2	2.32	119.14	109.91	3	2
4	A	330	PX4	C31-C30-C29	2.32	102.63	114.37	12	1
4	A	348	PX4	O5-C9-O6	2.32	117.82	123.63	5	1
4	A	388	PX4	C33-C32-C31	2.32	102.62	114.37	11	2
4	A	409	PX4	C5-N1-C2	2.32	119.14	109.91	13	2
4	A	419	PX4	C25-C24-C23	2.32	105.19	113.69	13	1
4	A	323	PX4	C33-C32-C31	2.32	102.64	114.37	7	1
4	A	333	PX4	O1-P1-O3	2.32	97.05	107.57	8	2
4	A	351	PX4	C3-N1-C2	2.32	119.13	109.91	10	1
4	A	430	PX4	O1-P1-O3	2.32	97.05	107.57	14	1
4	A	343	PX4	C34-C33-C32	2.32	102.65	114.37	11	2
4	A	362	PX4	C15-C14-C13	2.32	102.64	114.37	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	429	PX4	C5-N1-C3	2.32	102.88	108.98	9	5
4	A	331	PX4	C11-C10-C9	2.32	105.20	113.69	3	1
4	A	347	PX4	C17-C16-C15	2.32	102.66	114.37	7	2
4	A	354	PX4	C32-C31-C30	2.32	102.66	114.37	5	2
4	A	388	PX4	O8-C23-C24	2.32	114.72	123.78	7	3
4	A	390	PX4	C18-C17-C16	2.32	102.66	114.37	9	2
4	A	403	PX4	C27-C26-C25	2.32	102.66	114.37	8	1
4	A	315	PX4	C15-C14-C13	2.31	102.67	114.37	4	2
4	A	339	PX4	C12-C11-C10	2.31	104.62	113.13	11	2
4	A	355	PX4	C29-C28-C27	2.32	102.67	114.37	4	1
4	A	426	PX4	C18-C17-C16	2.32	102.67	114.37	13	1
4	A	333	PX4	C3-N1-C2	2.31	100.71	109.91	4	2
4	A	408	PX4	C16-C15-C14	2.31	102.68	114.37	9	1
4	A	411	PX4	C5-N1-C2	2.31	119.10	109.91	13	1
4	A	429	PX4	C30-C29-C28	2.31	102.67	114.37	1	2
4	A	384	PX4	C27-C26-C25	2.31	102.68	114.37	9	1
4	A	387	PX4	C34-C33-C32	2.31	102.68	114.37	10	2
4	A	414	PX4	C19-C18-C17	2.31	102.69	114.37	1	1
4	A	419	PX4	C18-C17-C16	2.31	102.68	114.37	10	4
4	A	316	PX4	C30-C29-C28	2.31	102.69	114.37	1	1
4	A	321	PX4	C4-N1-C2	2.31	119.09	109.91	1	1
4	A	329	PX4	C13-C12-C11	2.31	102.69	114.37	8	2
4	A	376	PX4	C1-C2-N1	2.31	123.24	115.82	11	2
4	A	418	PX4	C11-C10-C9	2.31	105.23	113.69	4	2
4	A	327	PX4	O3-P1-O2	2.31	99.79	108.94	14	1
4	A	329	PX4	C1-C2-N1	2.31	123.23	115.82	7	2
4	A	311	PX4	C5-N1-C3	2.31	102.92	108.98	2	2
4	A	345	PX4	C26-C25-C24	2.31	104.65	113.13	1	1
4	A	360	PX4	C15-C14-C13	2.31	102.70	114.37	12	2
4	A	366	PX4	O3-C1-C2	2.31	120.76	109.65	8	1
4	A	373	PX4	C4-N1-C2	2.31	119.08	109.91	13	1
4	A	319	PX4	C29-C28-C27	2.30	102.72	114.37	3	1
4	A	314	PX4	O4-P1-O2	2.30	99.81	108.94	12	2
4	A	363	PX4	C7-O7-C23	2.30	123.31	117.80	1	2
4	A	320	PX4	C34-C33-C32	2.30	102.73	114.37	2	1
4	A	365	PX4	C16-C15-C14	2.30	102.73	114.37	11	1
4	A	368	PX4	C15-C14-C13	2.30	102.72	114.37	12	2
4	A	386	PX4	C34-C33-C32	2.30	102.73	114.37	13	2
4	A	392	PX4	C5-N1-C2	2.30	119.07	109.91	6	2
4	A	425	PX4	C3-N1-C2	2.30	119.07	109.91	7	1
4	A	369	PX4	C4-N1-C3	2.30	102.93	108.98	11	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	309	PX4	C14-C13-C12	2.30	102.74	114.37	3	1
4	A	334	PX4	C5-N1-C2	2.30	100.76	109.91	1	2
4	A	374	PX4	O4-P1-O2	2.30	118.06	108.94	5	1
4	A	403	PX4	C28-C27-C26	2.30	102.73	114.37	1	1
4	A	337	PX4	C4-N1-C3	2.30	115.02	108.98	8	1
4	A	358	PX4	C8-O5-C9	2.30	108.71	117.12	7	2
4	A	405	PX4	C32-C31-C30	2.30	102.74	114.37	5	1
4	A	347	PX4	C25-C24-C23	2.30	105.27	113.69	14	3
4	A	381	PX4	C27-C26-C25	2.30	102.74	114.37	2	2
4	A	306	PX4	C17-C16-C15	2.30	102.76	114.37	10	1
4	A	355	PX4	C19-C18-C17	2.30	102.75	114.37	12	1
4	A	357	PX4	C19-C18-C17	2.30	102.75	114.37	11	1
4	A	374	PX4	C5-N1-C2	2.30	119.04	109.91	1	1
4	A	406	PX4	C29-C28-C27	2.30	102.75	114.37	3	1
4	A	415	PX4	C5-N1-C3	2.30	115.01	108.98	10	4
4	A	319	PX4	C32-C31-C30	2.30	102.76	114.37	10	1
4	A	362	PX4	C36-C35-C34	2.30	128.87	113.36	4	1
4	A	374	PX4	O7-C7-C6	2.30	116.58	108.34	1	4
4	A	421	PX4	C20-C19-C18	2.30	102.76	114.37	11	1
4	A	403	PX4	C15-C14-C13	2.29	102.77	114.37	13	3
4	A	422	PX4	C28-C27-C26	2.30	102.77	114.37	14	1
4	A	314	PX4	C13-C12-C11	2.29	102.77	114.37	4	1
4	A	325	PX4	C33-C32-C31	2.29	102.77	114.37	10	1
4	A	375	PX4	C29-C28-C27	2.29	102.77	114.37	11	1
4	A	373	PX4	C19-C18-C17	2.29	102.78	114.37	7	1
4	A	378	PX4	C5-N1-C2	2.29	119.02	109.91	10	1
4	A	381	PX4	C11-C10-C9	2.29	105.29	113.69	4	2
4	A	387	PX4	O7-C7-C8	2.29	116.57	108.34	7	1
4	A	410	PX4	C30-C29-C28	2.29	102.77	114.37	3	1
4	A	309	PX4	C19-C18-C17	2.29	102.78	114.37	5	1
4	A	313	PX4	C30-C29-C28	2.29	102.78	114.37	4	1
4	A	311	PX4	C3-N1-C2	2.29	119.02	109.91	12	4
4	A	344	PX4	C32-C31-C30	2.29	102.78	114.37	13	1
4	A	352	PX4	C8-O5-C9	2.29	108.74	117.12	7	2
4	A	361	PX4	C13-C12-C11	2.29	102.78	114.37	2	1
4	A	368	PX4	O6-C9-C10	2.29	114.82	123.78	8	2
4	A	398	PX4	C31-C30-C29	2.29	102.78	114.37	2	1
4	A	318	PX4	O1-P1-O3	2.29	97.19	107.57	4	1
4	A	325	PX4	C30-C29-C28	2.29	102.79	114.37	3	1
4	A	357	PX4	C28-C27-C26	2.29	102.79	114.37	13	1
4	A	399	PX4	C26-C25-C24	2.29	121.54	113.13	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	C27-C26-C25	2.29	102.80	114.37	9	2
4	A	415	PX4	C13-C12-C11	2.29	102.80	114.37	6	2
4	A	306	PX4	C30-C29-C28	2.29	102.81	114.37	6	1
4	A	346	PX4	C18-C17-C16	2.29	102.81	114.37	11	2
4	A	404	PX4	C8-O5-C9	2.29	108.76	117.12	5	2
4	A	412	PX4	C33-C32-C31	2.29	102.81	114.37	11	2
4	A	425	PX4	C17-C16-C15	2.29	102.81	114.37	9	2
4	A	337	PX4	C20-C19-C18	2.29	102.82	114.37	14	1
4	A	339	PX4	C32-C31-C30	2.28	102.82	114.37	5	1
4	A	342	PX4	C4-N1-C2	2.29	118.99	109.91	8	3
4	A	339	PX4	C5-N1-C2	2.28	118.99	109.91	13	1
4	A	391	PX4	O5-C9-C10	2.28	118.80	111.83	8	1
4	A	355	PX4	C13-C12-C11	2.28	102.83	114.37	4	3
4	A	363	PX4	C34-C33-C32	2.28	102.82	114.37	9	2
4	A	426	PX4	C32-C31-C30	2.28	102.82	114.37	6	2
4	A	371	PX4	C26-C25-C24	2.28	104.74	113.13	6	1
4	A	371	PX4	C30-C29-C28	2.28	125.91	114.37	9	1
4	A	345	PX4	C5-N1-C3	2.28	102.98	108.98	12	2
4	A	419	PX4	C11-C10-C9	2.28	122.06	113.69	3	3
4	A	310	PX4	C5-N1-C2	2.28	118.98	109.91	11	1
4	A	340	PX4	C16-C15-C14	2.28	102.84	114.37	12	1
4	A	320	PX4	C30-C29-C28	2.28	102.85	114.37	8	2
4	A	326	PX4	C3-N1-C2	2.28	118.96	109.91	8	2
4	A	337	PX4	C11-C10-C9	2.28	105.34	113.69	4	2
4	A	370	PX4	C12-C11-C10	2.28	104.75	113.13	5	1
4	A	372	PX4	C15-C14-C13	2.28	102.86	114.37	5	1
4	A	390	PX4	C15-C14-C13	2.28	102.85	114.37	5	1
4	A	397	PX4	C4-N1-C2	2.28	100.85	109.91	4	1
4	A	409	PX4	C8-O5-C9	2.28	108.79	117.12	4	1
4	A	339	PX4	C16-C15-C14	2.28	102.86	114.37	9	1
4	A	348	PX4	O1-P1-O4	2.28	117.89	107.57	2	3
4	A	316	PX4	O7-C7-C6	2.28	116.51	108.34	1	2
4	A	327	PX4	O1-P1-O4	2.28	117.89	107.57	3	2
4	A	341	PX4	C11-C10-C9	2.28	105.35	113.69	10	1
4	A	368	PX4	C4-N1-C3	2.28	102.99	108.98	10	2
4	A	379	PX4	C7-O7-C23	2.28	123.24	117.80	9	1
4	A	390	PX4	O8-C23-C24	2.28	114.88	123.78	6	1
4	A	414	PX4	C4-N1-C2	2.28	100.86	109.91	9	3
4	A	422	PX4	O1-P1-O4	2.27	117.88	107.57	5	5
4	A	315	PX4	C36-C35-C34	2.27	98.01	113.36	4	1
4	A	306	PX4	C4-N1-C3	2.27	103.01	108.98	14	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	310	PX4	O1-P1-O3	2.27	97.27	107.57	7	3
4	A	331	PX4	C26-C25-C24	2.27	104.78	113.13	2	3
4	A	385	PX4	C4-N1-C2	2.27	118.94	109.91	13	1
4	A	314	PX4	O3-P1-O2	2.27	117.93	108.94	7	2
4	A	341	PX4	C32-C31-C30	2.27	102.89	114.37	10	1
4	A	381	PX4	C5-N1-C2	2.27	100.89	109.91	7	1
4	A	388	PX4	C34-C33-C32	2.27	102.89	114.37	9	2
4	A	309	PX4	C29-C28-C27	2.27	102.90	114.37	6	2
4	A	365	PX4	C3-N1-C2	2.27	100.89	109.91	5	2
4	A	345	PX4	C29-C28-C27	2.27	102.90	114.37	1	1
4	A	345	PX4	C33-C32-C31	2.27	102.90	114.37	8	1
4	A	408	PX4	C8-O5-C9	2.27	108.83	117.12	10	1
4	A	411	PX4	C19-C18-C17	2.27	102.90	114.37	1	2
4	A	427	PX4	C11-C10-C9	2.27	105.38	113.69	11	1
4	A	378	PX4	C5-N1-C3	2.27	103.02	108.98	6	1
4	A	386	PX4	C8-O5-C9	2.27	108.83	117.12	3	2
4	A	355	PX4	C33-C32-C31	2.27	102.91	114.37	8	3
4	A	409	PX4	C28-C27-C26	2.27	102.92	114.37	3	1
4	A	410	PX4	O3-P1-O2	2.27	99.95	108.94	2	1
4	A	313	PX4	O7-C23-O8	2.26	118.41	123.70	10	1
4	A	327	PX4	C19-C18-C17	2.26	102.92	114.37	10	1
4	A	349	PX4	C30-C29-C28	2.27	102.92	114.37	10	1
4	A	414	PX4	O3-C1-C2	2.27	120.55	109.65	3	2
4	A	319	PX4	C13-C12-C11	2.26	102.94	114.37	3	1
4	A	345	PX4	C15-C14-C13	2.26	102.93	114.37	4	1
4	A	370	PX4	C25-C24-C23	2.26	121.98	113.69	9	2
4	A	395	PX4	O3-C1-C2	2.26	120.54	109.65	14	2
4	A	396	PX4	O5-C9-C10	2.26	118.73	111.83	6	2
4	A	407	PX4	C30-C29-C28	2.26	102.93	114.37	9	3
4	A	356	PX4	C15-C14-C13	2.26	102.94	114.37	4	2
4	A	315	PX4	C19-C18-C17	2.26	102.94	114.37	12	1
4	A	329	PX4	C16-C15-C14	2.26	102.94	114.37	5	2
4	A	331	PX4	C20-C19-C18	2.26	102.94	114.37	6	1
4	A	334	PX4	C12-C11-C10	2.26	104.83	113.13	12	2
4	A	338	PX4	C5-N1-C2	2.26	118.89	109.91	10	1
4	A	363	PX4	C4-N1-C3	2.26	114.91	108.98	14	5
4	A	367	PX4	C5-N1-C3	2.26	103.04	108.98	2	1
4	A	314	PX4	C29-C28-C27	2.26	102.96	114.37	8	2
4	A	349	PX4	C33-C32-C31	2.26	102.96	114.37	14	1
4	A	366	PX4	C15-C14-C13	2.26	102.95	114.37	4	1
4	A	341	PX4	C20-C19-C18	2.26	102.97	114.37	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	364	PX4	C17-C16-C15	2.25	102.97	114.37	13	2
4	A	372	PX4	C30-C29-C28	2.25	102.97	114.37	10	1
4	A	384	PX4	O5-C9-O6	2.25	117.99	123.63	5	1
4	A	385	PX4	C20-C19-C18	2.25	102.97	114.37	7	1
4	A	385	PX4	C28-C27-C26	2.25	102.97	114.37	8	1
4	A	407	PX4	C3-N1-C2	2.25	100.95	109.91	7	2
4	A	312	PX4	C33-C32-C31	2.25	102.98	114.37	12	2
4	A	342	PX4	C11-C10-C9	2.25	105.44	113.69	1	1
4	A	309	PX4	C8-O5-C9	2.25	108.89	117.12	6	2
4	A	315	PX4	C16-C15-C14	2.25	102.99	114.37	11	1
4	A	371	PX4	C28-C27-C26	2.25	102.99	114.37	1	2
4	A	371	PX4	C4-N1-C2	2.25	118.86	109.91	12	3
4	A	396	PX4	C30-C29-C28	2.25	102.99	114.37	6	1
4	A	401	PX4	C13-C12-C11	2.25	102.99	114.37	7	4
4	A	358	PX4	C25-C24-C23	2.25	105.45	113.69	5	2
4	A	380	PX4	C1-C2-N1	2.25	123.04	115.82	3	2
4	A	421	PX4	C12-C11-C10	2.25	121.39	113.13	7	2
4	A	310	PX4	C30-C29-C28	2.25	103.01	114.37	3	2
4	A	310	PX4	C31-C30-C29	2.25	103.01	114.37	13	1
4	A	321	PX4	C8-O5-C9	2.25	125.33	117.12	10	3
4	A	335	PX4	C33-C32-C31	2.25	103.00	114.37	7	1
4	A	358	PX4	C32-C31-C30	2.25	103.00	114.37	13	1
4	A	420	PX4	C26-C25-C24	2.25	104.87	113.13	8	2
4	A	347	PX4	C20-C19-C18	2.25	103.02	114.37	1	1
4	A	354	PX4	C3-N1-C2	2.25	118.84	109.91	1	2
4	A	366	PX4	C4-N1-C2	2.25	118.84	109.91	7	2
4	A	383	PX4	C28-C27-C26	2.25	103.01	114.37	11	1
4	A	355	PX4	C3-N1-C2	2.25	100.98	109.91	12	1
4	A	373	PX4	O7-C7-C8	2.25	116.40	108.34	4	3
4	A	396	PX4	C4-N1-C2	2.25	118.83	109.91	14	2
4	A	396	PX4	C15-C14-C13	2.25	103.02	114.37	4	1
4	A	363	PX4	C15-C14-C13	2.24	103.02	114.37	12	1
4	A	400	PX4	C34-C33-C32	2.24	103.02	114.37	4	3
4	A	419	PX4	C19-C18-C17	2.25	103.02	114.37	9	2
4	A	423	PX4	C16-C15-C14	2.24	103.02	114.37	6	2
4	A	311	PX4	C31-C30-C29	2.24	103.03	114.37	2	2
4	A	311	PX4	O6-C9-C10	2.24	115.01	123.78	3	3
4	A	396	PX4	C16-C15-C14	2.24	103.03	114.37	9	2
4	A	321	PX4	C16-C15-C14	2.24	103.04	114.37	3	1
4	A	330	PX4	O3-C1-C2	2.24	120.44	109.65	10	1
4	A	382	PX4	C1-C2-N1	2.24	123.02	115.82	3	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	407	PX4	O8-C23-C24	2.24	115.01	123.78	9	1
4	A	353	PX4	O3-C1-C2	2.24	120.44	109.65	6	2
4	A	391	PX4	O8-C23-C24	2.24	115.01	123.78	12	1
4	A	417	PX4	C16-C15-C14	2.24	103.04	114.37	6	1
4	A	421	PX4	C29-C28-C27	2.24	103.03	114.37	12	3
4	A	328	PX4	C31-C30-C29	2.24	103.05	114.37	8	2
4	A	357	PX4	C8-O5-C9	2.24	125.31	117.12	11	2
4	A	376	PX4	C4-N1-C2	2.24	118.81	109.91	14	3
4	A	378	PX4	C16-C15-C14	2.24	103.04	114.37	5	2
4	A	332	PX4	C8-O5-C9	2.24	108.94	117.12	3	2
4	A	386	PX4	C29-C28-C27	2.24	103.05	114.37	13	1
4	A	411	PX4	C11-C10-C9	2.24	105.49	113.69	10	2
4	A	417	PX4	C32-C31-C30	2.24	103.05	114.37	8	2
4	A	421	PX4	O5-C9-O6	2.24	118.03	123.63	14	4
4	A	312	PX4	O8-C23-C24	2.24	115.03	123.78	9	1
4	A	322	PX4	C27-C26-C25	2.24	103.06	114.37	4	1
4	A	306	PX4	C34-C33-C32	2.24	103.06	114.37	6	1
4	A	325	PX4	O5-C9-C10	2.24	118.65	111.83	11	3
4	A	346	PX4	C20-C19-C18	2.24	103.06	114.37	14	3
4	A	347	PX4	C29-C28-C27	2.24	103.06	114.37	14	1
4	A	393	PX4	C14-C13-C12	2.24	103.06	114.37	8	2
4	A	311	PX4	C19-C18-C17	2.24	103.07	114.37	6	3
4	A	314	PX4	C11-C10-C9	2.23	105.51	113.69	13	2
4	A	347	PX4	C22-C21-C20	2.23	98.27	113.36	6	1
4	A	360	PX4	C28-C27-C26	2.24	103.07	114.37	2	2
4	A	360	PX4	C32-C31-C30	2.24	103.07	114.37	3	1
4	A	369	PX4	C34-C33-C32	2.24	103.07	114.37	11	1
4	A	393	PX4	O7-C7-C6	2.24	116.36	108.34	14	1
4	A	408	PX4	O3-C1-C2	2.23	120.40	109.65	9	1
4	A	410	PX4	C4-N1-C3	2.24	103.10	108.98	9	1
4	A	419	PX4	O1-P1-O4	2.24	117.70	107.57	2	1
4	A	399	PX4	C4-N1-C2	2.24	118.80	109.91	12	1
4	A	411	PX4	O8-C23-C24	2.23	115.04	123.78	8	2
4	A	427	PX4	C15-C14-C13	2.23	103.07	114.37	13	3
4	A	335	PX4	C14-C13-C12	2.23	103.08	114.37	7	1
4	A	360	PX4	O8-C23-C24	2.23	115.05	123.78	10	1
4	A	357	PX4	C3-N1-C2	2.23	118.78	109.91	1	1
4	A	361	PX4	C27-C26-C25	2.23	103.08	114.37	3	2
4	A	381	PX4	C16-C15-C14	2.23	103.08	114.37	9	1
4	A	383	PX4	C15-C14-C13	2.23	103.08	114.37	8	1
4	A	400	PX4	C20-C19-C18	2.23	103.08	114.37	4	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	372	PX4	C8-O5-C9	2.23	108.96	117.12	12	1
4	A	374	PX4	C29-C28-C27	2.23	103.09	114.37	6	1
4	A	343	PX4	C3-N1-C2	2.23	118.78	109.91	14	1
4	A	395	PX4	C30-C29-C28	2.23	103.09	114.37	3	2
4	A	363	PX4	O1-P1-O4	2.23	117.67	107.57	3	1
4	A	389	PX4	C16-C15-C14	2.23	103.10	114.37	9	1
4	A	410	PX4	O5-C9-O6	2.23	118.05	123.63	10	3
4	A	430	PX4	C33-C32-C31	2.23	103.10	114.37	3	1
4	A	308	PX4	O3-C1-C2	2.23	120.37	109.65	5	1
4	A	310	PX4	C20-C19-C18	2.23	103.10	114.37	14	2
4	A	310	PX4	C4-N1-C2	2.23	118.77	109.91	7	2
4	A	311	PX4	C8-O5-C9	2.23	108.97	117.12	6	3
4	A	334	PX4	C13-C12-C11	2.23	103.11	114.37	9	3
4	A	357	PX4	C32-C31-C30	2.23	103.11	114.37	14	1
4	A	364	PX4	C16-C15-C14	2.23	103.11	114.37	14	1
4	A	368	PX4	C18-C17-C16	2.23	103.10	114.37	5	2
4	A	400	PX4	C27-C26-C25	2.23	103.11	114.37	7	4
4	A	422	PX4	C26-C25-C24	2.23	104.94	113.13	13	1
4	A	367	PX4	C29-C28-C27	2.23	103.11	114.37	7	2
4	A	374	PX4	O5-C9-C10	2.23	118.62	111.83	3	3
4	A	387	PX4	C5-N1-C2	2.23	118.76	109.91	14	2
4	A	339	PX4	O8-C23-C24	2.23	115.08	123.78	9	1
4	A	395	PX4	C13-C12-C11	2.22	103.13	114.37	14	1
4	A	398	PX4	C14-C13-C12	2.22	103.12	114.37	7	1
4	A	329	PX4	C8-O5-C9	2.22	108.99	117.12	6	2
4	A	333	PX4	C26-C25-C24	2.22	104.96	113.13	14	3
4	A	339	PX4	C26-C25-C24	2.22	104.97	113.13	9	2
4	A	323	PX4	O5-C9-C10	2.22	118.61	111.83	2	3
4	A	326	PX4	C16-C15-C14	2.22	103.14	114.37	10	1
4	A	359	PX4	O3-C1-C2	2.22	120.34	109.65	3	1
4	A	363	PX4	O3-C1-C2	2.22	120.34	109.65	2	1
4	A	388	PX4	C20-C19-C18	2.22	103.13	114.37	6	1
4	A	306	PX4	O3-C1-C2	2.22	120.33	109.65	2	1
4	A	351	PX4	C28-C27-C26	2.22	103.15	114.37	14	1
4	A	356	PX4	O1-P1-O3	2.22	117.63	107.57	11	2
4	A	367	PX4	C32-C31-C30	2.22	125.59	114.37	6	2
4	A	380	PX4	C19-C18-C17	2.22	103.14	114.37	4	1
4	A	385	PX4	C14-C13-C12	2.22	103.14	114.37	5	1
4	A	392	PX4	C19-C18-C17	2.22	103.15	114.37	11	2
4	A	401	PX4	C20-C19-C18	2.22	103.14	114.37	7	1
4	A	368	PX4	C19-C18-C17	2.22	103.15	114.37	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	412	PX4	C27-C26-C25	2.22	103.15	114.37	11	1
4	A	310	PX4	C17-C16-C15	2.22	103.16	114.37	3	1
4	A	329	PX4	C19-C18-C17	2.22	103.16	114.37	14	1
4	A	369	PX4	C20-C19-C18	2.22	103.16	114.37	9	1
4	A	371	PX4	O3-C1-C2	2.22	120.32	109.65	2	1
4	A	376	PX4	C15-C14-C13	2.22	103.16	114.37	2	1
4	A	405	PX4	C5-N1-C2	2.22	118.73	109.91	4	1
4	A	416	PX4	C30-C29-C28	2.22	103.15	114.37	10	1
4	A	346	PX4	C29-C28-C27	2.22	103.16	114.37	11	1
4	A	417	PX4	C26-C25-C24	2.22	104.98	113.13	13	2
4	A	424	PX4	C5-N1-C4	2.22	103.15	108.98	10	3
4	A	356	PX4	C25-C24-C23	2.22	105.57	113.69	12	1
4	A	380	PX4	C3-N1-C2	2.22	101.10	109.91	6	1
4	A	414	PX4	O1-P1-O4	2.22	117.62	107.57	1	2
4	A	333	PX4	C13-C12-C11	2.22	103.17	114.37	4	1
4	A	389	PX4	C8-O5-C9	2.22	109.02	117.12	9	1
4	A	309	PX4	C3-N1-C2	2.21	118.71	109.91	12	1
4	A	356	PX4	C8-O5-C9	2.21	109.03	117.12	10	1
4	A	418	PX4	O6-C9-C10	2.21	115.13	123.78	7	1
4	A	339	PX4	C14-C13-C12	2.21	103.19	114.37	1	1
4	A	394	PX4	C5-N1-C2	2.21	118.70	109.91	7	1
4	A	396	PX4	C11-C10-C9	2.21	121.80	113.69	14	1
4	A	418	PX4	O1-P1-O4	2.21	117.59	107.57	1	2
4	A	309	PX4	C17-C16-C15	2.21	103.20	114.37	7	2
4	A	355	PX4	C28-C27-C26	2.21	103.20	114.37	1	1
4	A	369	PX4	C25-C24-C23	2.21	105.60	113.69	3	2
4	A	374	PX4	C3-N1-C2	2.21	118.69	109.91	10	1
4	A	375	PX4	C13-C12-C11	2.21	103.20	114.37	1	1
4	A	370	PX4	C17-C16-C15	2.21	103.20	114.37	3	2
4	A	379	PX4	C17-C16-C15	2.21	103.20	114.37	10	1
4	A	406	PX4	C13-C12-C11	2.21	103.20	114.37	6	1
4	A	320	PX4	O5-C9-O6	2.21	118.10	123.63	11	2
4	A	332	PX4	C13-C12-C11	2.21	103.21	114.37	3	1
4	A	379	PX4	C16-C15-C14	2.21	103.22	114.37	11	2
4	A	381	PX4	O5-C9-C10	2.21	118.56	111.83	10	1
4	A	382	PX4	C13-C12-C11	2.21	103.22	114.37	7	2
4	A	385	PX4	C30-C29-C28	2.21	103.22	114.37	5	1
4	A	404	PX4	C3-N1-C2	2.21	118.68	109.91	1	1
4	A	323	PX4	O4-P1-O2	2.20	117.67	108.94	12	1
4	A	334	PX4	C4-N1-C2	2.20	101.15	109.91	14	1
4	A	349	PX4	C32-C31-C30	2.20	103.22	114.37	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	393	PX4	C8-O5-C9	2.21	109.06	117.12	4	1
4	A	428	PX4	O7-C7-C6	2.21	116.25	108.34	11	3
4	A	344	PX4	C4-N1-C2	2.20	118.67	109.91	9	1
4	A	379	PX4	O6-C9-C10	2.20	115.17	123.78	2	1
4	A	383	PX4	C3-N1-C2	2.20	101.15	109.91	10	1
4	A	309	PX4	C12-C11-C10	2.20	105.04	113.13	1	1
4	A	333	PX4	C11-C10-C9	2.20	121.76	113.69	1	1
4	A	376	PX4	C17-C16-C15	2.20	103.24	114.37	11	2
4	A	400	PX4	C4-N1-C2	2.20	118.67	109.91	7	5
4	A	404	PX4	C26-C25-C24	2.20	105.04	113.13	3	2
4	A	404	PX4	O8-C23-C24	2.20	115.17	123.78	9	1
4	A	426	PX4	O3-C1-C2	2.20	120.25	109.65	2	2
4	A	357	PX4	O3-P1-O2	2.20	100.21	108.94	4	1
4	A	314	PX4	C30-C29-C28	2.20	103.25	114.37	6	1
4	A	332	PX4	C33-C32-C31	2.20	103.24	114.37	2	1
4	A	315	PX4	C34-C33-C32	2.20	103.25	114.37	10	2
4	A	385	PX4	C33-C32-C31	2.20	103.25	114.37	6	2
4	A	388	PX4	C13-C12-C11	2.20	103.25	114.37	4	1
4	A	391	PX4	O1-P1-O4	2.20	117.54	107.57	8	2
4	A	398	PX4	C32-C31-C30	2.20	103.25	114.37	12	2
4	A	413	PX4	C14-C13-C12	2.20	103.25	114.37	4	1
4	A	329	PX4	O8-C23-C24	2.20	115.19	123.78	6	1
4	A	318	PX4	C19-C18-C17	2.20	103.26	114.37	11	1
4	A	322	PX4	C34-C33-C32	2.20	103.27	114.37	2	1
4	A	328	PX4	C8-O5-C9	2.20	109.09	117.12	1	1
4	A	356	PX4	C20-C19-C18	2.20	103.26	114.37	13	1
4	A	360	PX4	C17-C16-C15	2.20	103.26	114.37	7	1
4	A	361	PX4	O6-C9-C10	2.20	115.18	123.78	6	2
4	A	391	PX4	O7-C7-C8	2.20	116.23	108.34	2	1
4	A	383	PX4	C8-O5-C9	2.20	109.09	117.12	6	2
4	A	343	PX4	C16-C15-C14	2.20	103.27	114.37	9	2
4	A	400	PX4	C11-C10-C9	2.20	105.65	113.69	5	1
4	A	402	PX4	O6-C9-C10	2.20	115.19	123.78	8	1
4	A	317	PX4	C5-N1-C2	2.19	101.19	109.91	2	1
4	A	382	PX4	C3-N1-C2	2.19	118.63	109.91	1	1
4	A	415	PX4	C33-C32-C31	2.19	103.28	114.37	9	1
4	A	314	PX4	C8-O5-C9	2.19	109.11	117.12	7	1
4	A	322	PX4	C20-C19-C18	2.19	103.29	114.37	8	1
4	A	326	PX4	C32-C31-C30	2.19	103.29	114.37	8	1
4	A	337	PX4	C3-N1-C2	2.19	101.20	109.91	11	1
4	A	358	PX4	C14-C13-C12	2.19	103.29	114.37	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	O1-P1-O4	2.19	117.50	107.57	6	1
4	A	361	PX4	C28-C27-C26	2.19	103.29	114.37	3	1
4	A	405	PX4	O1-P1-O4	2.19	117.50	107.57	14	2
4	A	412	PX4	C16-C15-C14	2.19	103.29	114.37	1	2
4	A	417	PX4	C12-C11-C10	2.19	105.08	113.13	8	1
4	A	425	PX4	O3-P1-O2	2.19	100.25	108.94	14	2
4	A	311	PX4	C29-C28-C27	2.19	103.30	114.37	3	1
4	A	328	PX4	C33-C32-C31	2.19	103.30	114.37	4	1
4	A	338	PX4	O6-C9-C10	2.19	115.22	123.78	8	1
4	A	374	PX4	C26-C25-C24	2.19	121.17	113.13	13	1
4	A	376	PX4	C27-C26-C25	2.19	103.31	114.37	7	1
4	A	384	PX4	O1-P1-O3	2.19	97.65	107.57	7	1
4	A	402	PX4	C5-N1-C2	2.19	118.61	109.91	12	1
4	A	410	PX4	C20-C19-C18	2.19	103.30	114.37	4	1
4	A	317	PX4	C28-C27-C26	2.19	103.31	114.37	12	2
4	A	357	PX4	O1-P1-O3	2.19	117.48	107.57	8	2
4	A	419	PX4	C29-C28-C27	2.19	103.31	114.37	11	1
4	A	358	PX4	C26-C25-C24	2.19	105.09	113.13	9	3
4	A	364	PX4	C11-C10-C9	2.19	105.68	113.69	6	2
4	A	383	PX4	C29-C28-C27	2.19	103.32	114.37	11	1
4	A	402	PX4	C4-N1-C3	2.19	103.23	108.98	9	2
4	A	405	PX4	C33-C32-C31	2.19	103.32	114.37	6	2
4	A	410	PX4	O1-P1-O3	2.19	117.48	107.57	14	1
4	A	425	PX4	C28-C27-C26	2.19	103.31	114.37	6	1
4	A	315	PX4	C13-C12-C11	2.18	103.32	114.37	5	2
4	A	347	PX4	C31-C30-C29	2.18	103.32	114.37	8	1
4	A	369	PX4	C18-C17-C16	2.19	103.32	114.37	4	1
4	A	347	PX4	C28-C27-C26	2.18	103.33	114.37	11	1
4	A	349	PX4	C8-O5-C9	2.18	109.13	117.12	3	3
4	A	364	PX4	C12-C11-C10	2.18	105.10	113.13	12	1
4	A	393	PX4	O8-C23-C24	2.18	115.24	123.78	7	1
4	A	393	PX4	C32-C31-C30	2.18	103.33	114.37	10	1
4	A	427	PX4	C30-C29-C28	2.18	103.33	114.37	9	1
4	A	313	PX4	O1-P1-O3	2.18	97.68	107.57	11	3
4	A	319	PX4	O1-P1-O4	2.18	117.46	107.57	8	1
4	A	332	PX4	C25-C24-C23	2.18	105.70	113.69	3	2
4	A	414	PX4	C34-C33-C32	2.18	125.40	114.37	5	1
4	A	335	PX4	O8-C23-C24	2.18	115.25	123.78	9	1
4	A	348	PX4	C28-C27-C26	2.18	103.35	114.37	12	2
4	A	357	PX4	C16-C15-C14	2.18	103.35	114.37	11	1
4	A	358	PX4	O5-C9-O6	2.18	118.17	123.63	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	C11-C10-C9	2.18	121.69	113.69	8	1
4	A	362	PX4	O5-C9-O6	2.18	118.17	123.63	8	2
4	A	379	PX4	C5-N1-C2	2.18	101.25	109.91	3	1
4	A	393	PX4	O5-C9-C10	2.18	118.48	111.83	14	2
4	A	408	PX4	C25-C24-C23	2.18	105.71	113.69	11	1
4	A	425	PX4	C32-C31-C30	2.18	103.35	114.37	4	1
4	A	354	PX4	C4-N1-C2	2.18	118.57	109.91	10	1
4	A	377	PX4	C32-C31-C30	2.18	103.36	114.37	7	2
4	A	395	PX4	C8-O5-C9	2.18	109.16	117.12	12	1
4	A	402	PX4	C34-C33-C32	2.18	103.36	114.37	8	1
4	A	310	PX4	O4-P1-O2	2.18	117.56	108.94	4	1
4	A	320	PX4	C1-C2-N1	2.18	122.81	115.82	6	1
4	A	322	PX4	O3-C1-C2	2.18	120.11	109.65	1	1
4	A	351	PX4	C19-C18-C17	2.18	103.37	114.37	2	1
4	A	389	PX4	O6-C9-C10	2.18	115.27	123.78	4	1
4	A	399	PX4	O3-C1-C2	2.17	120.11	109.65	2	2
4	A	407	PX4	C13-C12-C11	2.18	103.37	114.37	13	1
4	A	426	PX4	C5-N1-C2	2.18	118.56	109.91	5	2
4	A	427	PX4	C3-N1-C2	2.17	118.55	109.91	2	2
4	A	427	PX4	C19-C18-C17	2.18	103.37	114.37	6	1
4	A	317	PX4	O3-C1-C2	2.17	120.11	109.65	10	1
4	A	384	PX4	C3-N1-C2	2.17	118.55	109.91	2	1
4	A	418	PX4	C28-C27-C26	2.17	103.38	114.37	14	2
4	A	306	PX4	C32-C31-C30	2.17	103.39	114.37	7	1
4	A	325	PX4	C16-C15-C14	2.17	103.39	114.37	13	1
4	A	332	PX4	C14-C13-C12	2.17	103.39	114.37	9	1
4	A	346	PX4	C12-C11-C10	2.17	105.15	113.13	9	1
4	A	355	PX4	O1-P1-O3	2.17	117.41	107.57	4	3
4	A	362	PX4	C25-C24-C23	2.17	105.74	113.69	4	4
4	A	395	PX4	C16-C15-C14	2.17	103.39	114.37	13	1
4	A	398	PX4	C28-C27-C26	2.17	103.39	114.37	7	1
4	A	402	PX4	C33-C32-C31	2.17	103.39	114.37	9	1
4	A	420	PX4	C29-C28-C27	2.17	103.39	114.37	13	2
4	A	381	PX4	O1-P1-O4	2.17	117.40	107.57	6	2
4	A	384	PX4	C22-C21-C20	2.17	98.71	113.36	12	1
4	A	401	PX4	O6-C9-C10	2.17	115.30	123.78	4	2
4	A	403	PX4	C18-C17-C16	2.17	103.40	114.37	1	1
4	A	318	PX4	C30-C29-C28	2.17	103.40	114.37	14	1
4	A	346	PX4	C30-C29-C28	2.17	103.40	114.37	14	1
4	A	420	PX4	C33-C32-C31	2.17	103.40	114.37	10	1
4	A	308	PX4	C15-C14-C13	2.17	103.41	114.37	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	C34-C33-C32	2.17	103.41	114.37	4	1
4	A	363	PX4	C16-C15-C14	2.17	103.41	114.37	9	2
4	A	392	PX4	C27-C26-C25	2.17	103.41	114.37	2	1
4	A	394	PX4	C17-C16-C15	2.17	103.41	114.37	2	1
4	A	397	PX4	C8-O5-C9	2.17	109.19	117.12	9	1
4	A	407	PX4	C31-C30-C29	2.17	103.41	114.37	11	1
4	A	426	PX4	C3-N1-C2	2.17	118.53	109.91	9	1
4	A	415	PX4	C19-C18-C17	2.17	103.41	114.37	1	2
4	A	332	PX4	C28-C27-C26	2.17	103.42	114.37	8	1
4	A	399	PX4	C25-C24-C23	2.17	105.76	113.69	2	2
4	A	424	PX4	C8-O5-C9	2.17	109.20	117.12	6	1
4	A	425	PX4	C18-C17-C16	2.17	103.42	114.37	4	1
4	A	348	PX4	C34-C33-C32	2.16	103.42	114.37	11	1
4	A	355	PX4	C14-C13-C12	2.17	103.42	114.37	6	1
4	A	359	PX4	C30-C29-C28	2.17	103.42	114.37	6	1
4	A	382	PX4	C31-C30-C29	2.16	103.43	114.37	1	1
4	A	397	PX4	C36-C35-C34	2.16	98.75	113.36	10	1
4	A	307	PX4	C5-N1-C4	2.16	103.30	108.98	13	1
4	A	350	PX4	C25-C24-C23	2.16	105.77	113.69	6	1
4	A	369	PX4	C27-C26-C25	2.16	103.44	114.37	2	1
4	A	371	PX4	C17-C16-C15	2.16	103.44	114.37	8	1
4	A	387	PX4	C19-C18-C17	2.16	103.44	114.37	12	1
4	A	306	PX4	O1-P1-O3	2.16	117.36	107.57	12	1
4	A	365	PX4	O6-C9-C10	2.16	115.34	123.78	6	2
4	A	376	PX4	C14-C13-C12	2.16	103.45	114.37	5	1
4	A	397	PX4	C29-C28-C27	2.16	103.45	114.37	6	1
4	A	308	PX4	C27-C26-C25	2.16	103.46	114.37	1	1
4	A	408	PX4	C13-C12-C11	2.16	103.46	114.37	1	3
4	A	423	PX4	C13-C12-C11	2.16	103.46	114.37	9	1
4	A	408	PX4	C31-C30-C29	2.16	103.47	114.37	8	1
4	A	424	PX4	O3-C1-C2	2.16	120.03	109.65	8	2
4	A	371	PX4	C5-N1-C2	2.16	118.48	109.91	9	1
4	A	397	PX4	O3-P1-O2	2.16	100.39	108.94	6	3
4	A	398	PX4	C33-C32-C31	2.16	103.47	114.37	11	1
4	A	321	PX4	C32-C31-C30	2.15	103.47	114.37	10	1
4	A	330	PX4	O8-C23-C24	2.15	115.35	123.78	11	1
4	A	338	PX4	C28-C27-C26	2.15	103.47	114.37	6	1
4	A	417	PX4	C33-C32-C31	2.15	103.47	114.37	5	1
4	A	419	PX4	C28-C27-C26	2.16	103.47	114.37	10	2
4	A	358	PX4	O7-C23-O8	2.15	118.67	123.70	9	1
4	A	385	PX4	C13-C12-C11	2.15	103.48	114.37	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	392	PX4	O8-C23-C24	2.15	115.35	123.78	5	1
4	A	393	PX4	C33-C32-C31	2.15	103.48	114.37	7	1
4	A	338	PX4	C17-C16-C15	2.15	103.49	114.37	13	1
4	A	355	PX4	C16-C15-C14	2.15	103.49	114.37	13	2
4	A	365	PX4	O5-C9-O6	2.15	118.24	123.63	3	1
4	A	381	PX4	C30-C29-C28	2.15	103.49	114.37	1	2
4	A	411	PX4	C3-N1-C2	2.15	118.47	109.91	1	1
4	A	314	PX4	O8-C23-C24	2.15	115.37	123.78	13	1
4	A	319	PX4	C17-C16-C15	2.15	103.50	114.37	12	1
4	A	306	PX4	C5-N1-C3	2.15	103.33	108.98	4	1
4	A	319	PX4	C11-C10-C9	2.15	105.82	113.69	1	1
4	A	327	PX4	O1-P1-O3	2.15	117.31	107.57	13	1
4	A	336	PX4	O7-C7-C6	2.15	116.05	108.34	1	2
4	A	346	PX4	O1-P1-O3	2.15	117.31	107.57	6	1
4	A	392	PX4	C13-C12-C11	2.15	103.50	114.37	1	3
4	A	362	PX4	C33-C32-C31	2.15	103.51	114.37	2	1
4	A	371	PX4	C12-C11-C10	2.15	105.23	113.13	10	1
4	A	376	PX4	C13-C12-C11	2.15	103.51	114.37	7	1
4	A	404	PX4	O6-C9-C10	2.15	115.38	123.78	7	1
4	A	324	PX4	C17-C16-C15	2.15	103.51	114.37	14	1
4	A	368	PX4	C12-C11-C10	2.15	105.24	113.13	7	2
4	A	308	PX4	C29-C28-C27	2.15	103.52	114.37	2	1
4	A	361	PX4	O8-C23-C24	2.15	115.39	123.78	8	1
4	A	362	PX4	O1-P1-O4	2.15	117.30	107.57	2	1
4	A	319	PX4	O6-C9-C10	2.14	115.39	123.78	5	1
4	A	320	PX4	O6-C9-C10	2.15	115.39	123.78	2	3
4	A	342	PX4	C30-C29-C28	2.14	103.53	114.37	11	1
4	A	344	PX4	C29-C28-C27	2.14	103.53	114.37	11	1
4	A	348	PX4	C18-C17-C16	2.15	103.52	114.37	4	1
4	A	382	PX4	C16-C15-C14	2.15	103.52	114.37	13	1
4	A	395	PX4	C28-C27-C26	2.14	103.53	114.37	4	1
4	A	401	PX4	O3-P1-O2	2.15	100.43	108.94	3	2
4	A	426	PX4	C27-C26-C25	2.15	103.52	114.37	4	1
4	A	307	PX4	C22-C21-C20	2.14	98.90	113.36	3	1
4	A	356	PX4	O3-C1-C2	2.14	119.96	109.65	7	1
4	A	371	PX4	C20-C19-C18	2.14	103.54	114.37	4	1
4	A	379	PX4	C36-C35-C34	2.14	98.90	113.36	12	1
4	A	403	PX4	C17-C16-C15	2.14	103.54	114.37	11	1
4	A	326	PX4	C28-C27-C26	2.14	103.54	114.37	1	1
4	A	412	PX4	C32-C31-C30	2.14	103.54	114.37	3	1
4	A	352	PX4	C20-C19-C18	2.14	103.55	114.37	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	372	PX4	C3-N1-C2	2.14	118.42	109.91	3	1
4	A	403	PX4	O6-C9-C10	2.14	115.41	123.78	10	2
4	A	406	PX4	C31-C30-C29	2.14	103.55	114.37	1	1
4	A	426	PX4	C35-C34-C33	2.14	96.47	115.25	8	1
4	A	314	PX4	C3-N1-C2	2.14	101.41	109.91	5	1
4	A	373	PX4	C26-C25-C24	2.14	105.26	113.13	7	1
4	A	343	PX4	C31-C30-C29	2.14	103.56	114.37	12	1
4	A	344	PX4	O1-P1-O3	2.14	97.87	107.57	6	1
4	A	394	PX4	C29-C28-C27	2.14	103.56	114.37	3	1
4	A	419	PX4	C33-C32-C31	2.14	103.56	114.37	8	1
4	A	328	PX4	C32-C31-C30	2.14	103.57	114.37	8	1
4	A	332	PX4	C12-C11-C10	2.14	120.97	113.13	11	1
4	A	334	PX4	C16-C15-C14	2.14	103.57	114.37	1	3
4	A	346	PX4	C17-C16-C15	2.14	103.57	114.37	13	1
4	A	350	PX4	C27-C26-C25	2.14	103.57	114.37	8	1
4	A	353	PX4	C18-C17-C16	2.14	103.57	114.37	2	1
4	A	385	PX4	C4-N1-C3	2.13	114.58	108.98	9	1
4	A	398	PX4	O8-C23-C24	2.14	115.43	123.78	12	1
4	A	403	PX4	C12-C11-C10	2.14	105.28	113.13	12	1
4	A	341	PX4	O8-C23-C24	2.13	115.43	123.78	7	1
4	A	357	PX4	C34-C33-C32	2.13	103.58	114.37	4	1
4	A	313	PX4	O3-P1-O2	2.13	100.48	108.94	14	2
4	A	323	PX4	C25-C24-C23	2.13	105.88	113.69	9	1
4	A	327	PX4	O5-C9-C10	2.13	118.34	111.83	6	1
4	A	400	PX4	O3-P1-O2	2.13	117.39	108.94	10	1
4	A	316	PX4	C8-O5-C9	2.13	109.33	117.12	6	1
4	A	334	PX4	O3-C1-C2	2.13	119.91	109.65	3	1
4	A	349	PX4	C25-C24-C23	2.13	121.50	113.69	1	1
4	A	384	PX4	C17-C16-C15	2.13	103.60	114.37	6	1
4	A	391	PX4	C20-C19-C18	2.13	103.59	114.37	1	1
4	A	402	PX4	C5-N1-C3	2.13	103.38	108.98	7	2
4	A	408	PX4	C15-C14-C13	2.13	103.59	114.37	6	1
4	A	423	PX4	C32-C31-C30	2.13	103.59	114.37	2	1
4	A	315	PX4	C4-N1-C2	2.13	101.44	109.91	9	1
4	A	334	PX4	O8-C23-C24	2.13	132.12	123.78	11	1
4	A	324	PX4	C25-C24-C23	2.13	105.89	113.69	12	1
4	A	350	PX4	C8-O5-C9	2.13	109.33	117.12	12	1
4	A	360	PX4	C19-C18-C17	2.13	103.60	114.37	1	1
4	A	368	PX4	C26-C25-C24	2.13	105.30	113.13	1	1
4	A	424	PX4	C18-C17-C16	2.13	103.60	114.37	11	1
4	A	380	PX4	C5-N1-C2	2.13	118.37	109.91	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	406	PX4	C3-N1-C2	2.13	118.37	109.91	12	1
4	A	422	PX4	C11-C10-C9	2.13	105.89	113.69	11	1
4	A	429	PX4	C4-N1-C2	2.13	118.37	109.91	6	1
4	A	364	PX4	C3-N1-C2	2.13	101.45	109.91	5	2
4	A	382	PX4	C20-C19-C18	2.13	103.61	114.37	4	1
4	A	408	PX4	C33-C32-C31	2.13	103.61	114.37	14	2
4	A	412	PX4	C4-N1-C2	2.13	118.37	109.91	13	1
4	A	391	PX4	C16-C15-C14	2.13	103.61	114.37	11	1
4	A	373	PX4	C32-C31-C30	2.13	103.62	114.37	5	1
4	A	376	PX4	C29-C28-C27	2.13	103.62	114.37	13	1
4	A	421	PX4	C13-C12-C11	2.13	103.61	114.37	9	1
4	A	307	PX4	O3-C1-C2	2.13	119.88	109.65	2	1
4	A	342	PX4	C34-C33-C32	2.13	103.62	114.37	5	1
4	A	369	PX4	C33-C32-C31	2.13	103.62	114.37	10	1
4	A	374	PX4	C13-C12-C11	2.13	103.63	114.37	7	2
4	A	383	PX4	C5-N1-C2	2.13	118.36	109.91	11	1
4	A	422	PX4	C5-N1-C2	2.13	118.36	109.91	5	1
4	A	327	PX4	C16-C15-C14	2.12	103.63	114.37	12	1
4	A	344	PX4	C19-C18-C17	2.12	103.63	114.37	8	1
4	A	351	PX4	C4-N1-C2	2.12	101.47	109.91	5	1
4	A	353	PX4	C20-C19-C18	2.12	103.64	114.37	10	2
4	A	366	PX4	C5-N1-C2	2.12	101.47	109.91	5	1
4	A	398	PX4	C27-C26-C25	2.12	103.63	114.37	5	1
4	A	350	PX4	C18-C17-C16	2.12	103.64	114.37	3	1
4	A	362	PX4	C19-C18-C17	2.12	103.64	114.37	7	1
4	A	366	PX4	O6-C9-C10	2.12	115.48	123.78	10	1
4	A	387	PX4	O8-C23-C24	2.12	115.48	123.78	3	1
4	A	394	PX4	C13-C12-C11	2.12	103.64	114.37	7	1
4	A	320	PX4	C28-C27-C26	2.12	103.65	114.37	11	1
4	A	354	PX4	C34-C33-C32	2.12	103.65	114.37	1	1
4	A	378	PX4	O6-C9-C10	2.12	115.49	123.78	1	2
4	A	406	PX4	C18-C17-C16	2.12	103.65	114.37	3	1
4	A	410	PX4	C27-C26-C25	2.12	103.65	114.37	6	1
4	A	312	PX4	O1-P1-O4	2.12	117.17	107.57	6	1
4	A	390	PX4	O4-P1-O2	2.12	117.33	108.94	9	1
4	A	412	PX4	C29-C28-C27	2.12	103.66	114.37	14	1
4	A	347	PX4	C4-N1-C2	2.12	101.49	109.91	14	1
4	A	322	PX4	C3-N1-C2	2.12	118.33	109.91	13	1
4	A	324	PX4	O5-C9-C10	2.12	118.29	111.83	12	1
4	A	397	PX4	C33-C32-C31	2.12	103.67	114.37	14	2
4	A	417	PX4	O3-C1-C2	2.12	119.84	109.65	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	429	PX4	O1-P1-O4	2.12	117.16	107.57	7	1
4	A	330	PX4	C4-N1-C2	2.12	101.50	109.91	6	1
4	A	353	PX4	C11-C10-C9	2.12	105.94	113.69	2	1
4	A	429	PX4	C11-C10-C9	2.12	105.94	113.69	9	1
4	A	386	PX4	C19-C18-C17	2.12	103.67	114.37	12	1
4	A	371	PX4	C18-C17-C16	2.11	103.68	114.37	2	1
4	A	404	PX4	O1-P1-O4	2.11	117.15	107.57	11	1
4	A	422	PX4	C34-C33-C32	2.12	103.67	114.37	9	1
4	A	411	PX4	C4-N1-C2	2.11	118.31	109.91	3	1
4	A	414	PX4	C29-C28-C27	2.11	103.69	114.37	4	1
4	A	415	PX4	C27-C26-C25	2.11	103.68	114.37	13	1
4	A	424	PX4	C13-C12-C11	2.11	103.68	114.37	11	2
4	A	357	PX4	C27-C26-C25	2.11	103.69	114.37	5	1
4	A	370	PX4	O8-C23-C24	2.11	115.52	123.78	5	1
4	A	353	PX4	O1-P1-O3	2.11	117.14	107.57	10	1
4	A	361	PX4	C16-C15-C14	2.11	103.70	114.37	6	1
4	A	378	PX4	C28-C27-C26	2.11	103.69	114.37	8	1
4	A	306	PX4	C28-C27-C26	2.11	103.71	114.37	4	2
4	A	331	PX4	O4-P1-O2	2.11	117.29	108.94	4	1
4	A	345	PX4	C4-N1-C2	2.11	118.30	109.91	12	2
4	A	371	PX4	C13-C12-C11	2.11	103.71	114.37	13	1
4	A	372	PX4	C32-C31-C30	2.11	103.70	114.37	13	1
4	A	418	PX4	C5-N1-C4	2.11	114.52	108.98	14	2
4	A	317	PX4	C19-C18-C17	2.11	103.72	114.37	5	1
4	A	330	PX4	C18-C17-C16	2.11	103.72	114.37	12	1
4	A	361	PX4	C12-C11-C10	2.11	105.38	113.13	14	1
4	A	376	PX4	O3-C1-C2	2.11	119.79	109.65	2	1
4	A	381	PX4	C28-C27-C26	2.11	103.71	114.37	1	1
4	A	401	PX4	O1-P1-O4	2.11	117.12	107.57	12	1
4	A	341	PX4	C19-C18-C17	2.11	103.72	114.37	5	1
4	A	373	PX4	C31-C30-C29	2.11	103.72	114.37	1	1
4	A	350	PX4	C35-C34-C33	2.10	96.79	115.25	3	2
4	A	351	PX4	C8-O5-C9	2.11	109.42	117.12	13	1
4	A	375	PX4	O1-P1-O4	2.11	117.11	107.57	14	2
4	A	389	PX4	C34-C33-C32	2.11	103.72	114.37	6	1
4	A	429	PX4	C29-C28-C27	2.11	103.72	114.37	2	1
4	A	360	PX4	C34-C33-C32	2.10	103.73	114.37	3	1
4	A	373	PX4	O5-C9-C10	2.10	118.25	111.83	14	1
4	A	401	PX4	C32-C31-C30	2.10	103.74	114.37	12	2
4	A	323	PX4	C17-C16-C15	2.10	103.75	114.37	8	1
4	A	338	PX4	C5-N1-C3	2.10	103.46	108.98	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	375	PX4	C31-C30-C29	2.10	103.75	114.37	1	1
4	A	388	PX4	C18-C17-C16	2.10	103.75	114.37	3	1
4	A	339	PX4	C15-C14-C13	2.10	103.75	114.37	6	1
4	A	362	PX4	C31-C30-C29	2.10	103.75	114.37	11	2
4	A	328	PX4	C12-C11-C10	2.10	105.42	113.13	10	1
4	A	379	PX4	C33-C32-C31	2.10	103.76	114.37	2	1
4	A	381	PX4	C31-C30-C29	2.10	103.76	114.37	14	2
4	A	381	PX4	C15-C14-C13	2.10	103.76	114.37	11	1
4	A	401	PX4	O1-P1-O3	2.10	98.06	107.57	10	1
4	A	430	PX4	O1-P1-O4	2.10	117.08	107.57	9	1
4	A	312	PX4	C5-N1-C2	2.10	101.58	109.91	13	2
4	A	342	PX4	C20-C19-C18	2.10	103.77	114.37	13	1
4	A	308	PX4	C3-N1-C2	2.09	118.24	109.91	3	1
4	A	313	PX4	O1-P1-O4	2.10	117.06	107.57	1	1
4	A	316	PX4	C4-N1-C2	2.10	101.58	109.91	11	1
4	A	318	PX4	C11-C10-C9	2.10	106.01	113.69	8	1
4	A	340	PX4	O4-P1-O2	2.09	100.63	108.94	11	2
4	A	309	PX4	C5-N1-C2	2.09	118.23	109.91	7	1
4	A	318	PX4	C4-N1-C2	2.09	118.23	109.91	9	1
4	A	320	PX4	C20-C19-C18	2.09	103.78	114.37	9	1
4	A	354	PX4	C33-C32-C31	2.09	103.78	114.37	14	1
4	A	357	PX4	C13-C12-C11	2.10	103.78	114.37	1	1
4	A	388	PX4	C4-N1-C2	2.10	118.24	109.91	13	1
4	A	411	PX4	C26-C25-C24	2.09	120.82	113.13	7	1
4	A	419	PX4	C14-C13-C12	2.10	103.78	114.37	11	2
4	A	310	PX4	C14-C13-C12	2.09	103.79	114.37	2	1
4	A	322	PX4	O1-P1-O4	2.09	117.06	107.57	4	1
4	A	331	PX4	C30-C29-C28	2.09	103.78	114.37	13	1
4	A	341	PX4	C33-C32-C31	2.09	103.79	114.37	4	1
4	A	348	PX4	O1-P1-O3	2.09	98.08	107.57	5	1
4	A	361	PX4	C1-C2-N1	2.09	122.54	115.82	12	1
4	A	370	PX4	C11-C10-C9	2.09	121.36	113.69	9	1
4	A	323	PX4	C15-C14-C13	2.09	103.80	114.37	4	1
4	A	323	PX4	C19-C18-C17	2.09	103.80	114.37	6	2
4	A	375	PX4	C32-C31-C30	2.09	103.79	114.37	3	1
4	A	397	PX4	C19-C18-C17	2.09	103.79	114.37	11	1
4	A	324	PX4	C4-N1-C3	2.09	103.48	108.98	9	1
4	A	307	PX4	O1-P1-O3	2.09	98.10	107.57	2	1
4	A	314	PX4	C14-C13-C12	2.09	103.81	114.37	9	1
4	A	422	PX4	C17-C16-C15	2.09	103.80	114.37	11	1
4	A	310	PX4	C22-C21-C20	2.09	99.27	113.36	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	321	PX4	C20-C19-C18	2.09	103.81	114.37	2	1
4	A	350	PX4	C5-N1-C4	2.09	103.49	108.98	10	2
4	A	377	PX4	C29-C28-C27	2.09	124.92	114.37	5	1
4	A	311	PX4	C33-C32-C31	2.09	103.82	114.37	13	1
4	A	417	PX4	C30-C29-C28	2.09	103.81	114.37	7	1
4	A	426	PX4	C33-C32-C31	2.09	103.81	114.37	14	1
4	A	328	PX4	C13-C12-C11	2.09	103.82	114.37	3	1
4	A	331	PX4	C36-C35-C34	2.08	99.29	113.36	1	1
4	A	361	PX4	C20-C19-C18	2.09	103.83	114.37	7	2
4	A	364	PX4	C30-C29-C28	2.09	103.82	114.37	6	1
4	A	370	PX4	C16-C15-C14	2.09	103.82	114.37	12	1
4	A	372	PX4	O6-C9-C10	2.09	115.62	123.78	8	2
4	A	398	PX4	C8-O5-C9	2.09	109.49	117.12	7	1
4	A	405	PX4	C4-N1-C2	2.09	118.20	109.91	5	1
4	A	405	PX4	C18-C17-C16	2.09	103.82	114.37	5	1
4	A	412	PX4	O8-C23-C24	2.09	115.62	123.78	4	1
4	A	416	PX4	C29-C28-C27	2.09	103.83	114.37	2	2
4	A	425	PX4	C33-C32-C31	2.09	103.83	114.37	9	1
4	A	337	PX4	C16-C15-C14	2.08	103.84	114.37	1	1
4	A	347	PX4	O6-C9-C10	2.08	115.63	123.78	14	1
4	A	378	PX4	C25-C24-C23	2.08	106.06	113.69	4	1
4	A	413	PX4	C19-C18-C17	2.08	103.83	114.37	13	2
4	A	352	PX4	C18-C17-C16	2.08	103.84	114.37	2	1
4	A	376	PX4	O1-P1-O4	2.08	117.01	107.57	12	1
4	A	423	PX4	C7-O7-C23	2.08	112.81	117.80	13	2
4	A	425	PX4	C20-C19-C18	2.08	103.83	114.37	14	1
4	A	356	PX4	C17-C16-C15	2.08	103.84	114.37	6	1
4	A	367	PX4	O4-P1-O2	2.08	117.19	108.94	6	2
4	A	407	PX4	C14-C13-C12	2.08	103.85	114.37	14	1
4	A	412	PX4	C19-C18-C17	2.08	103.84	114.37	1	1
4	A	327	PX4	C13-C12-C11	2.08	103.86	114.37	5	2
4	A	333	PX4	C15-C14-C13	2.08	103.85	114.37	3	1
4	A	377	PX4	C20-C19-C18	2.08	103.85	114.37	13	1
4	A	413	PX4	C15-C14-C13	2.08	103.85	114.37	13	1
4	A	311	PX4	O1-P1-O4	2.08	116.98	107.57	7	2
4	A	317	PX4	C13-C12-C11	2.08	103.87	114.37	10	2
4	A	322	PX4	C31-C30-C29	2.08	103.86	114.37	13	2
4	A	325	PX4	O3-C1-C2	2.08	119.64	109.65	14	1
4	A	334	PX4	C36-C35-C34	2.08	99.34	113.36	8	1
4	A	338	PX4	O4-P1-O2	2.08	100.70	108.94	10	1
4	A	359	PX4	O8-C23-C24	2.08	115.66	123.78	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	387	PX4	C3-N1-C2	2.08	101.65	109.91	3	2
4	A	371	PX4	C11-C10-C9	2.08	106.09	113.69	10	1
4	A	424	PX4	O1-P1-O4	2.08	116.98	107.57	6	1
4	A	317	PX4	C18-C17-C16	2.07	103.88	114.37	10	1
4	A	328	PX4	C36-C35-C34	2.07	99.36	113.36	1	1
4	A	336	PX4	C14-C13-C12	2.07	103.88	114.37	5	2
4	A	383	PX4	C27-C26-C25	2.07	103.89	114.37	2	1
4	A	414	PX4	C27-C26-C25	2.07	103.89	114.37	9	1
4	A	327	PX4	C34-C33-C32	2.07	103.89	114.37	5	1
4	A	369	PX4	C15-C14-C13	2.07	103.89	114.37	3	1
4	A	398	PX4	C5-N1-C2	2.07	118.15	109.91	4	1
4	A	429	PX4	C20-C19-C18	2.07	103.89	114.37	1	1
4	A	325	PX4	C29-C28-C27	2.07	103.90	114.37	3	1
4	A	369	PX4	C14-C13-C12	2.07	103.90	114.37	14	1
4	A	346	PX4	C3-N1-C2	2.07	118.14	109.91	3	1
4	A	412	PX4	C15-C14-C13	2.07	103.90	114.37	10	1
4	A	307	PX4	C29-C28-C27	2.07	103.91	114.37	7	1
4	A	323	PX4	C29-C28-C27	2.07	103.91	114.37	10	1
4	A	376	PX4	C7-O7-C23	2.07	122.75	117.80	1	1
4	A	382	PX4	O6-C9-C10	2.07	115.69	123.78	1	1
4	A	390	PX4	C33-C32-C31	2.07	103.91	114.37	4	1
4	A	391	PX4	C8-O5-C9	2.07	109.56	117.12	1	1
4	A	392	PX4	O3-C1-C2	2.07	119.60	109.65	11	1
4	A	420	PX4	C3-N1-C2	2.07	118.14	109.91	9	1
4	A	429	PX4	O7-C7-C8	2.07	115.77	108.34	12	1
4	A	323	PX4	O1-P1-O3	2.07	98.20	107.57	2	1
4	A	329	PX4	C15-C14-C13	2.07	103.92	114.37	6	1
4	A	339	PX4	O1-P1-O4	2.07	116.94	107.57	8	1
4	A	342	PX4	C13-C12-C11	2.07	103.92	114.37	8	1
4	A	394	PX4	C25-C24-C23	2.07	106.12	113.69	3	1
4	A	402	PX4	C20-C19-C18	2.07	103.92	114.37	5	1
4	A	412	PX4	C28-C27-C26	2.07	103.92	114.37	14	1
4	A	414	PX4	C11-C10-C9	2.07	106.12	113.69	2	2
4	A	366	PX4	C27-C26-C25	2.07	103.92	114.37	11	1
4	A	318	PX4	C33-C32-C31	2.06	103.93	114.37	13	1
4	A	321	PX4	C13-C12-C11	2.07	103.93	114.37	10	2
4	A	371	PX4	C3-N1-C2	2.07	101.70	109.91	7	1
4	A	376	PX4	O8-C23-C24	2.06	115.71	123.78	12	1
4	A	392	PX4	C34-C33-C32	2.06	103.93	114.37	6	1
4	A	394	PX4	C16-C15-C14	2.07	103.92	114.37	8	1
4	A	410	PX4	C17-C16-C15	2.07	103.92	114.37	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	412	PX4	C31-C30-C29	2.07	103.93	114.37	5	1
4	A	430	PX4	C18-C17-C16	2.07	103.92	114.37	8	1
4	A	331	PX4	C5-N1-C2	2.06	118.12	109.91	13	1
4	A	339	PX4	C18-C17-C16	2.06	103.93	114.37	5	1
4	A	346	PX4	C31-C30-C29	2.06	103.93	114.37	9	1
4	A	408	PX4	C30-C29-C28	2.06	103.94	114.37	14	1
4	A	410	PX4	C15-C14-C13	2.06	103.94	114.37	3	1
4	A	413	PX4	C5-N1-C2	2.06	118.12	109.91	1	1
4	A	315	PX4	C18-C17-C16	2.06	103.94	114.37	2	1
4	A	324	PX4	C26-C25-C24	2.06	120.70	113.13	1	1
4	A	338	PX4	C3-N1-C2	2.06	101.72	109.91	3	1
4	A	346	PX4	C13-C12-C11	2.06	103.95	114.37	12	1
4	A	357	PX4	C14-C13-C12	2.06	103.94	114.37	10	1
4	A	374	PX4	C16-C15-C14	2.06	103.94	114.37	4	1
4	A	426	PX4	C34-C33-C32	2.06	103.94	114.37	5	1
4	A	330	PX4	C15-C14-C13	2.06	103.95	114.37	4	1
4	A	356	PX4	C3-N1-C2	2.06	118.10	109.91	2	1
4	A	365	PX4	C5-N1-C4	2.06	103.56	108.98	3	1
4	A	370	PX4	C22-C21-C20	2.06	99.44	113.36	13	1
4	A	384	PX4	C16-C15-C14	2.06	103.95	114.37	1	3
4	A	374	PX4	C14-C13-C12	2.06	103.96	114.37	3	1
4	A	379	PX4	O8-C23-C24	2.06	115.72	123.78	5	1
4	A	408	PX4	C28-C27-C26	2.06	103.95	114.37	14	1
4	A	419	PX4	C20-C19-C18	2.06	103.95	114.37	13	1
4	A	420	PX4	C13-C12-C11	2.06	103.95	114.37	1	1
4	A	339	PX4	C20-C19-C18	2.06	103.96	114.37	1	2
4	A	339	PX4	O6-C9-C10	2.06	115.73	123.78	12	1
4	A	367	PX4	C14-C13-C12	2.06	103.96	114.37	1	1
4	A	392	PX4	O1-P1-O4	2.06	116.90	107.57	1	1
4	A	401	PX4	C15-C14-C13	2.06	103.96	114.37	12	1
4	A	402	PX4	C18-C17-C16	2.06	103.96	114.37	13	1
4	A	331	PX4	C16-C15-C14	2.06	103.97	114.37	10	1
4	A	350	PX4	C12-C11-C10	2.06	105.56	113.13	13	1
4	A	414	PX4	C32-C31-C30	2.06	103.97	114.37	11	1
4	A	311	PX4	C34-C33-C32	2.06	103.97	114.37	12	1
4	A	319	PX4	C33-C32-C31	2.06	103.97	114.37	11	1
4	A	353	PX4	C4-N1-C2	2.06	118.08	109.91	1	1
4	A	362	PX4	C12-C11-C10	2.06	105.57	113.13	1	1
4	A	364	PX4	C1-C2-N1	2.06	109.22	115.82	13	2
4	A	315	PX4	O1-P1-O3	2.05	116.88	107.57	4	1
4	A	365	PX4	C27-C26-C25	2.06	103.98	114.37	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	387	PX4	C20-C19-C18	2.06	103.98	114.37	5	1
4	A	419	PX4	O6-C9-C10	2.05	115.75	123.78	1	1
4	A	429	PX4	O3-C1-C2	2.05	119.53	109.65	3	1
4	A	307	PX4	C3-N1-C2	2.05	101.75	109.91	4	1
4	A	348	PX4	O4-P1-O2	2.05	100.80	108.94	13	1
4	A	349	PX4	C5-N1-C2	2.05	101.75	109.91	14	1
4	A	361	PX4	C25-C24-C23	2.05	106.17	113.69	4	1
4	A	382	PX4	C34-C33-C32	2.05	104.00	114.37	2	1
4	A	383	PX4	C31-C30-C29	2.05	104.00	114.37	12	2
4	A	416	PX4	C28-C27-C26	2.05	103.99	114.37	10	1
4	A	357	PX4	C18-C17-C16	2.05	104.00	114.37	6	1
4	A	385	PX4	O1-P1-O3	2.05	98.27	107.57	9	1
4	A	391	PX4	C3-N1-C2	2.05	101.76	109.91	1	1
4	A	395	PX4	C11-C10-C9	2.05	106.18	113.69	3	1
4	A	406	PX4	C5-N1-C2	2.05	101.76	109.91	12	1
4	A	425	PX4	C31-C30-C29	2.05	104.00	114.37	7	1
4	A	318	PX4	C5-N1-C2	2.05	118.05	109.91	10	1
4	A	331	PX4	O1-P1-O3	2.05	116.86	107.57	2	1
4	A	349	PX4	C28-C27-C26	2.05	104.01	114.37	14	1
4	A	375	PX4	C15-C14-C13	2.05	104.01	114.37	5	1
4	A	409	PX4	C31-C30-C29	2.05	104.01	114.37	14	3
4	A	320	PX4	C5-N1-C2	2.05	101.77	109.91	2	1
4	A	321	PX4	C30-C29-C28	2.05	104.02	114.37	1	1
4	A	346	PX4	C8-O5-C9	2.05	109.63	117.12	4	2
4	A	370	PX4	C8-O5-C9	2.05	109.63	117.12	12	1
4	A	376	PX4	C5-N1-C2	2.05	101.77	109.91	6	1
4	A	380	PX4	C15-C14-C13	2.05	104.02	114.37	4	1
4	A	386	PX4	C4-N1-C2	2.05	101.77	109.91	12	1
4	A	404	PX4	C11-C10-C9	2.05	106.19	113.69	10	1
4	A	317	PX4	C27-C26-C25	2.05	104.03	114.37	8	1
4	A	324	PX4	C31-C30-C29	2.05	104.03	114.37	6	2
4	A	329	PX4	C33-C32-C31	2.05	104.02	114.37	4	1
4	A	330	PX4	O3-P1-O2	2.05	100.83	108.94	3	1
4	A	331	PX4	O3-C1-C2	2.05	119.50	109.65	12	1
4	A	405	PX4	O8-C23-C24	2.04	115.78	123.78	10	1
4	A	414	PX4	C13-C12-C11	2.05	104.03	114.37	10	1
4	A	423	PX4	C33-C32-C31	2.05	104.02	114.37	3	2
4	A	331	PX4	C12-C11-C10	2.04	105.61	113.13	8	1
4	A	426	PX4	C13-C12-C11	2.05	104.03	114.37	1	1
4	A	339	PX4	O3-C1-C2	2.04	119.48	109.65	7	1
4	A	309	PX4	C11-C10-C9	2.04	106.22	113.69	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	311	PX4	C14-C13-C12	2.04	104.05	114.37	11	1
4	A	320	PX4	C17-C16-C15	2.04	104.05	114.37	1	1
4	A	374	PX4	C32-C31-C30	2.04	104.04	114.37	3	1
4	A	375	PX4	C34-C33-C32	2.04	104.04	114.37	1	1
4	A	377	PX4	C27-C26-C25	2.04	104.05	114.37	3	1
4	A	396	PX4	C32-C31-C30	2.04	104.05	114.37	5	1
4	A	398	PX4	C16-C15-C14	2.04	104.04	114.37	7	1
4	A	333	PX4	C18-C17-C16	2.04	104.05	114.37	12	1
4	A	312	PX4	C32-C31-C30	2.04	104.07	114.37	13	1
4	A	343	PX4	C18-C17-C16	2.04	104.06	114.37	8	1
4	A	430	PX4	O6-C9-C10	2.04	115.81	123.78	9	1
4	A	400	PX4	O8-C23-C24	2.04	115.81	123.78	9	1
4	A	314	PX4	O1-P1-O3	2.04	98.33	107.57	8	1
4	A	329	PX4	C25-C24-C23	2.04	106.23	113.69	2	1
4	A	393	PX4	C30-C29-C28	2.04	104.07	114.37	8	1
4	A	401	PX4	C29-C28-C27	2.04	104.07	114.37	14	1
4	A	419	PX4	C13-C12-C11	2.04	104.07	114.37	3	1
4	A	317	PX4	C4-N1-C2	2.03	118.00	109.91	2	1
4	A	346	PX4	C14-C13-C12	2.04	104.08	114.37	12	1
4	A	366	PX4	C14-C13-C12	2.04	104.07	114.37	5	1
4	A	372	PX4	C19-C18-C17	2.03	104.08	114.37	8	1
4	A	374	PX4	O3-C1-C2	2.04	119.44	109.65	14	1
4	A	382	PX4	C29-C28-C27	2.04	124.66	114.37	4	1
4	A	402	PX4	O3-C1-C2	2.04	119.44	109.65	2	1
4	A	405	PX4	C25-C24-C23	2.04	106.24	113.69	4	1
4	A	419	PX4	C27-C26-C25	2.04	104.08	114.37	7	1
4	A	340	PX4	C32-C31-C30	2.03	104.09	114.37	8	1
4	A	383	PX4	C4-N1-C2	2.03	118.00	109.91	10	1
4	A	342	PX4	C8-O5-C9	2.03	109.69	117.12	4	1
4	A	311	PX4	C32-C31-C30	2.03	104.09	114.37	14	1
4	A	355	PX4	C30-C29-C28	2.03	104.09	114.37	1	1
4	A	388	PX4	C30-C29-C28	2.03	104.09	114.37	12	1
4	A	405	PX4	C26-C25-C24	2.03	105.65	113.13	4	1
4	A	340	PX4	O6-C9-C10	2.03	115.83	123.78	8	1
4	A	394	PX4	O1-P1-O4	2.03	116.78	107.57	2	1
4	A	401	PX4	O4-P1-O2	2.03	116.99	108.94	13	1
4	A	424	PX4	C19-C18-C17	2.03	104.09	114.37	4	1
4	A	310	PX4	O3-C1-C2	2.03	119.42	109.65	8	1
4	A	336	PX4	C20-C19-C18	2.03	104.11	114.37	5	1
4	A	343	PX4	O3-P1-O2	2.03	100.89	108.94	12	1
4	A	355	PX4	C31-C30-C29	2.03	104.10	114.37	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	399	PX4	C16-C15-C14	2.03	104.10	114.37	3	1
4	A	411	PX4	C27-C26-C25	2.03	104.10	114.37	11	1
4	A	418	PX4	C33-C32-C31	2.03	104.10	114.37	10	1
4	A	351	PX4	C17-C16-C15	2.03	104.11	114.37	8	1
4	A	364	PX4	C19-C18-C17	2.03	104.11	114.37	10	1
4	A	423	PX4	C27-C26-C25	2.03	104.10	114.37	13	1
4	A	322	PX4	C4-N1-C2	2.03	117.97	109.91	7	1
4	A	328	PX4	C27-C26-C25	2.03	104.12	114.37	2	1
4	A	337	PX4	C30-C29-C28	2.03	104.12	114.37	4	1
4	A	365	PX4	C30-C29-C28	2.03	104.12	114.37	2	1
4	A	368	PX4	C32-C31-C30	2.03	104.12	114.37	12	1
4	A	374	PX4	C17-C16-C15	2.03	104.11	114.37	4	1
4	A	389	PX4	C13-C12-C11	2.03	104.11	114.37	10	1
4	A	403	PX4	C13-C12-C11	2.03	104.12	114.37	3	1
4	A	419	PX4	C31-C30-C29	2.03	104.12	114.37	10	2
4	A	395	PX4	C32-C31-C30	2.03	104.12	114.37	8	1
4	A	323	PX4	C31-C30-C29	2.02	104.14	114.37	14	1
4	A	330	PX4	C5-N1-C4	2.02	114.29	108.98	6	1
4	A	348	PX4	C7-O7-C23	2.02	122.64	117.80	12	1
4	A	341	PX4	C5-N1-C2	2.02	117.95	109.91	6	1
4	A	353	PX4	C27-C26-C25	2.02	104.14	114.37	13	1
4	A	368	PX4	C34-C33-C32	2.02	104.13	114.37	2	1
4	A	373	PX4	O1-P1-O3	2.02	116.74	107.57	12	1
4	A	375	PX4	C18-C17-C16	2.02	104.14	114.37	9	1
4	A	361	PX4	C5-N1-C2	2.02	117.95	109.91	7	1
4	A	333	PX4	C16-C15-C14	2.02	104.15	114.37	8	1
4	A	335	PX4	O5-C9-C10	2.02	118.00	111.83	7	1
4	A	335	PX4	C4-N1-C2	2.02	117.94	109.91	12	1
4	A	350	PX4	C3-N1-C2	2.02	117.94	109.91	4	1
4	A	394	PX4	C4-N1-C2	2.02	117.94	109.91	6	1
4	A	330	PX4	C32-C31-C30	2.02	104.17	114.37	3	1
4	A	340	PX4	O1-P1-O3	2.02	116.72	107.57	14	1
4	A	373	PX4	C28-C27-C26	2.02	104.16	114.37	12	1
4	A	377	PX4	O1-P1-O3	2.02	116.72	107.57	2	1
4	A	405	PX4	C28-C27-C26	2.02	104.16	114.37	3	1
4	A	347	PX4	C11-C10-C9	2.02	121.09	113.69	9	1
4	A	374	PX4	C18-C17-C16	2.02	104.17	114.37	7	1
4	A	397	PX4	C30-C29-C28	2.02	104.17	114.37	3	1
4	A	401	PX4	C30-C29-C28	2.02	104.17	114.37	12	1
4	A	407	PX4	C27-C26-C25	2.02	104.17	114.37	12	1
4	A	427	PX4	C14-C13-C12	2.02	104.17	114.37	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	321	PX4	C19-C18-C17	2.02	104.18	114.37	11	1
4	A	329	PX4	O3-C1-C2	2.01	119.34	109.65	3	1
4	A	338	PX4	C20-C19-C18	2.02	104.18	114.37	3	1
4	A	338	PX4	O7-C7-C6	2.01	115.57	108.34	14	1
4	A	341	PX4	C36-C35-C34	2.01	99.76	113.36	6	1
4	A	386	PX4	C13-C12-C11	2.02	104.18	114.37	13	1
4	A	363	PX4	C28-C27-C26	2.01	104.19	114.37	13	1
4	A	395	PX4	C15-C14-C13	2.01	104.19	114.37	3	1
4	A	335	PX4	C20-C19-C18	2.01	104.20	114.37	4	1
4	A	383	PX4	C14-C13-C12	2.01	104.19	114.37	10	1
4	A	390	PX4	O3-C1-C2	2.01	119.33	109.65	1	1
4	A	312	PX4	C16-C15-C14	2.01	104.21	114.37	8	1
4	A	315	PX4	C5-N1-C3	2.01	103.70	108.98	12	1
4	A	332	PX4	C29-C28-C27	2.01	104.22	114.37	9	1
4	A	389	PX4	C30-C29-C28	2.01	104.21	114.37	5	1
4	A	318	PX4	C20-C19-C18	2.01	104.22	114.37	2	1
4	A	319	PX4	C14-C13-C12	2.01	104.22	114.37	1	1
4	A	332	PX4	C31-C30-C29	2.01	104.23	114.37	13	1
4	A	341	PX4	C26-C25-C24	2.01	105.75	113.13	14	1
4	A	349	PX4	C14-C13-C12	2.01	104.23	114.37	12	1
4	A	377	PX4	C5-N1-C2	2.01	117.88	109.91	10	1
4	A	392	PX4	C16-C15-C14	2.01	104.23	114.37	4	1
4	A	396	PX4	O1-P1-O4	2.01	116.66	107.57	13	1
4	A	420	PX4	C17-C16-C15	2.01	104.23	114.37	8	1
4	A	317	PX4	C33-C32-C31	2.00	104.23	114.37	8	1
4	A	429	PX4	C17-C16-C15	2.01	104.23	114.37	8	1
4	A	331	PX4	C15-C14-C13	2.00	104.24	114.37	5	1
4	A	340	PX4	C18-C17-C16	2.00	104.24	114.37	4	1
4	A	346	PX4	O7-C7-C6	2.00	115.53	108.34	6	1
4	A	332	PX4	O3-C1-C2	2.00	119.28	109.65	8	1
4	A	364	PX4	O5-C9-C10	2.00	117.94	111.83	5	1
4	A	418	PX4	C13-C12-C11	2.00	104.24	114.37	1	1
4	A	326	PX4	O3-C1-C2	2.00	119.28	109.65	1	1
4	A	333	PX4	C32-C31-C30	2.00	104.25	114.37	8	1
4	A	341	PX4	C17-C16-C15	2.00	104.25	114.37	14	1
4	A	349	PX4	O8-C23-C24	2.00	115.95	123.78	2	1
4	A	383	PX4	C25-C24-C23	2.00	121.03	113.69	3	1
4	A	393	PX4	C34-C33-C32	2.00	104.25	114.37	2	1
4	A	337	PX4	C15-C14-C13	2.00	104.25	114.37	7	1
4	A	352	PX4	C19-C18-C17	2.00	104.25	114.37	7	1
4	A	423	PX4	C29-C28-C27	2.00	104.25	114.37	11	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	428	PX4	C18-C17-C16	2.00	104.25	114.37	4	1

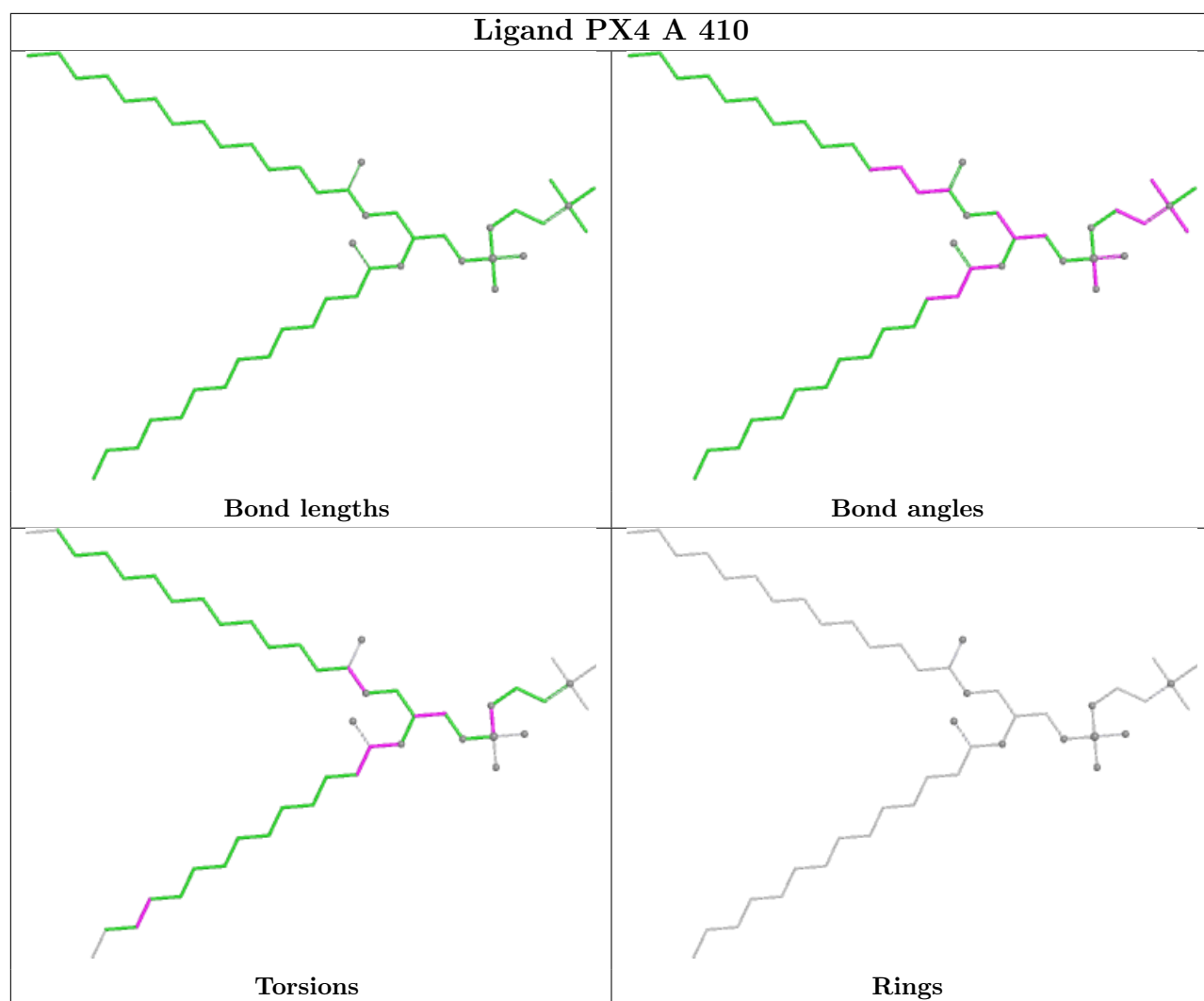
There are no chirality outliers.

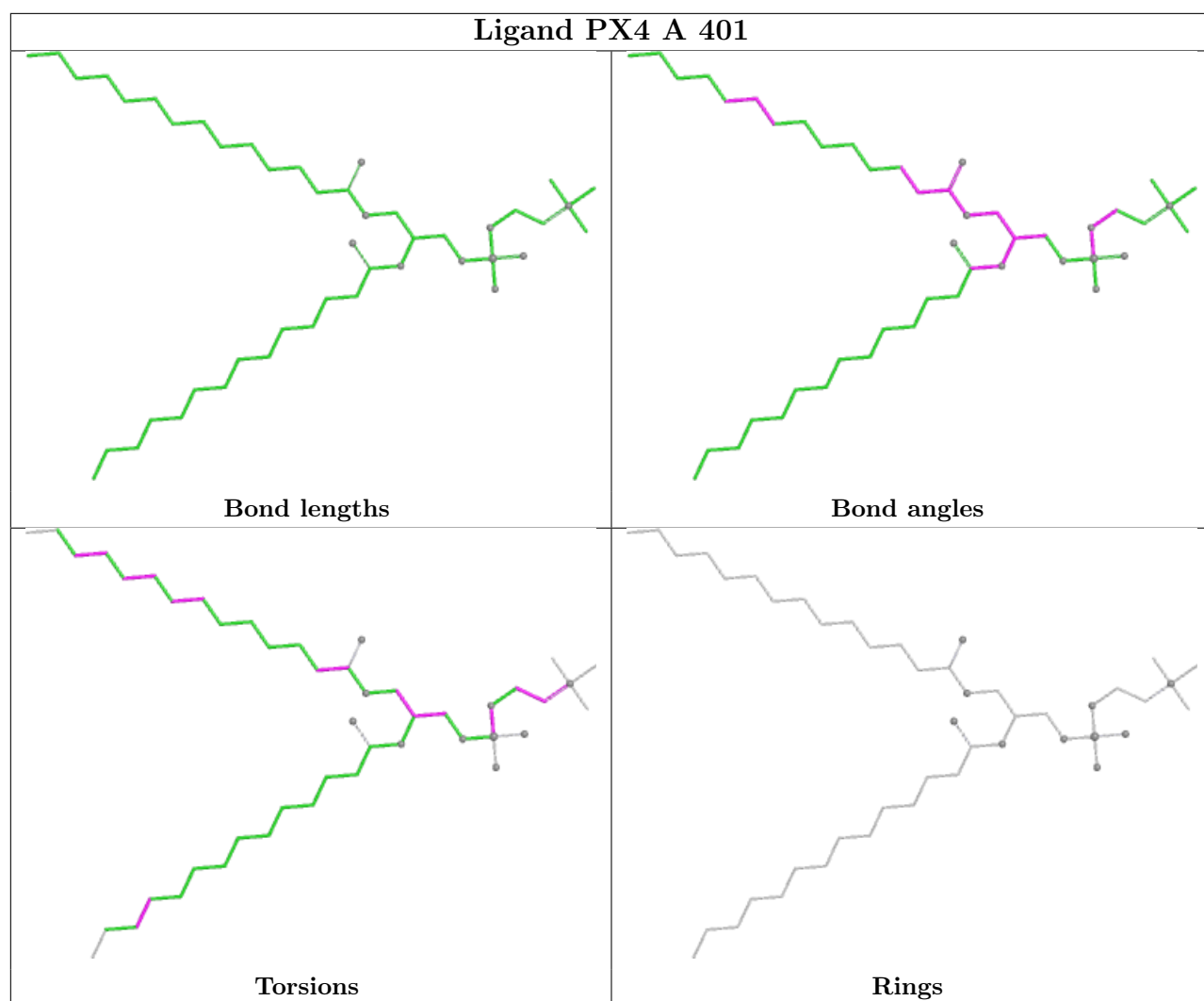
All unique torsion outliers are listed below.

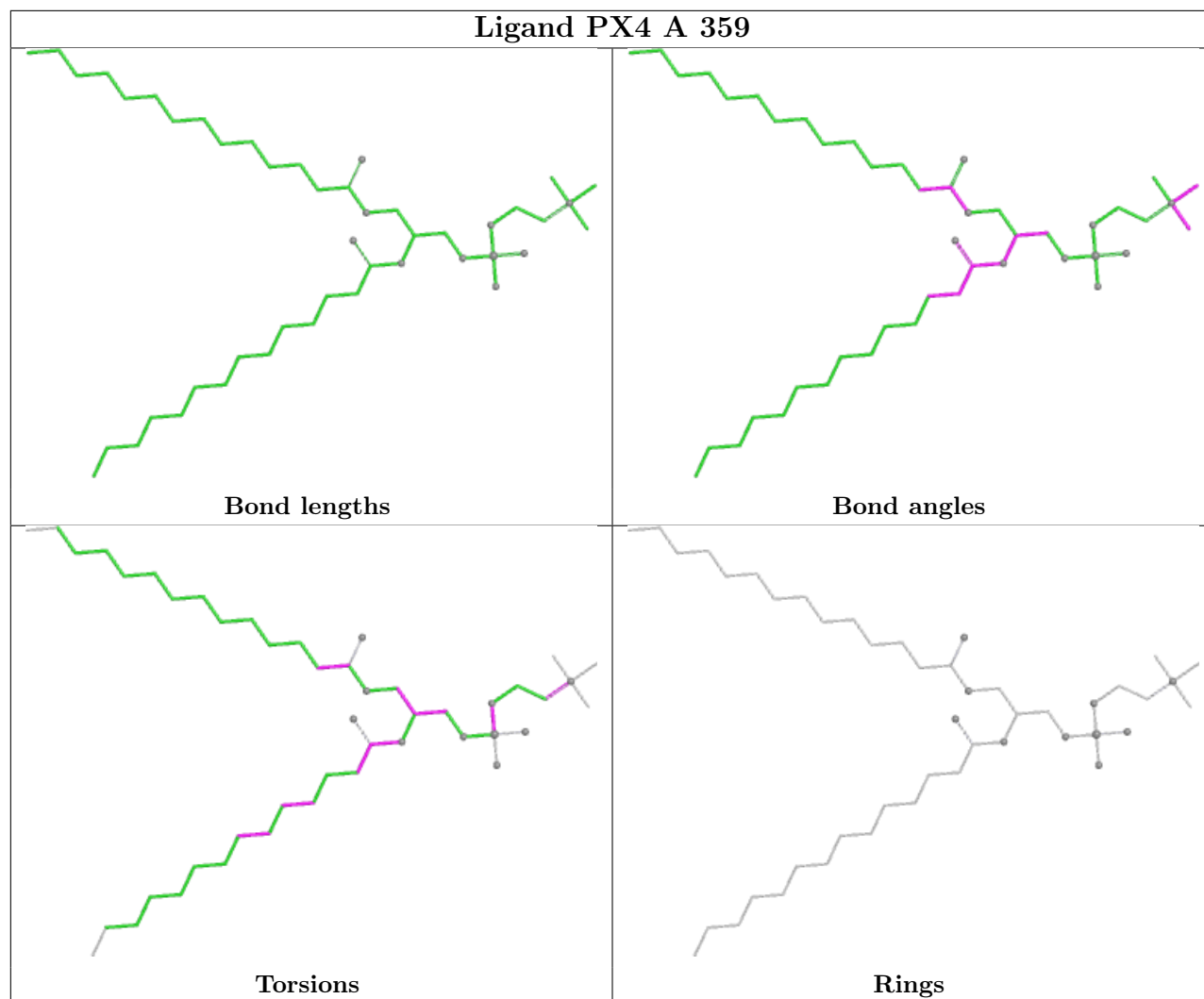
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	335	PX4	O8-C23-O7-C7	2

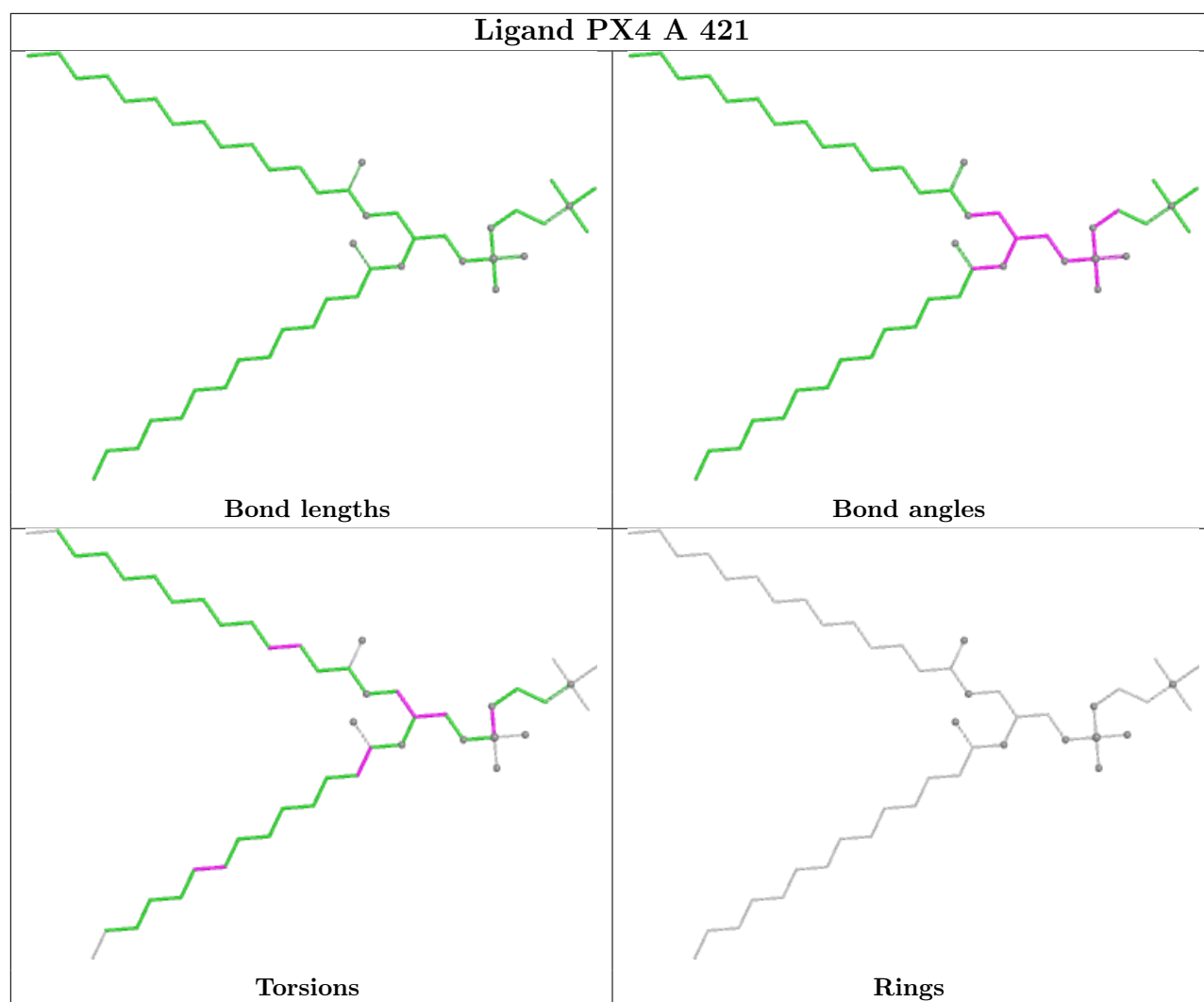
There are no ring outliers.

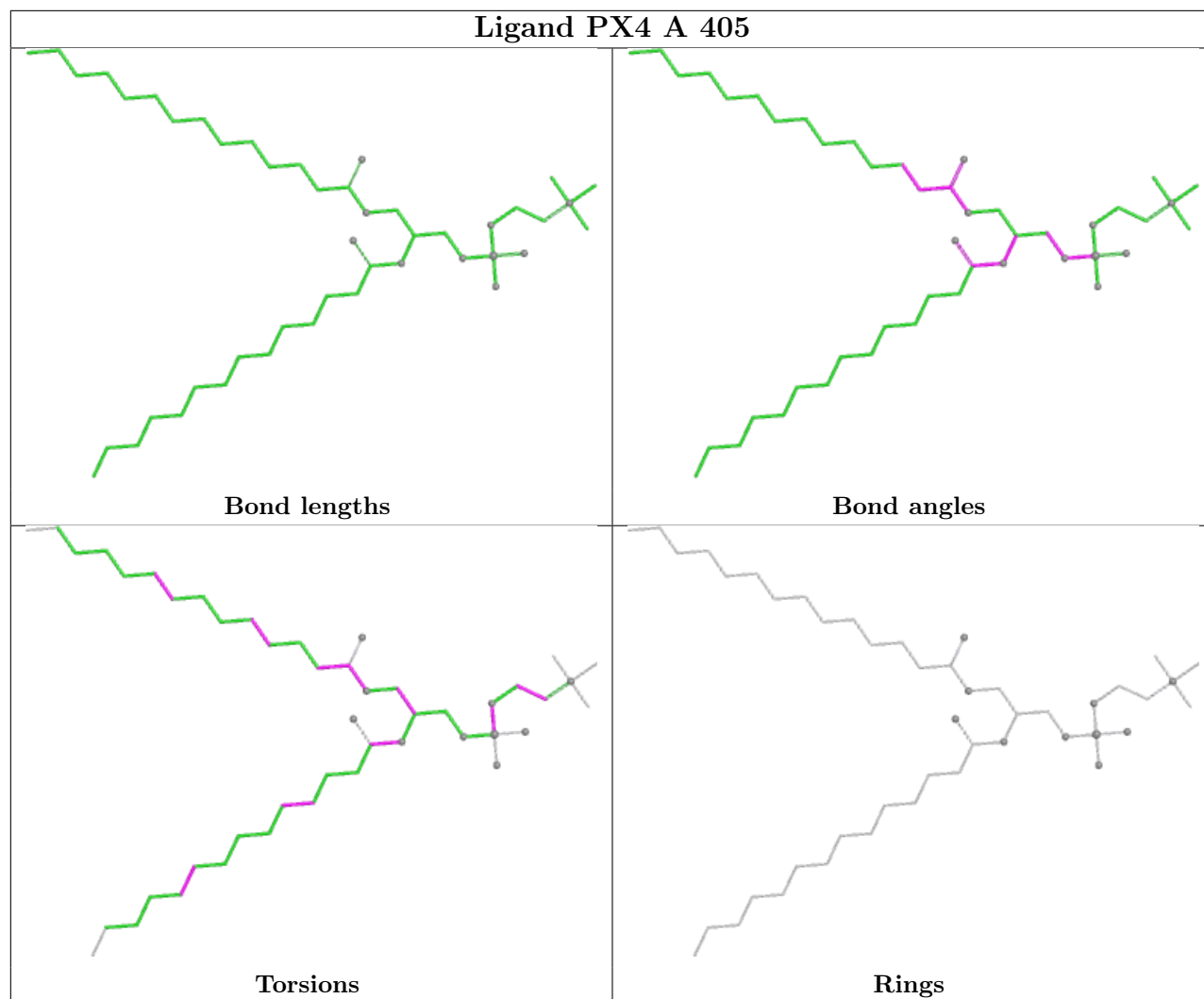
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

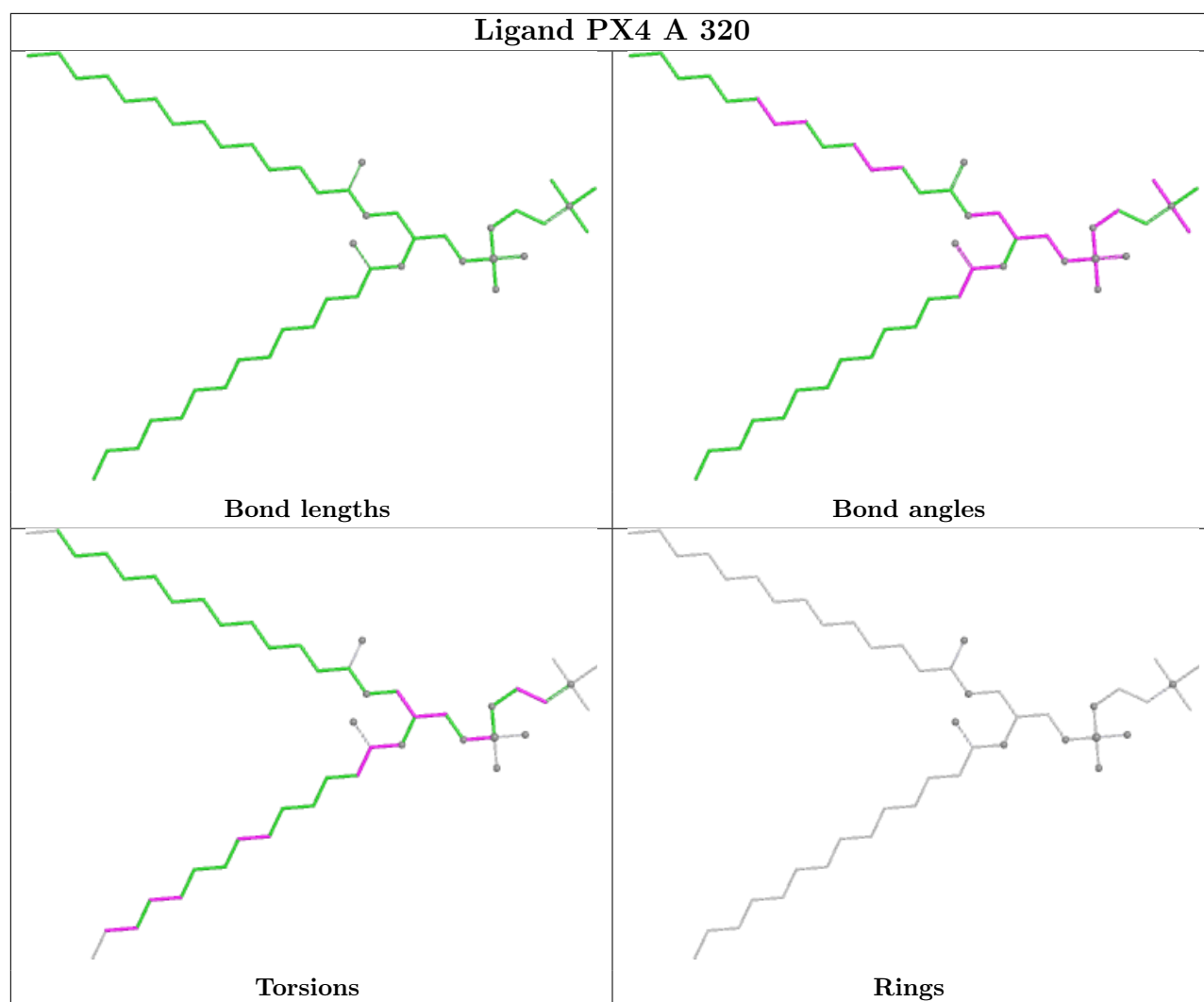


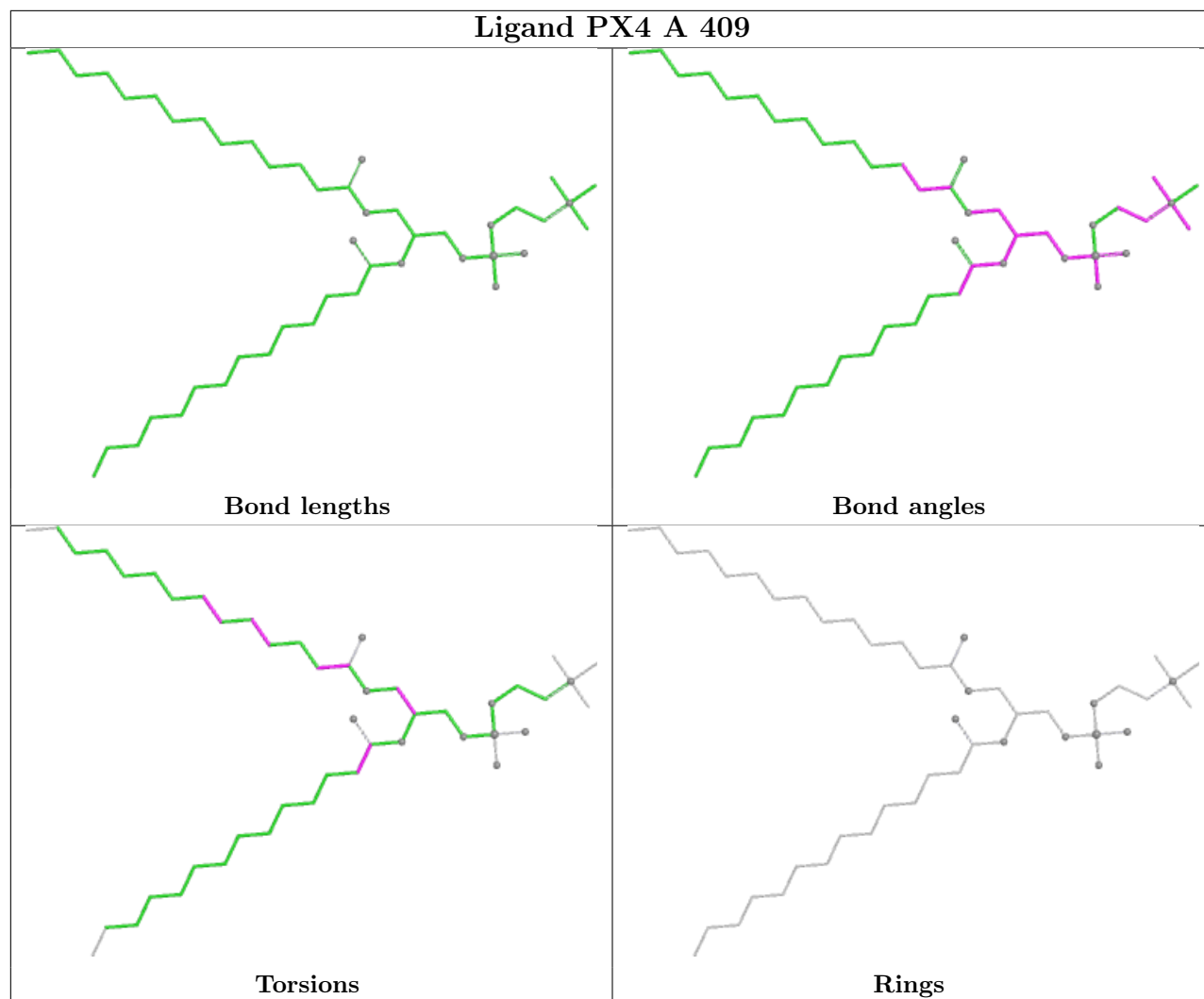


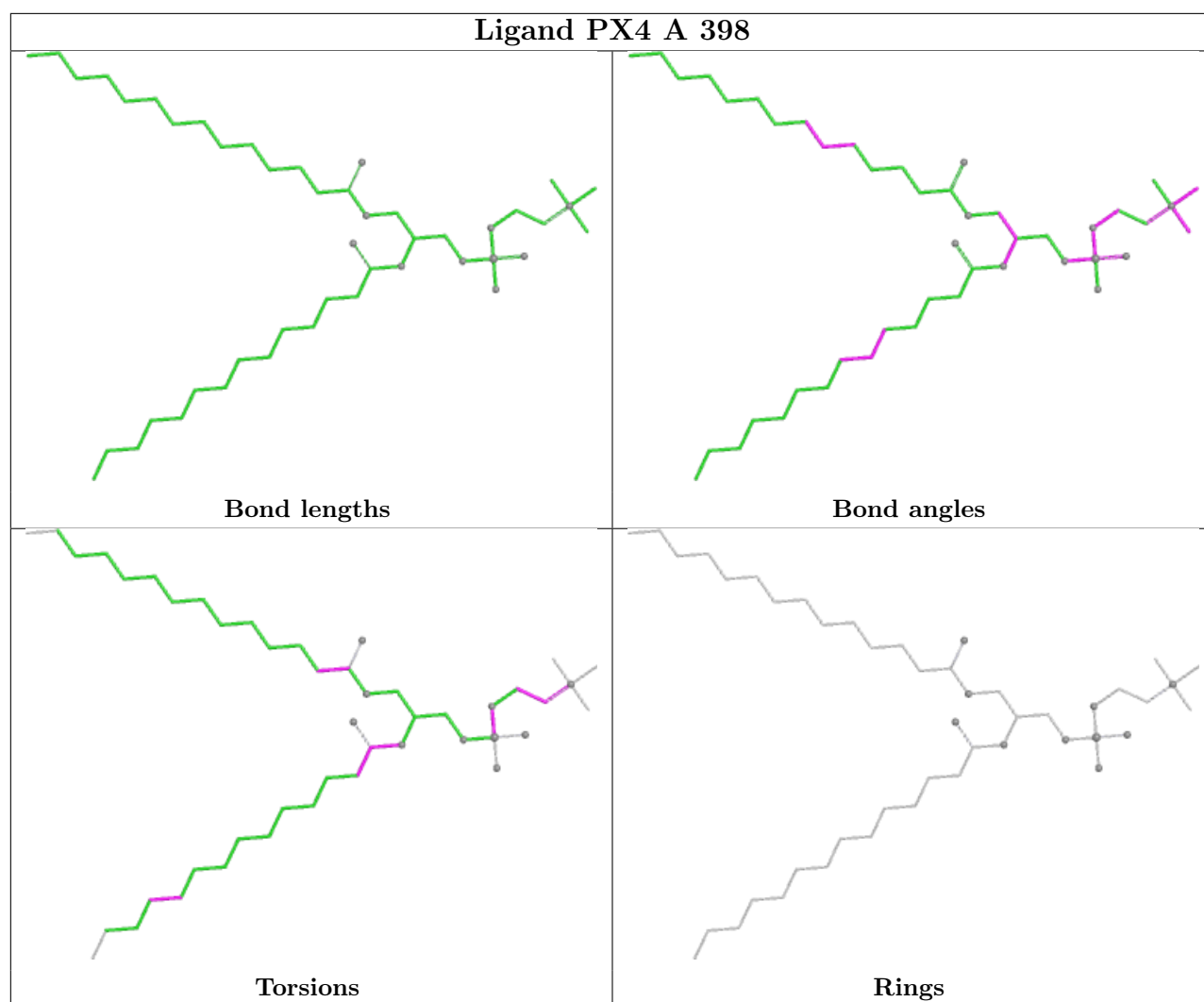


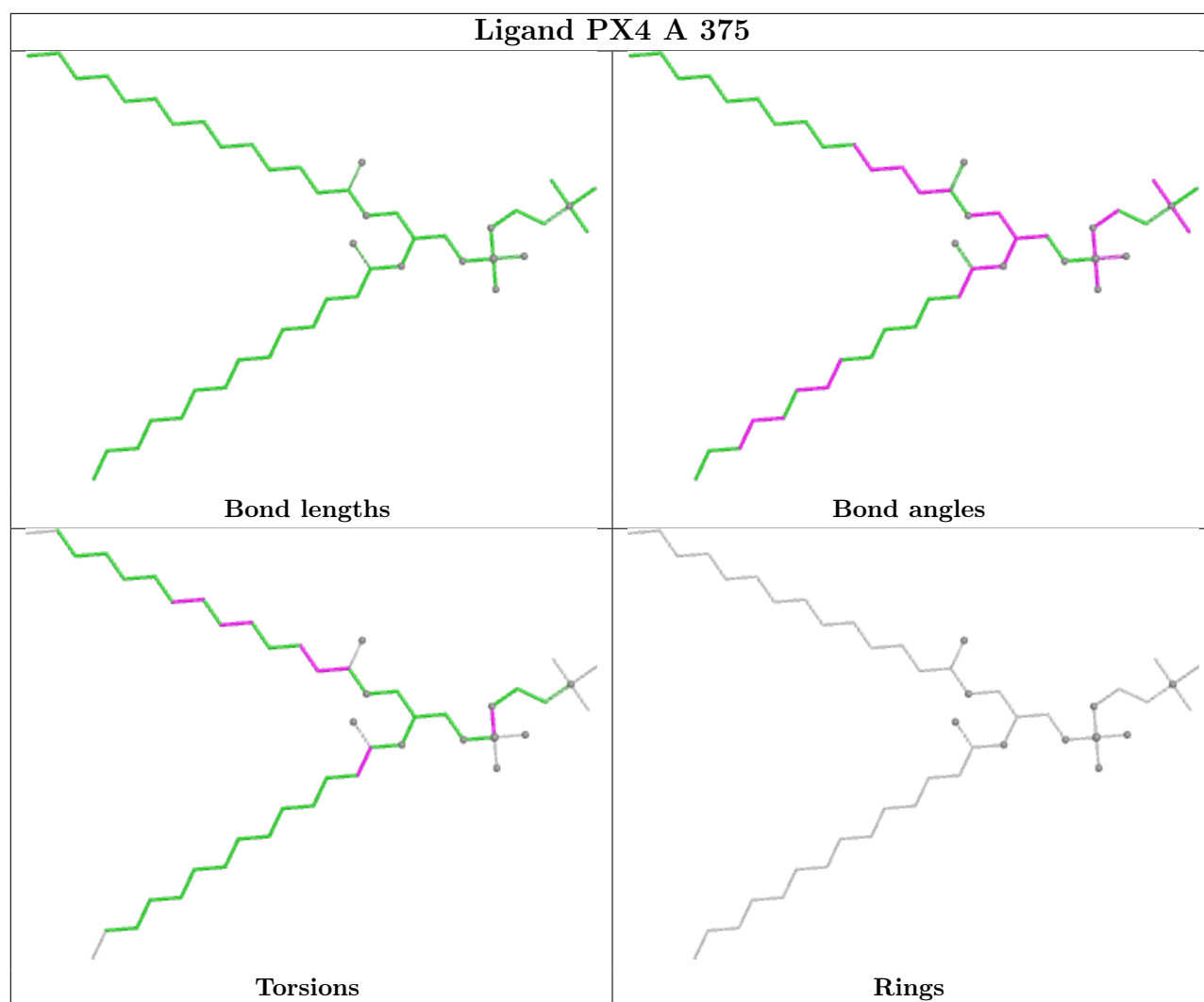


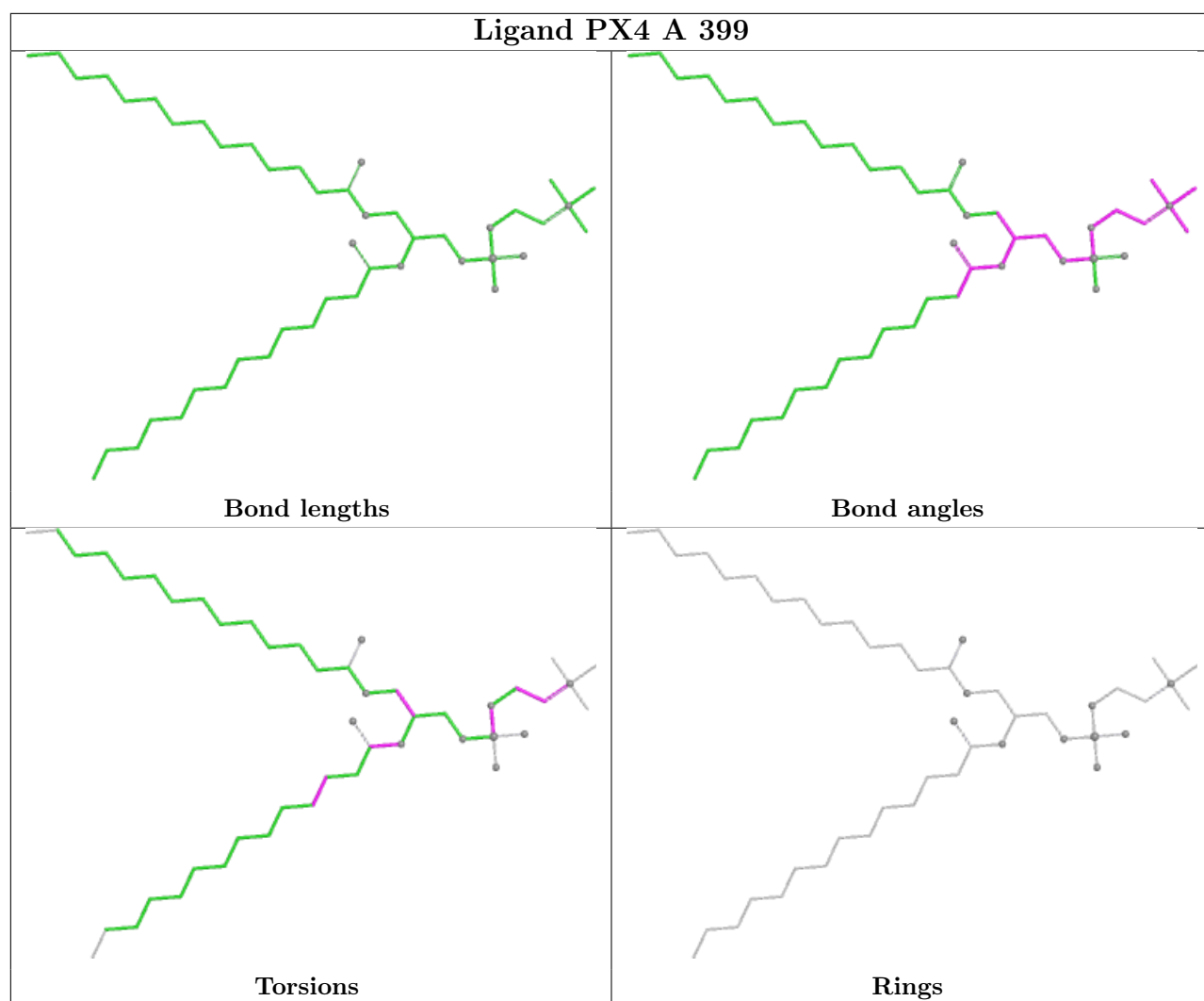


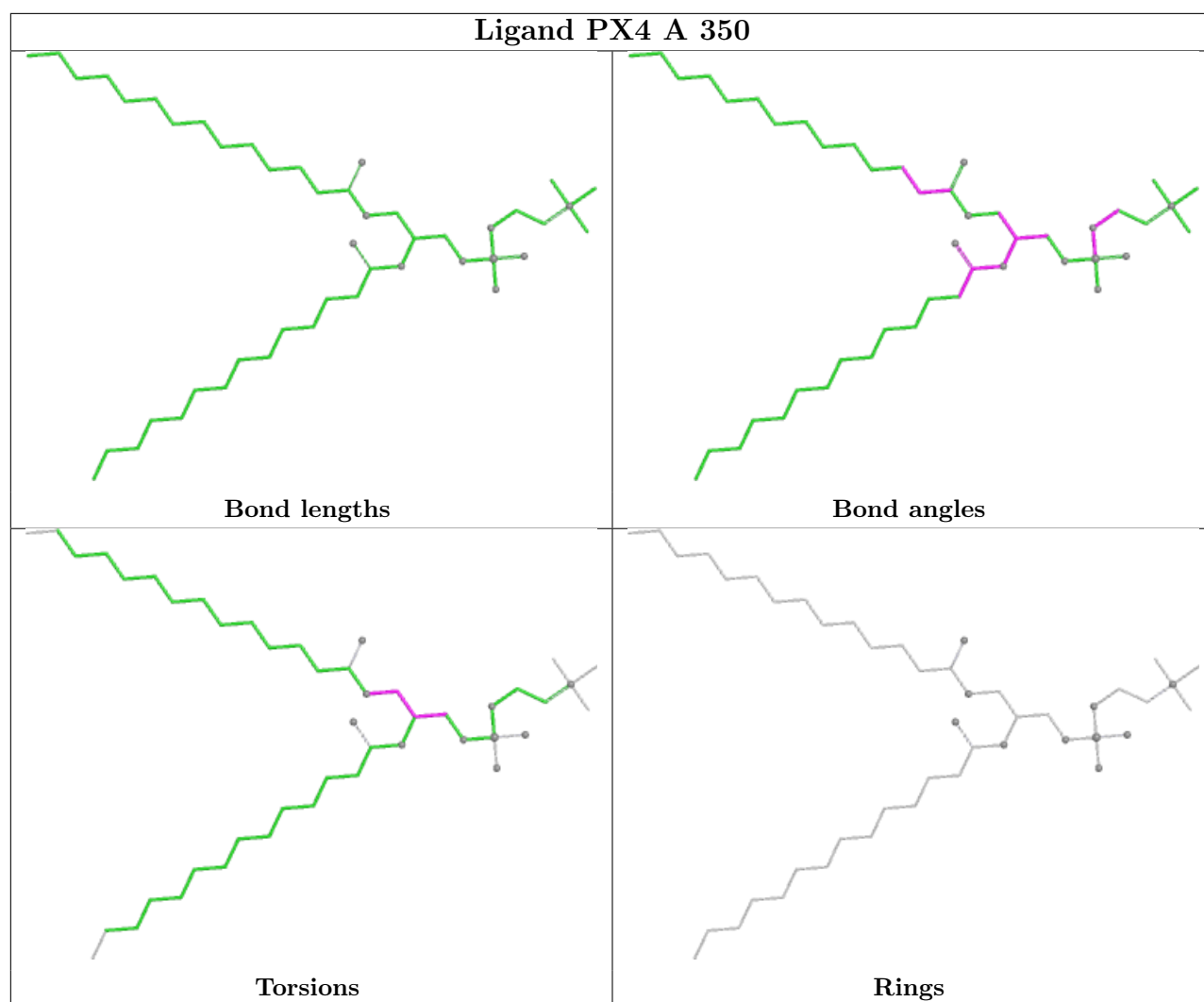


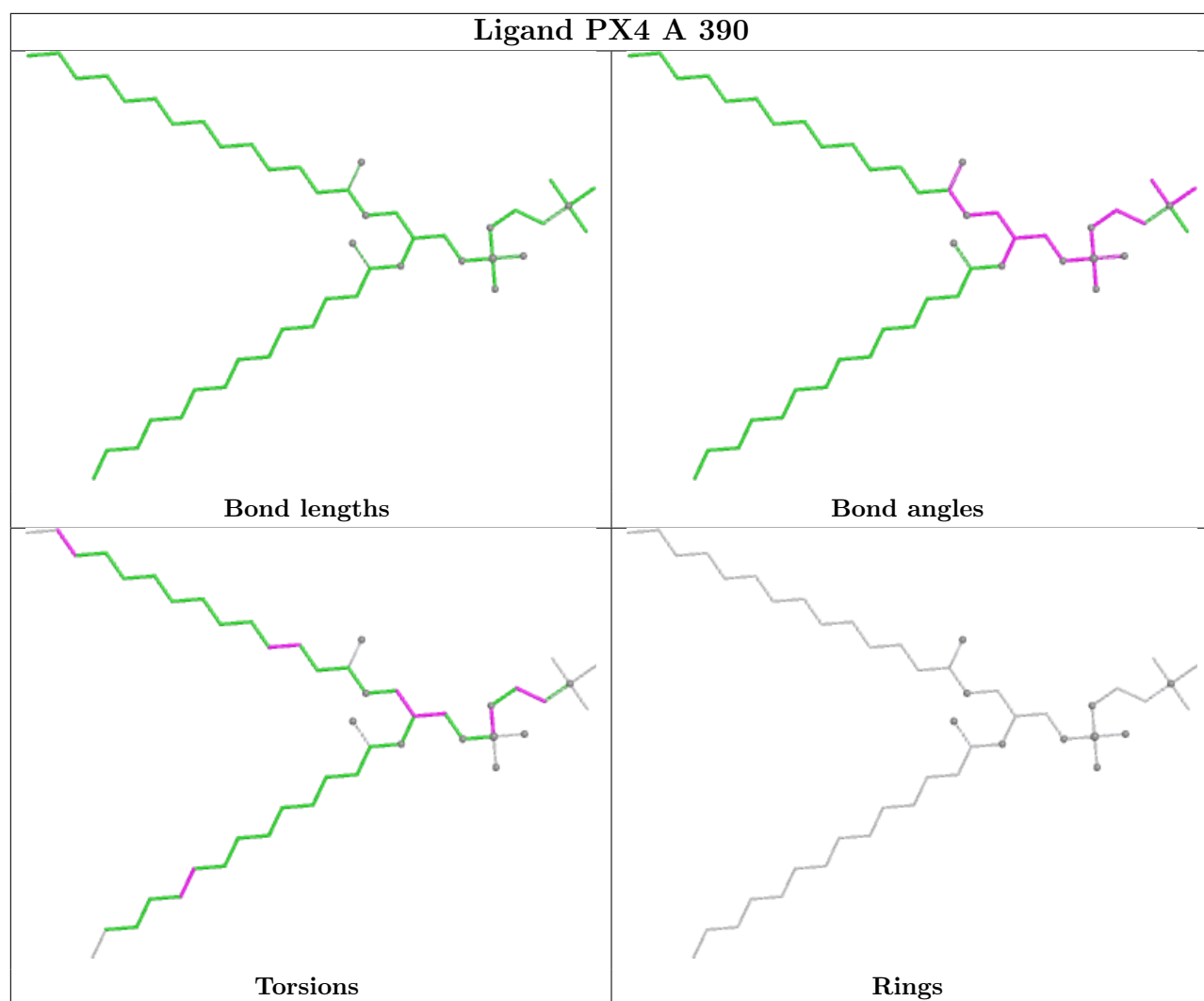


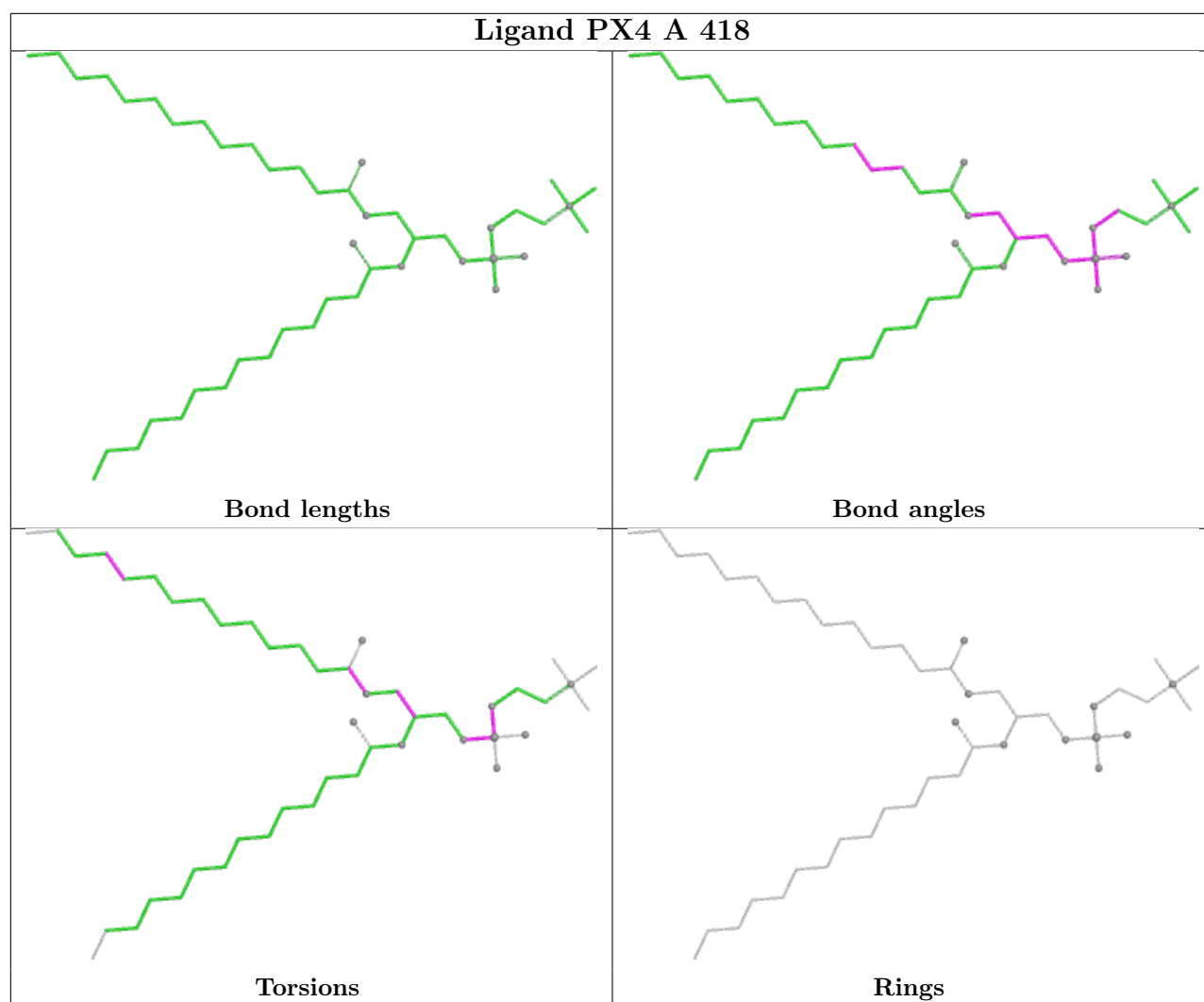


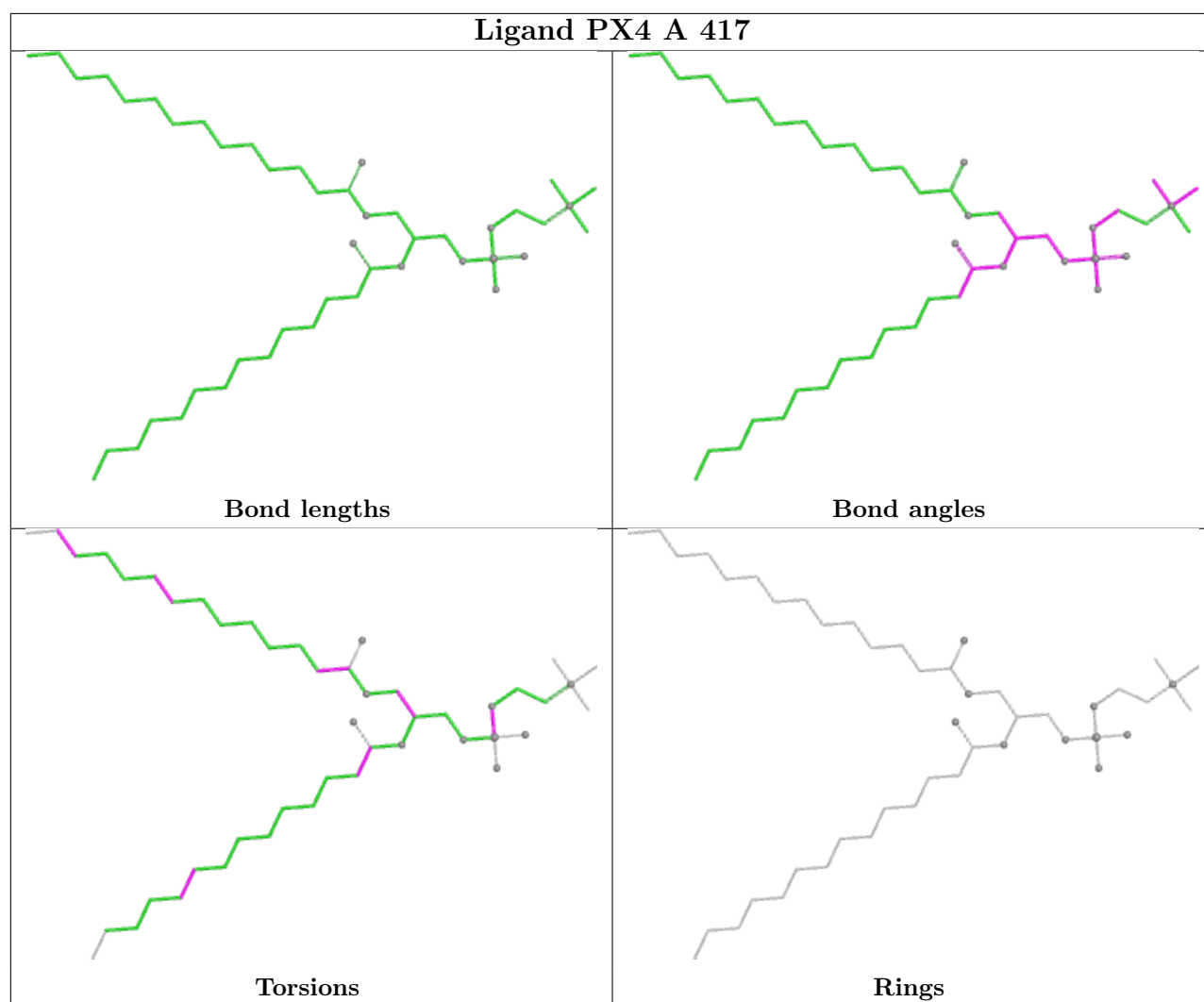


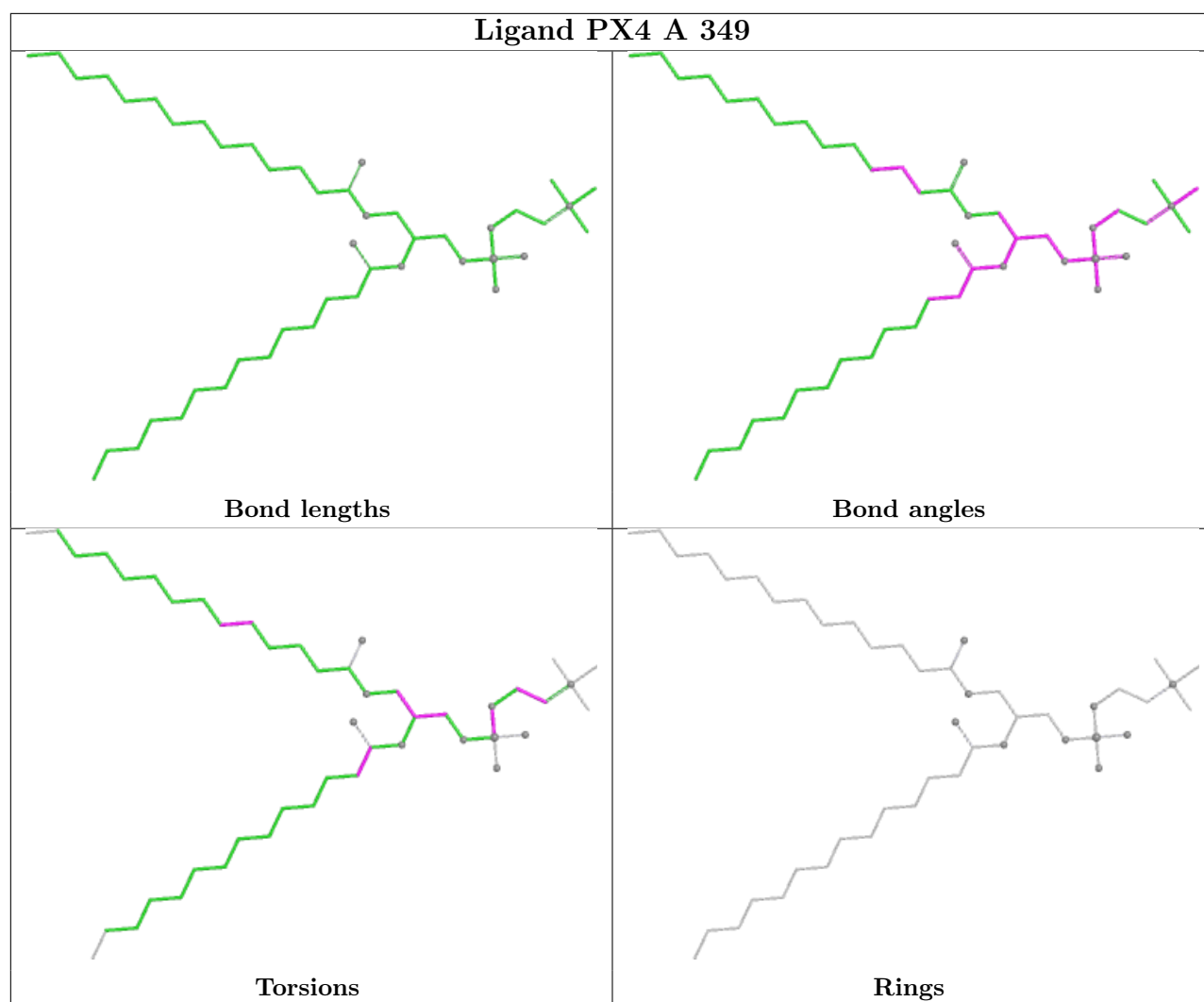


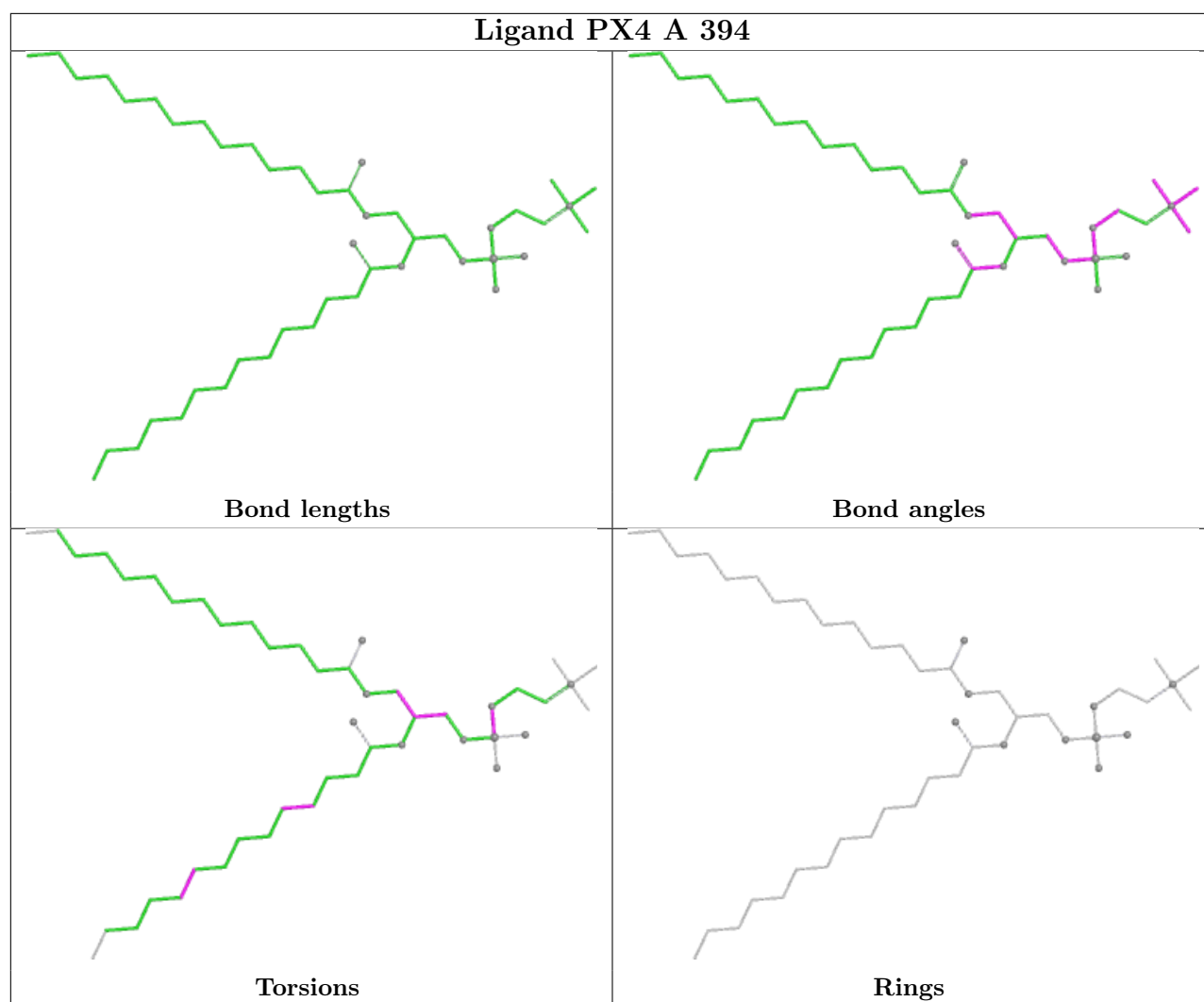


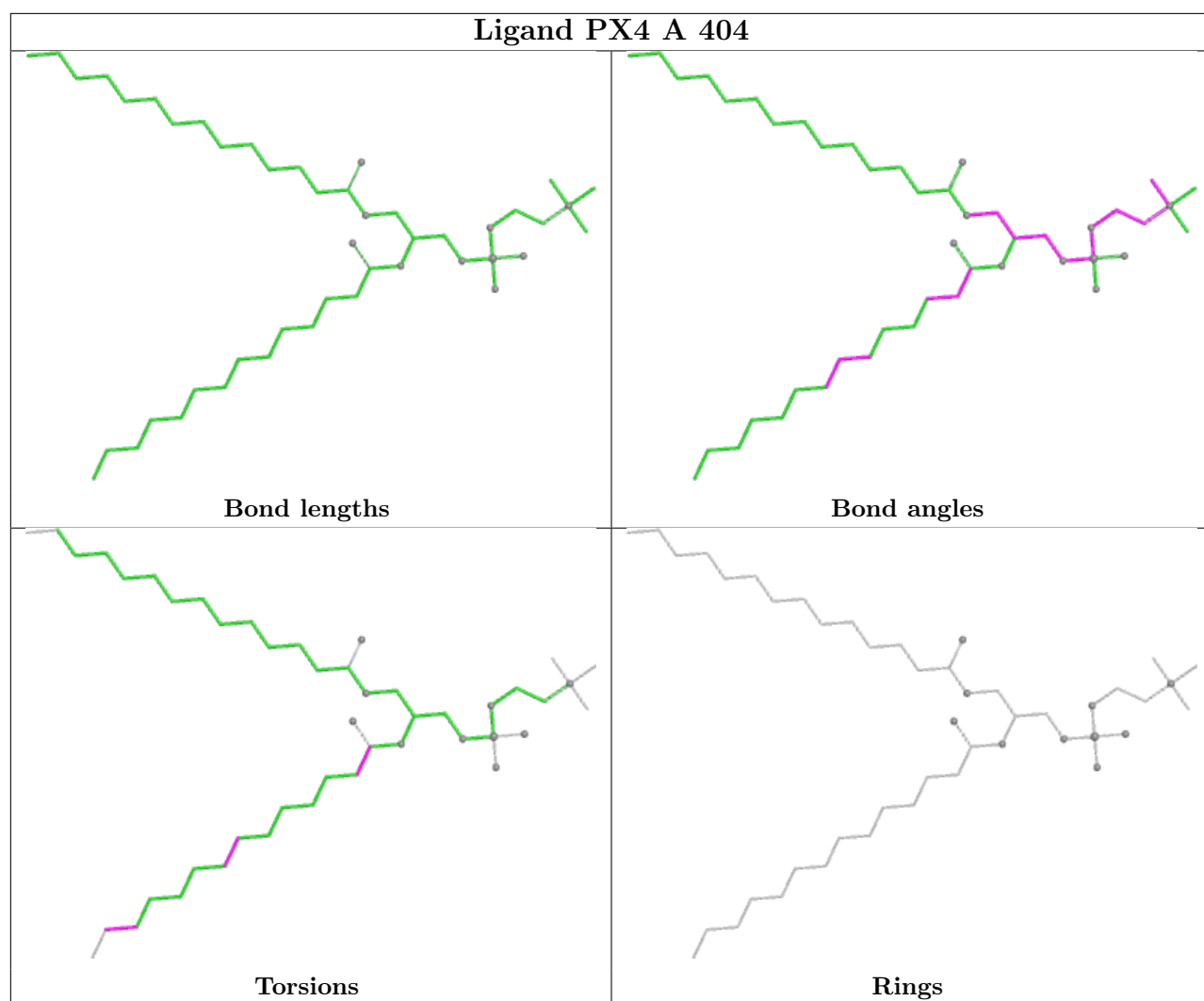


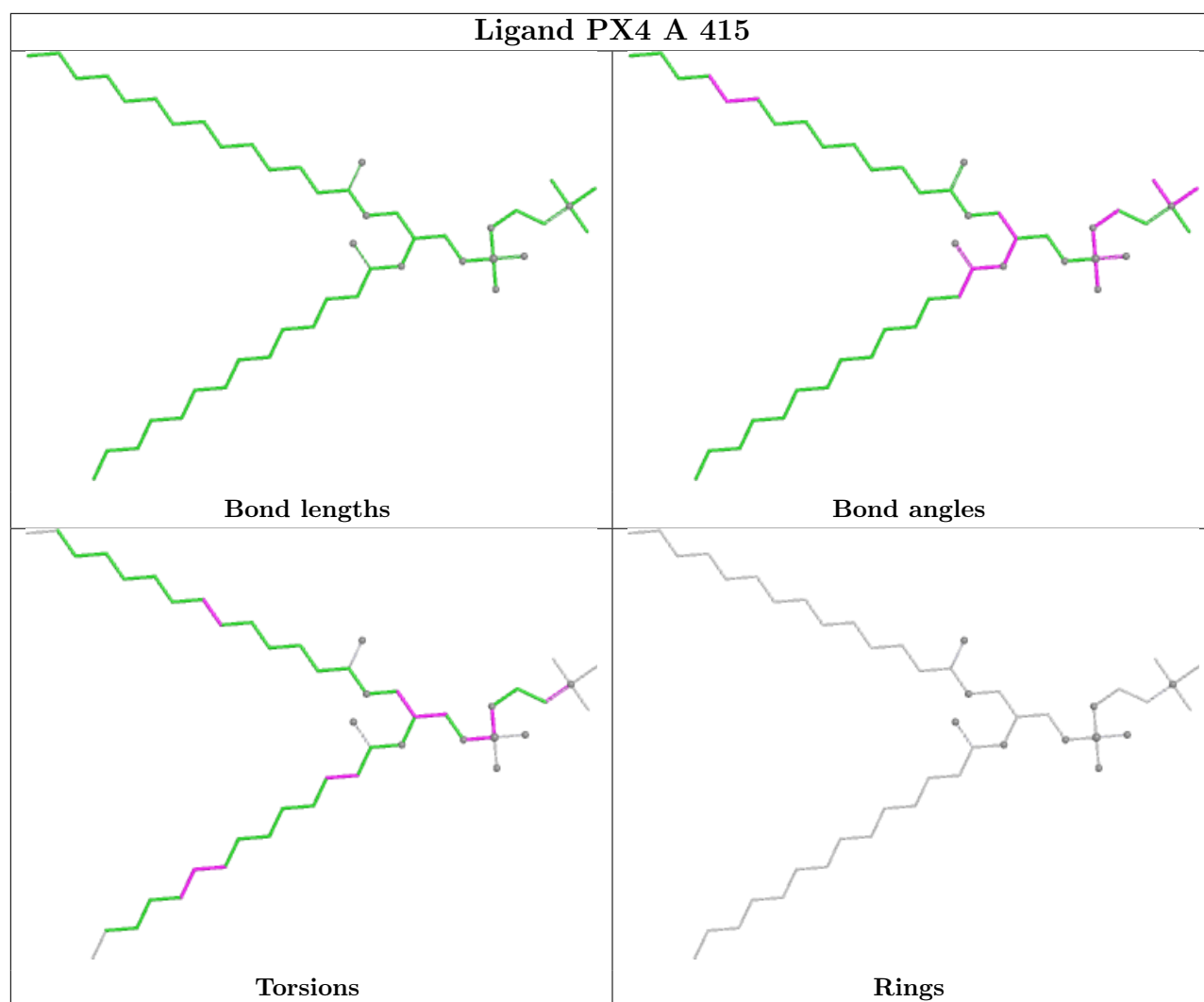


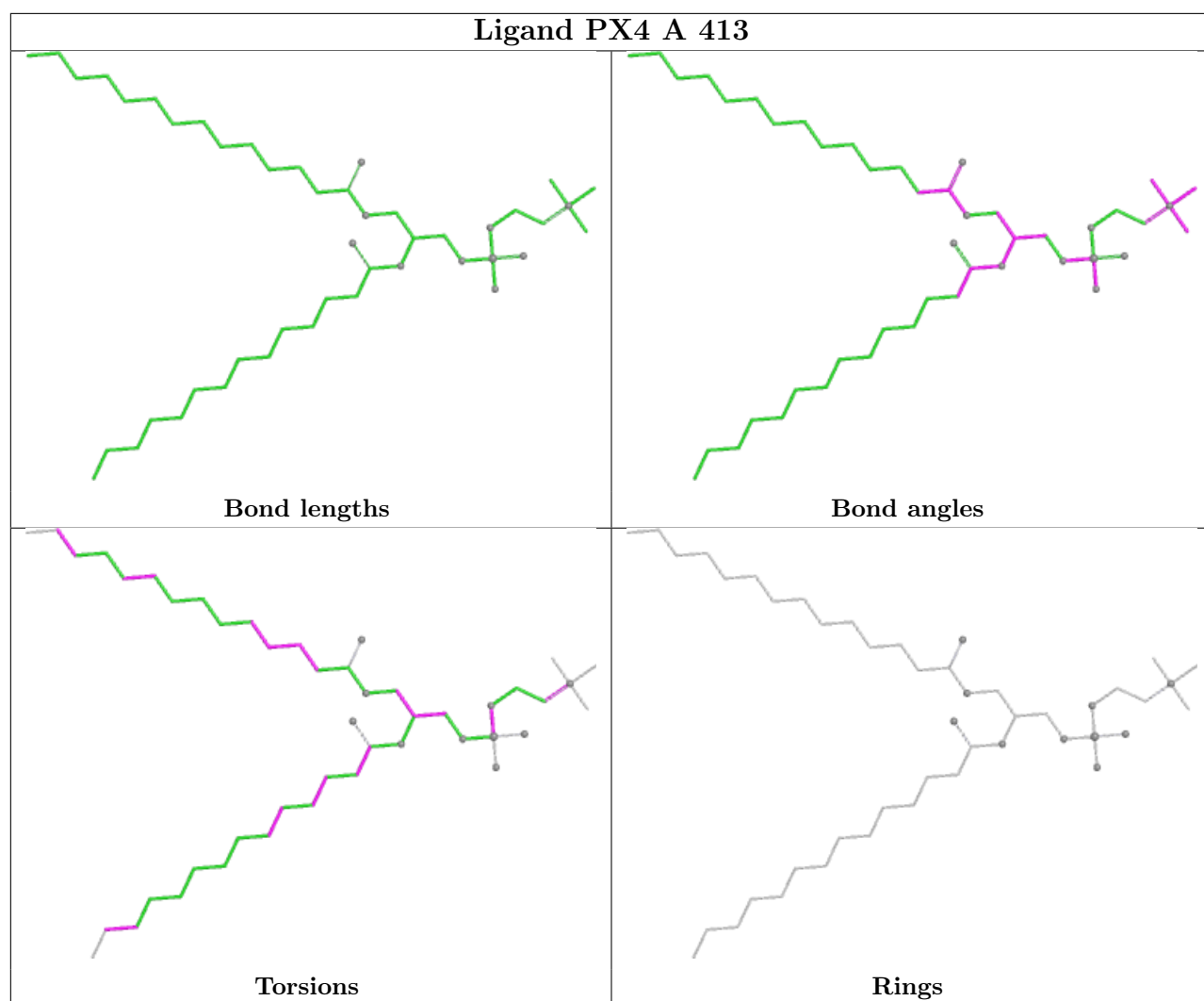


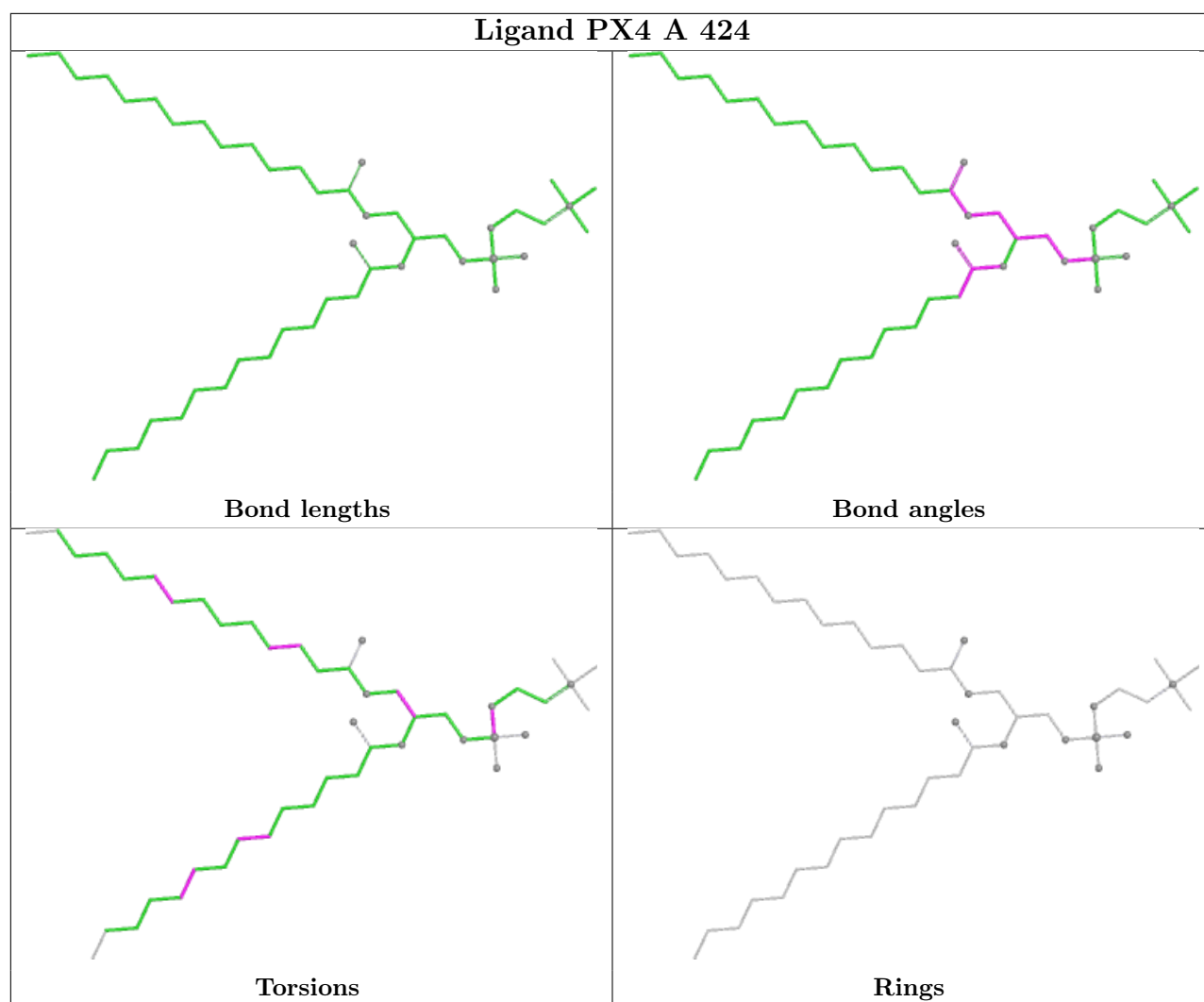


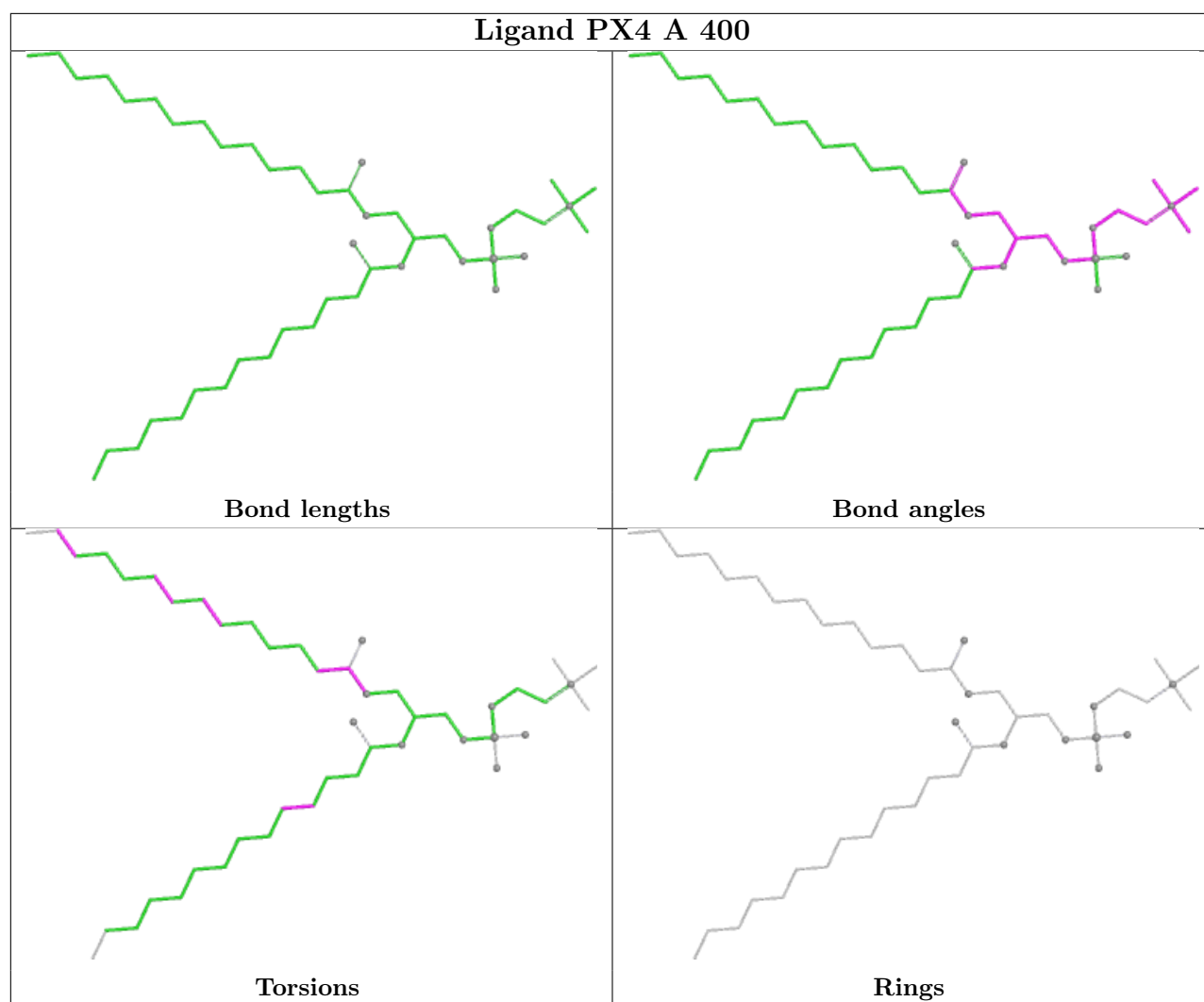


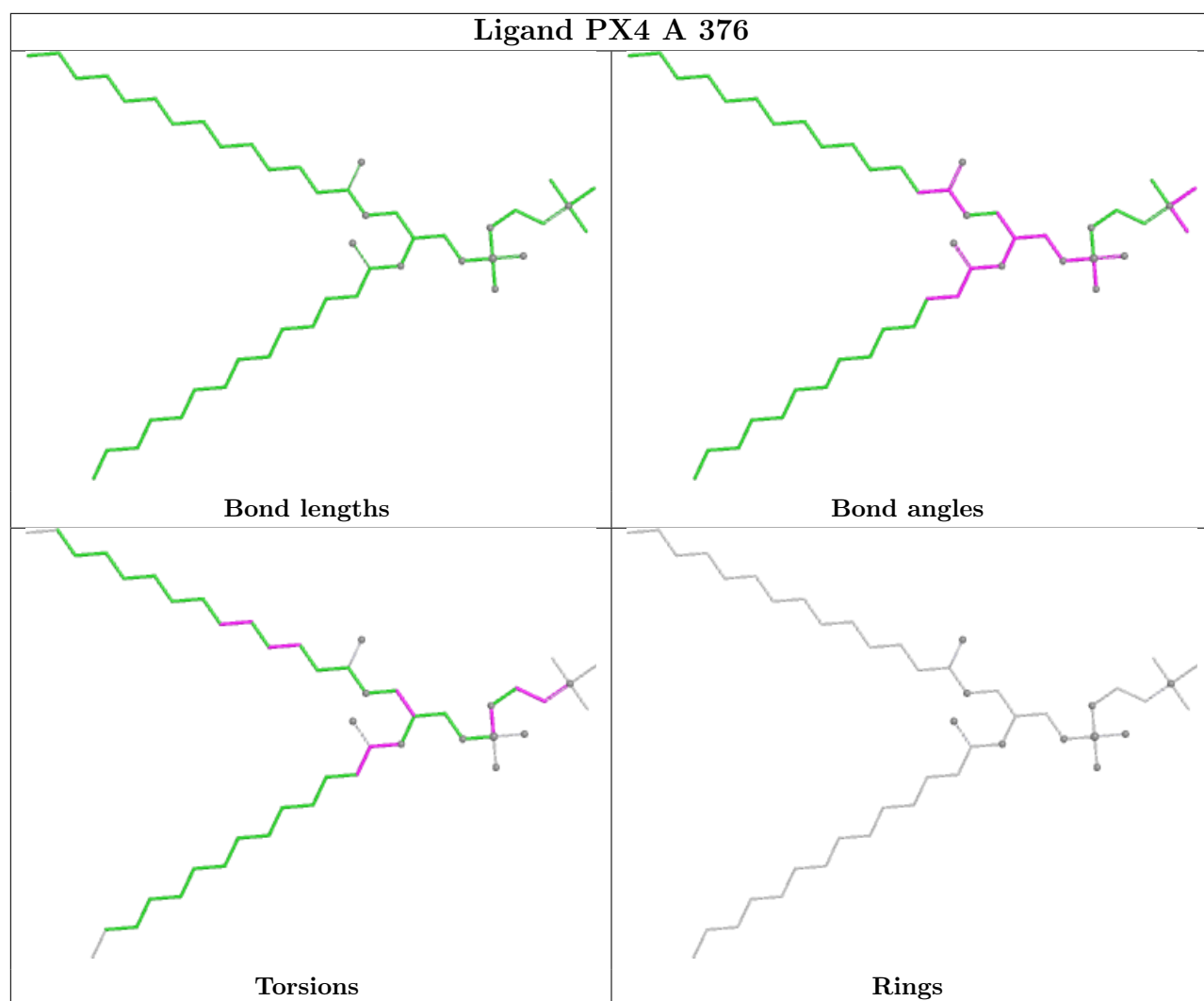


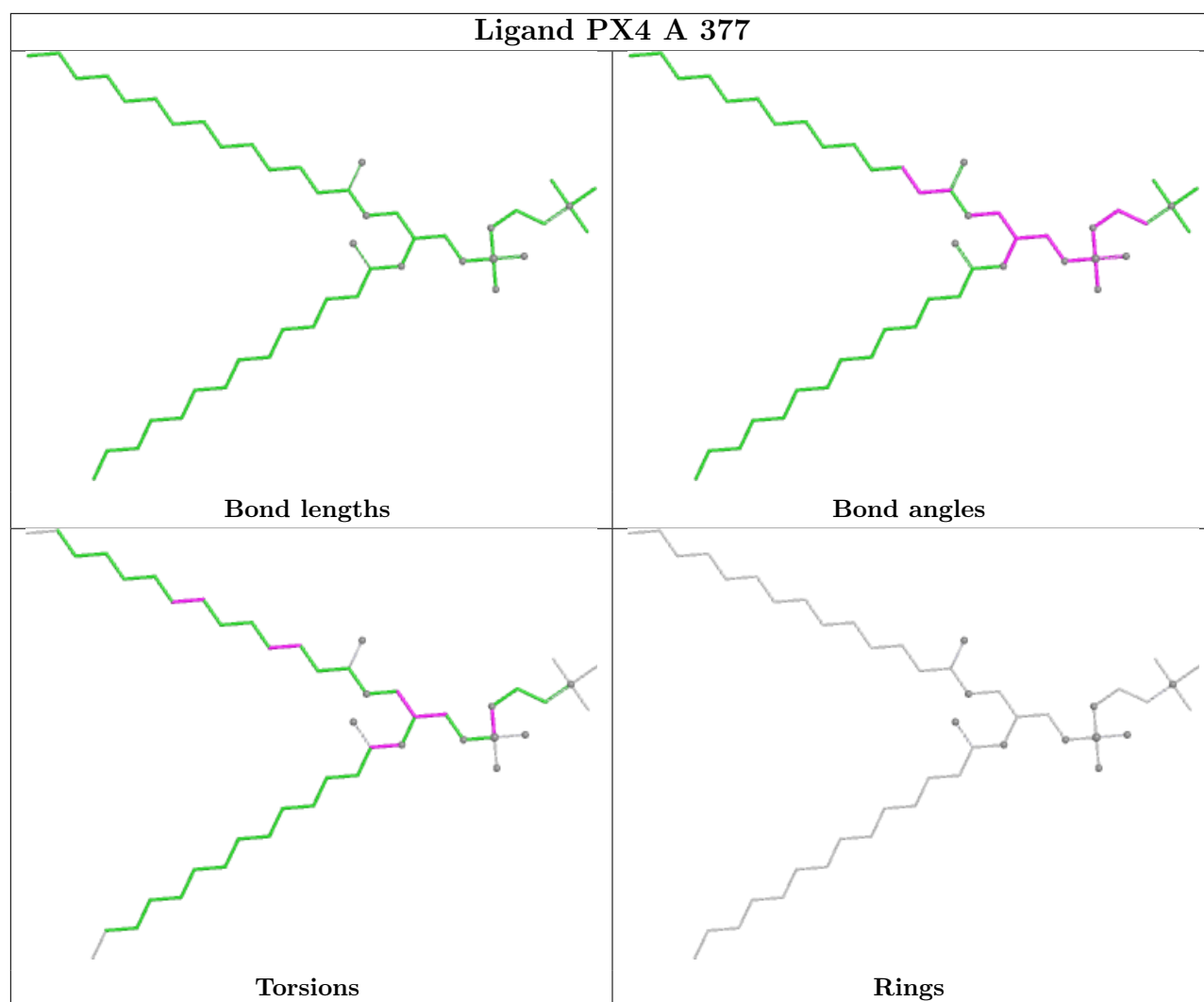


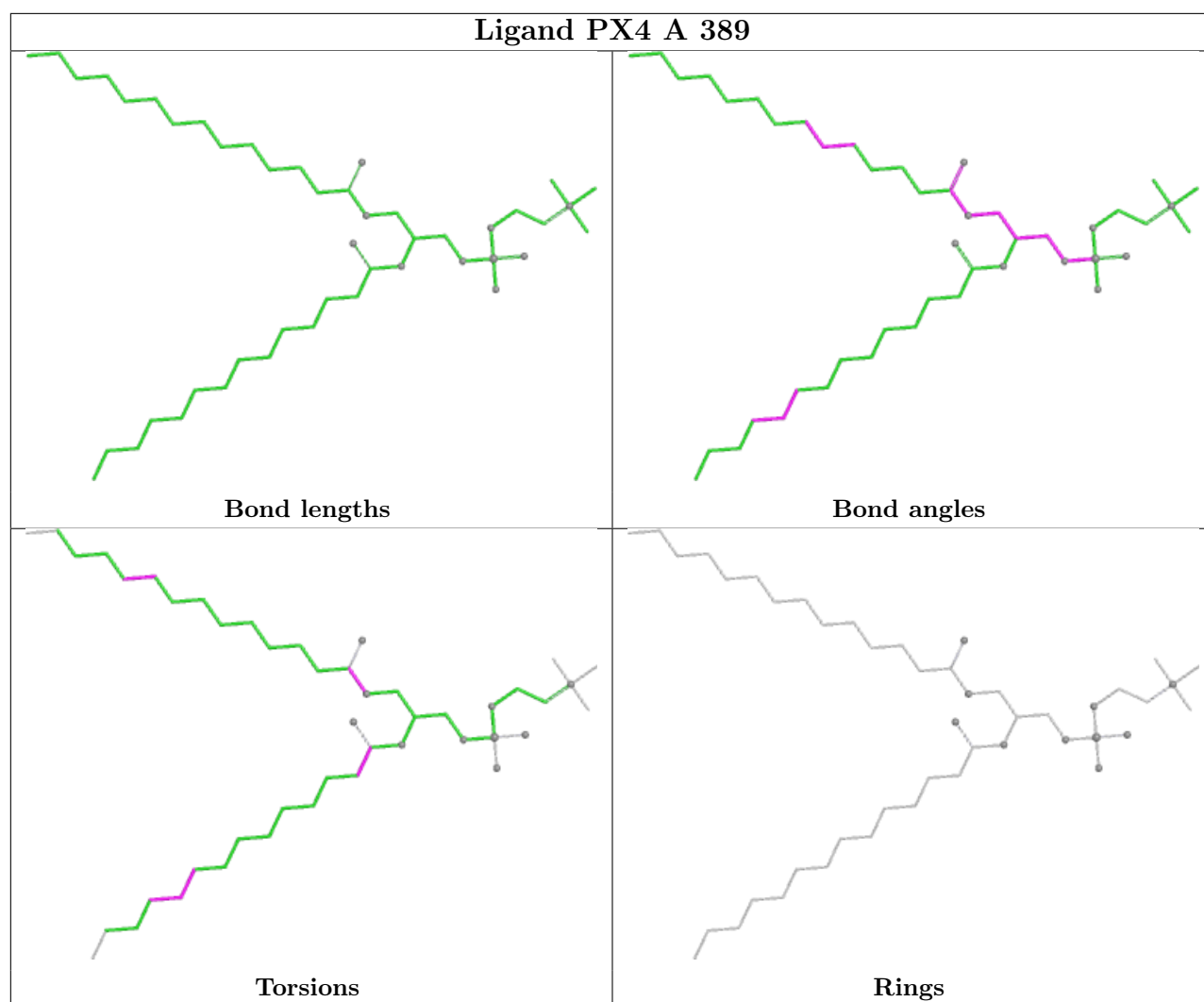


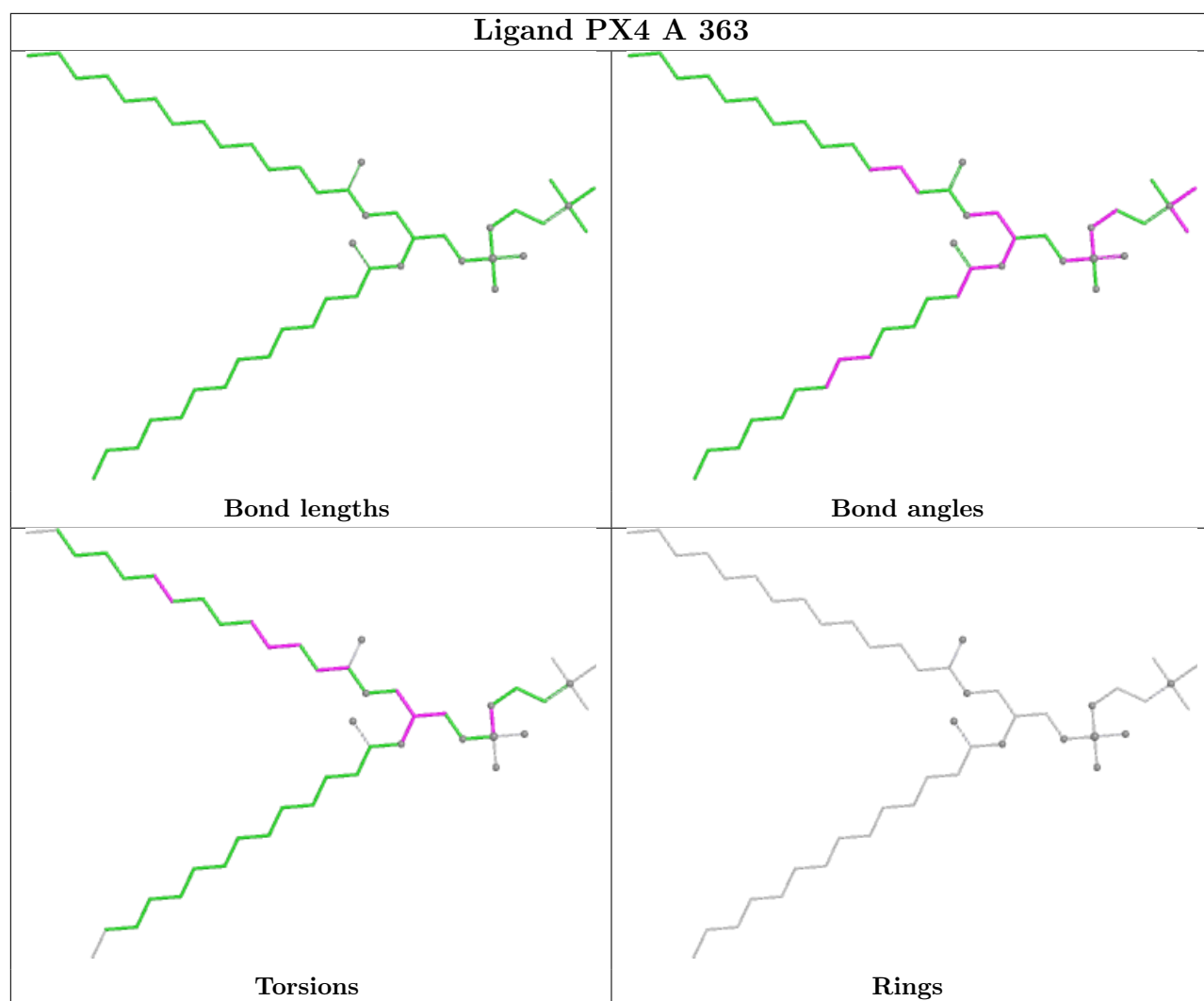


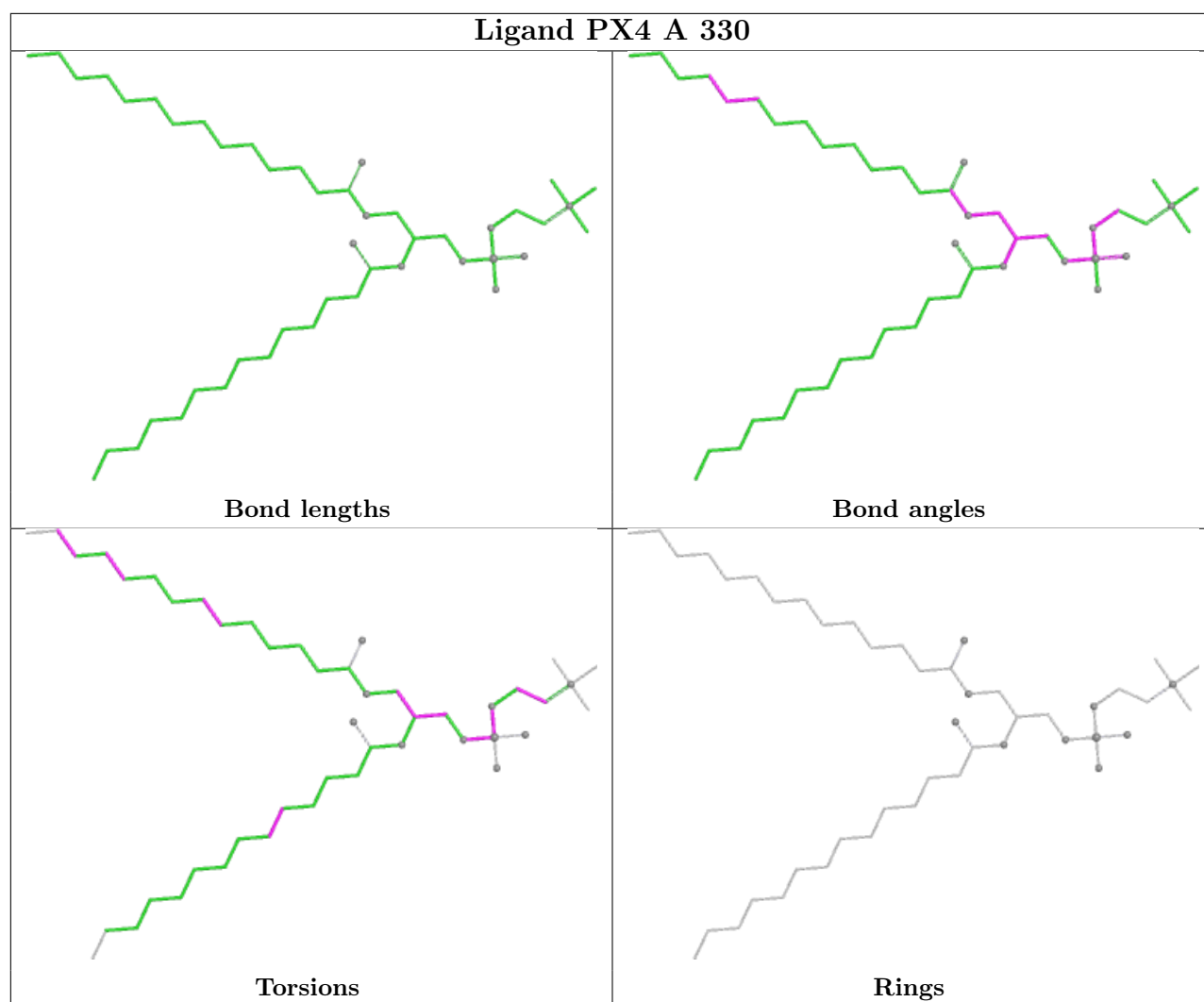


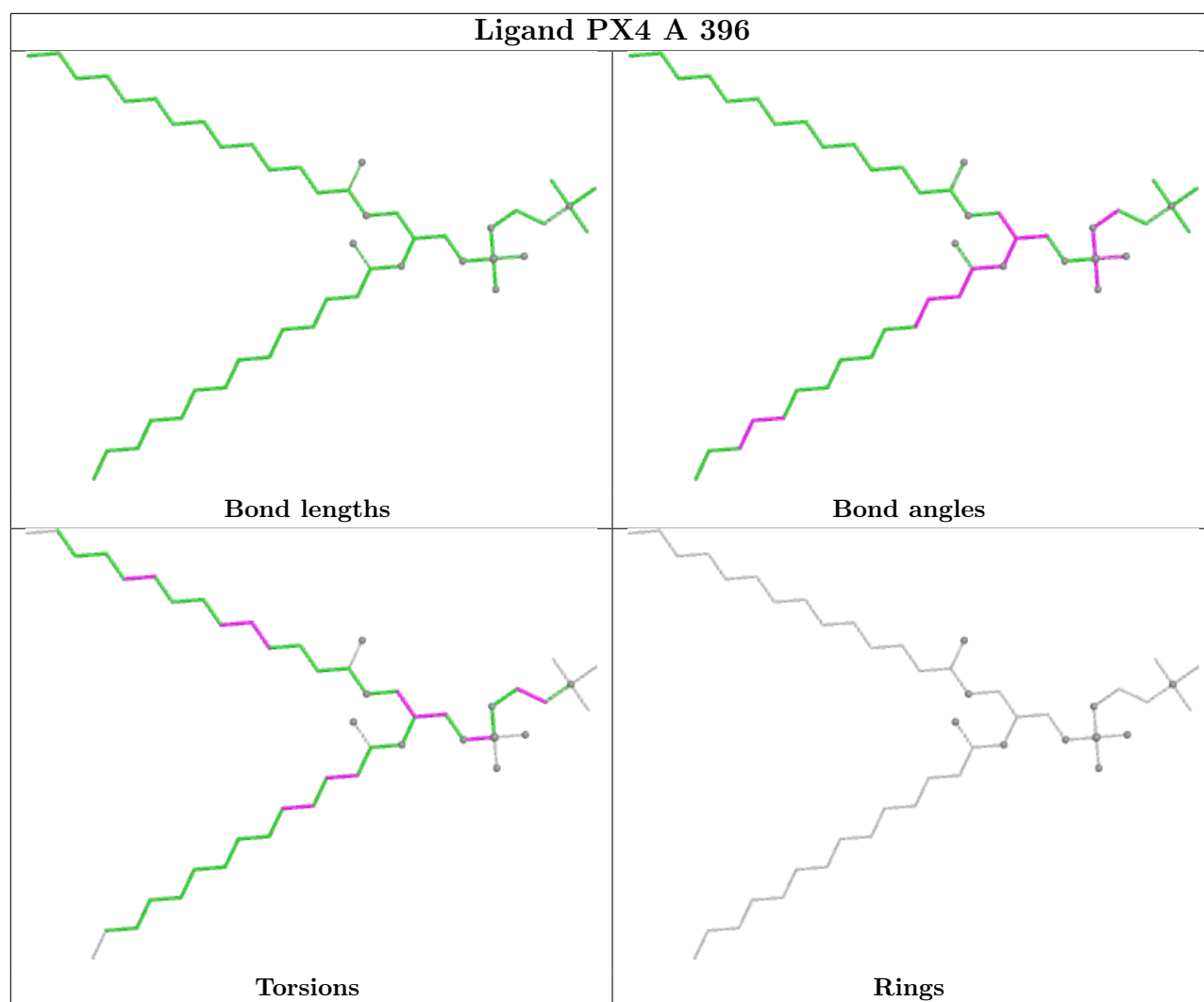


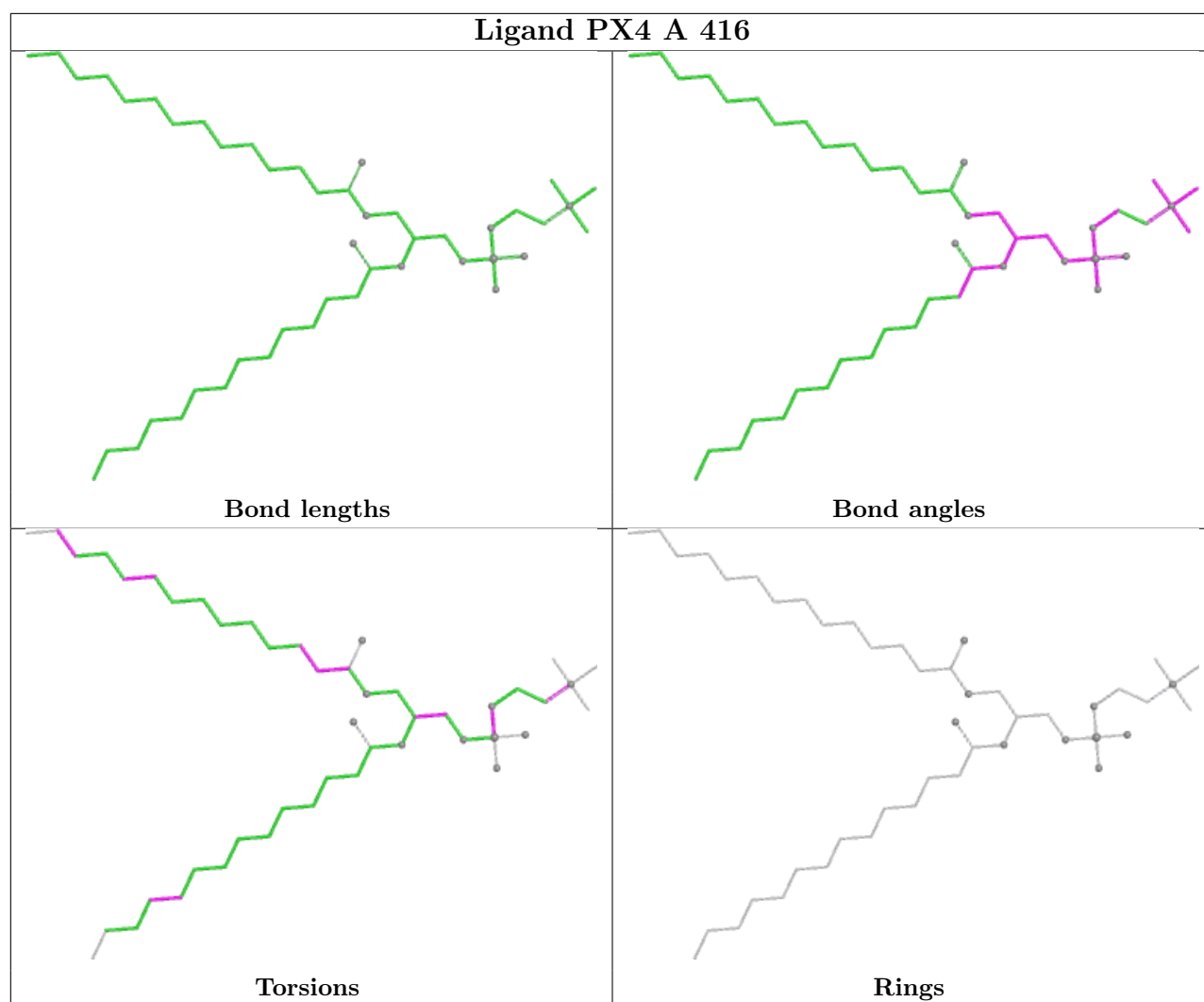


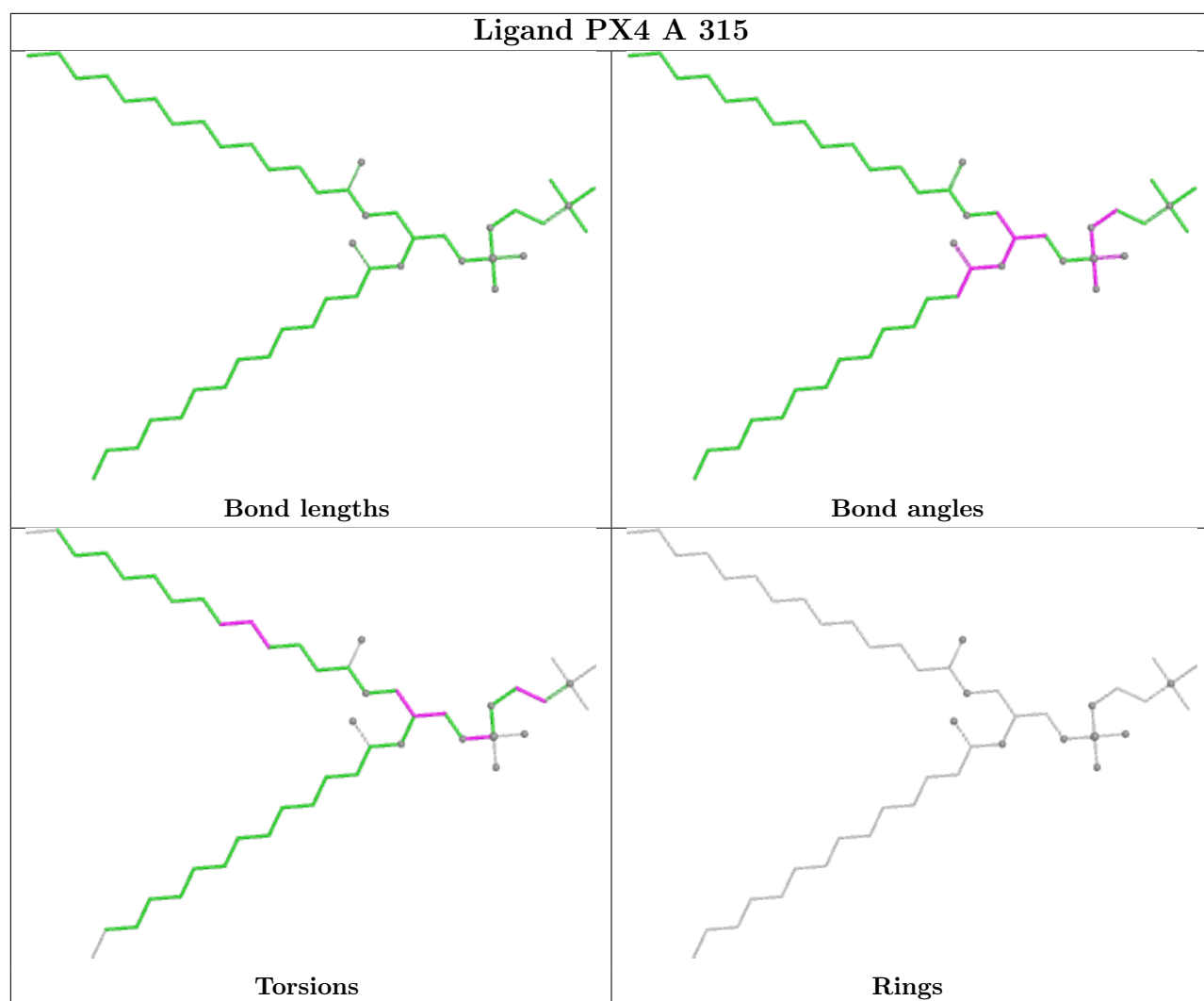


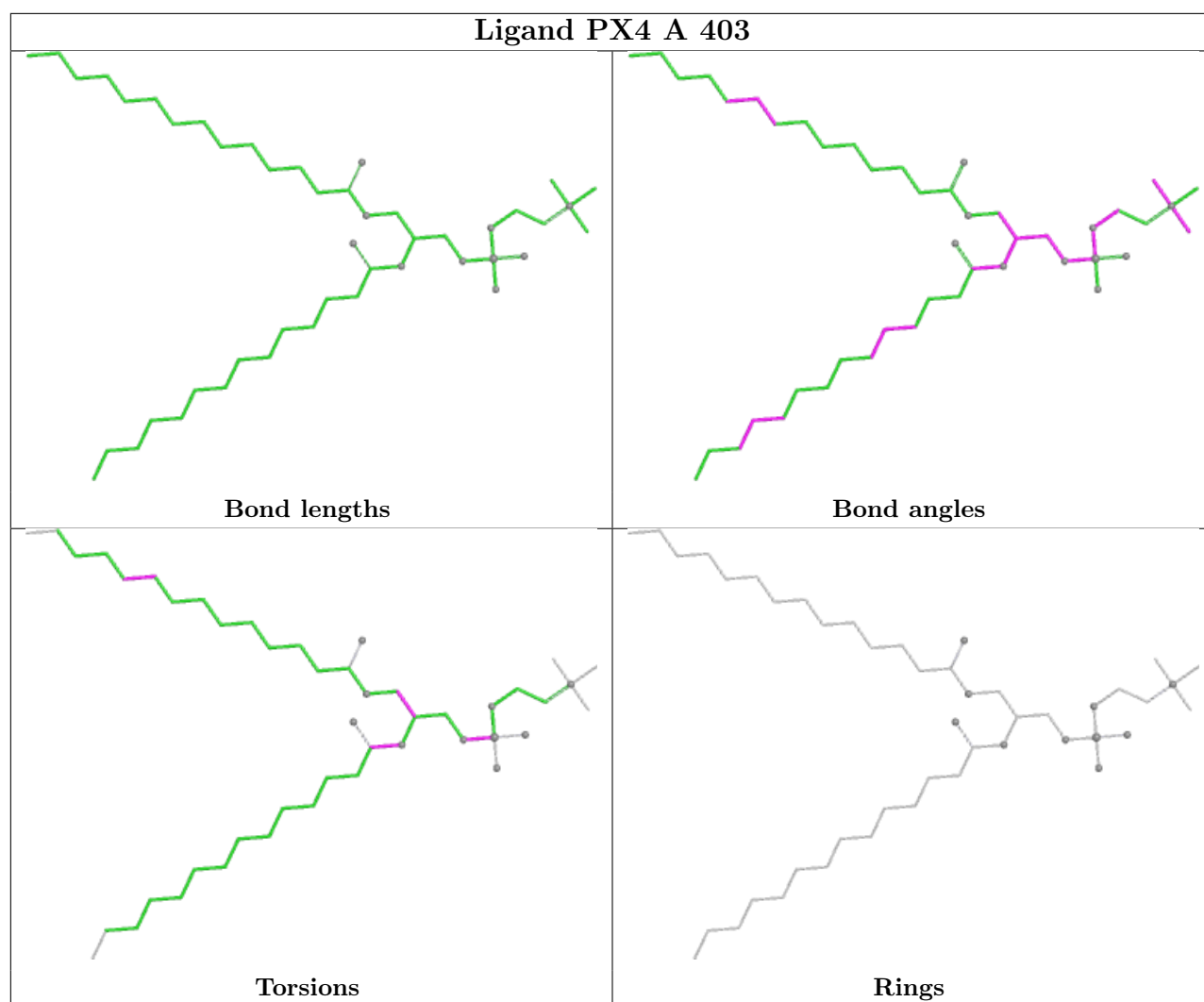


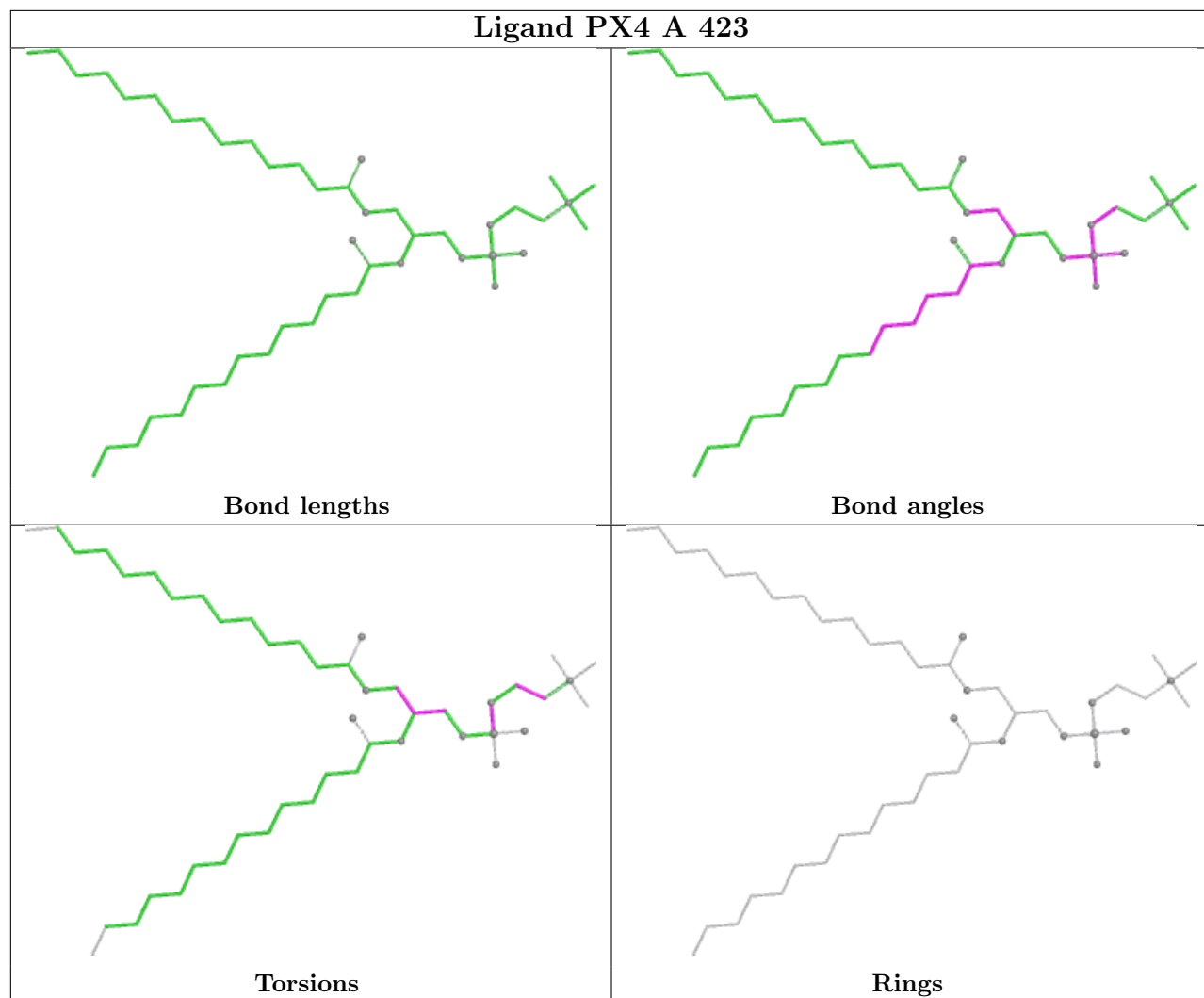


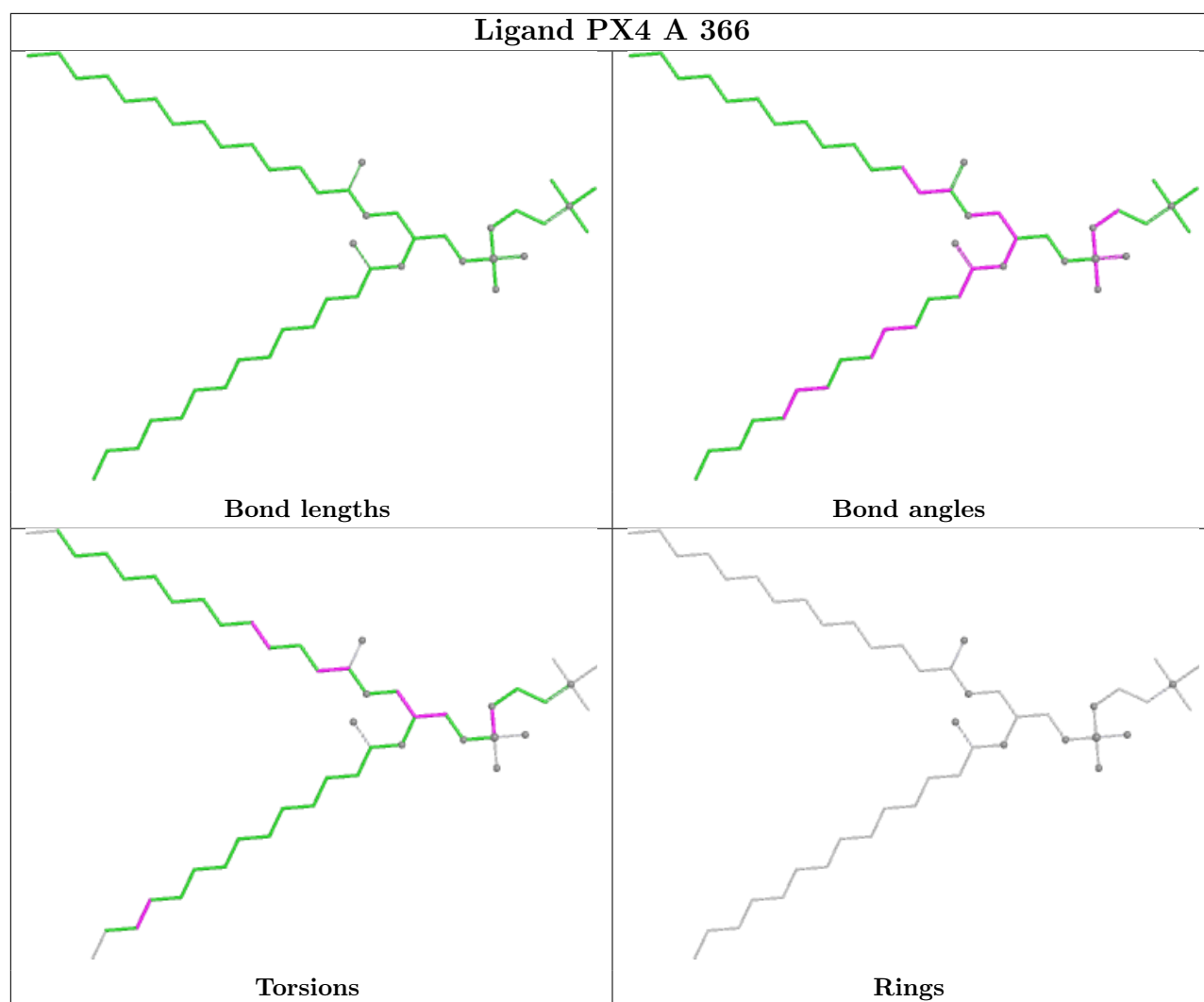


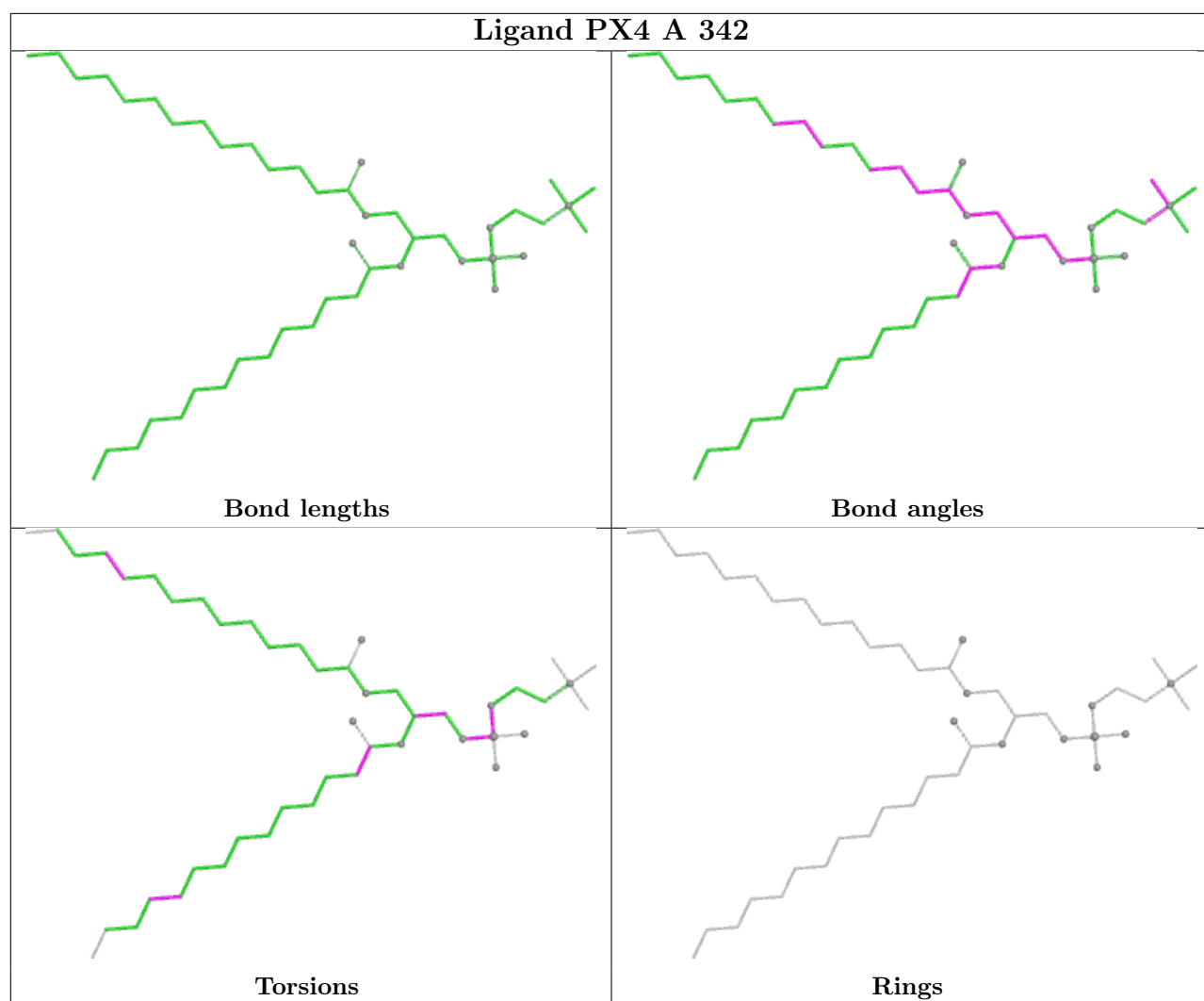


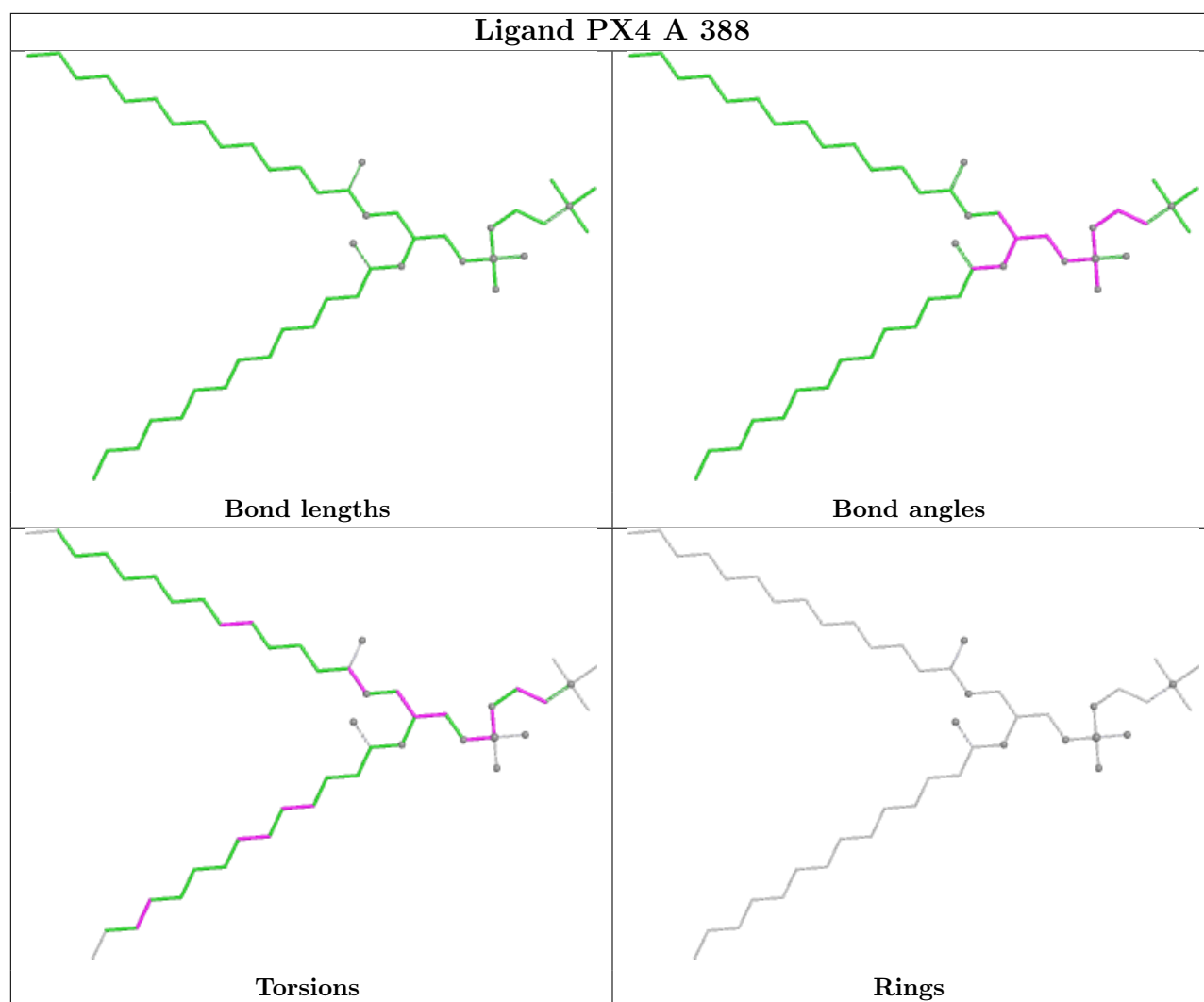


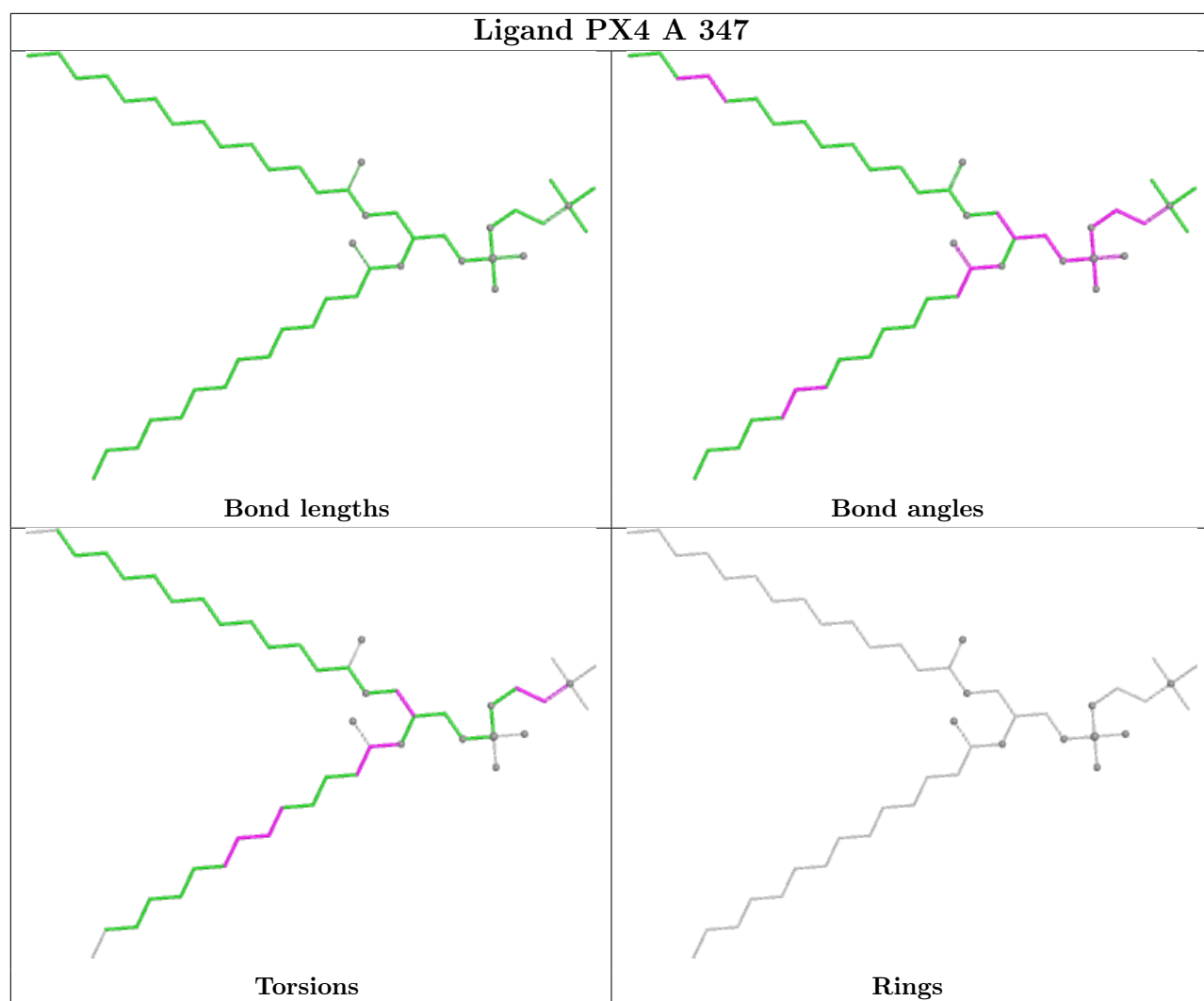


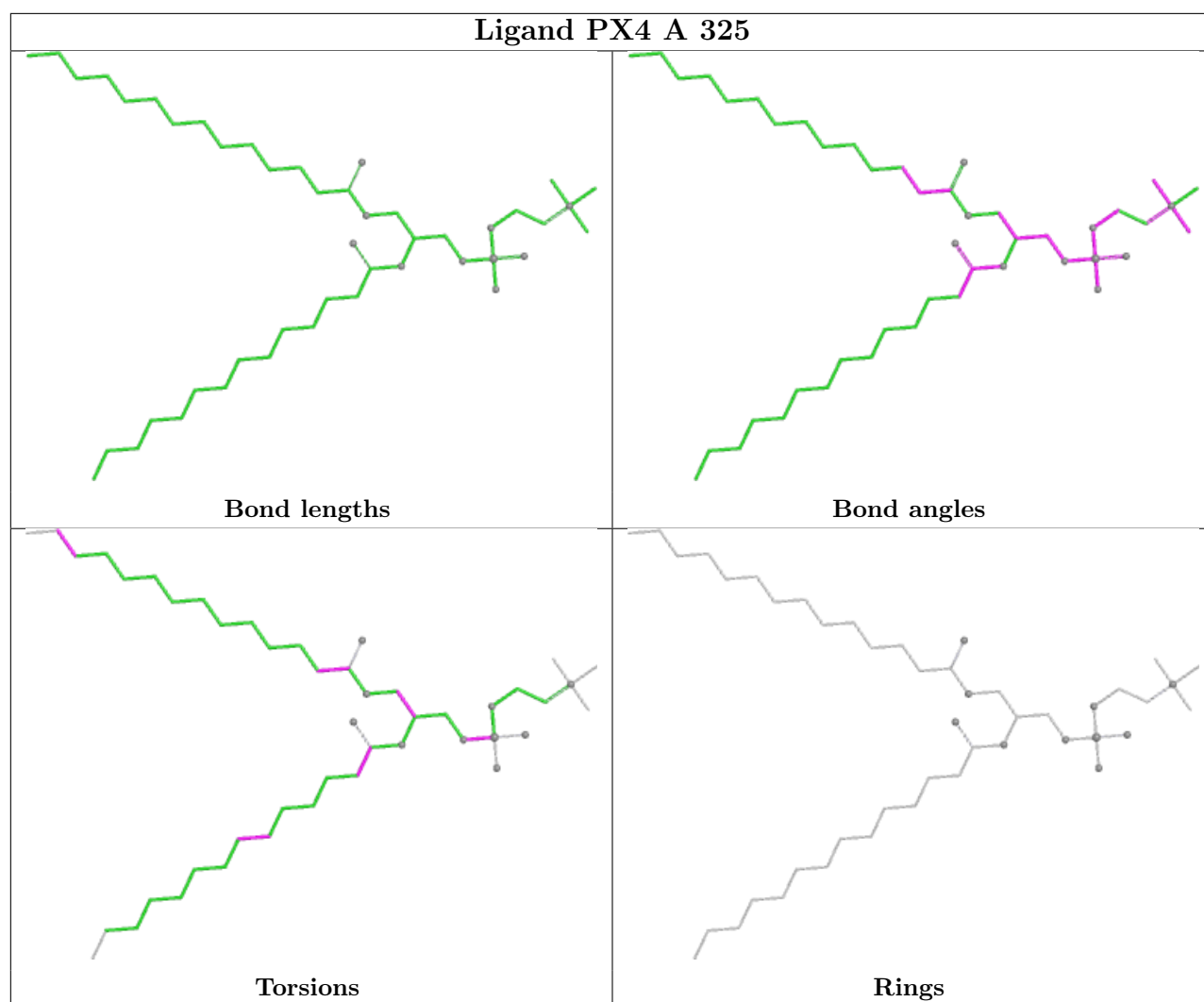


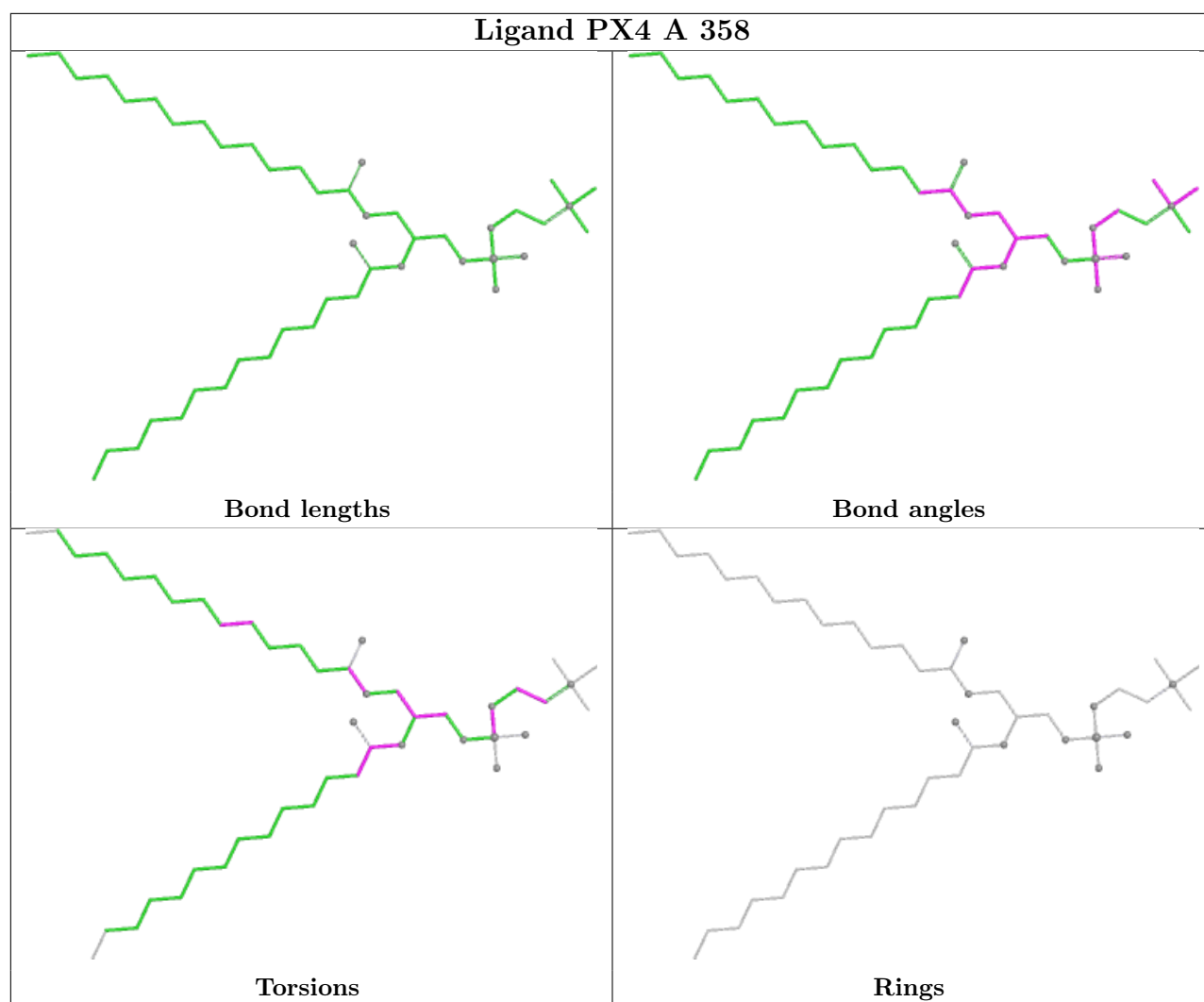


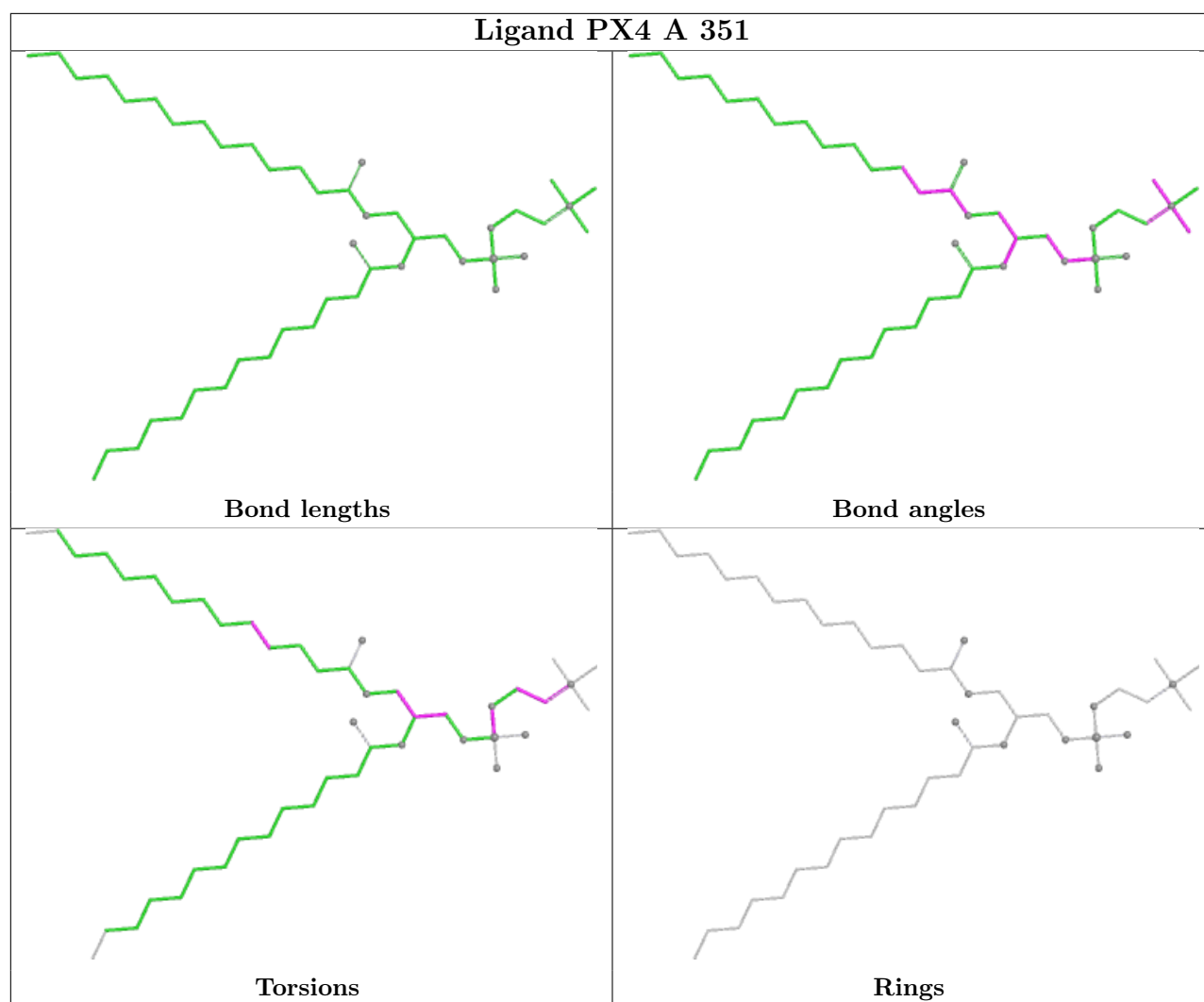


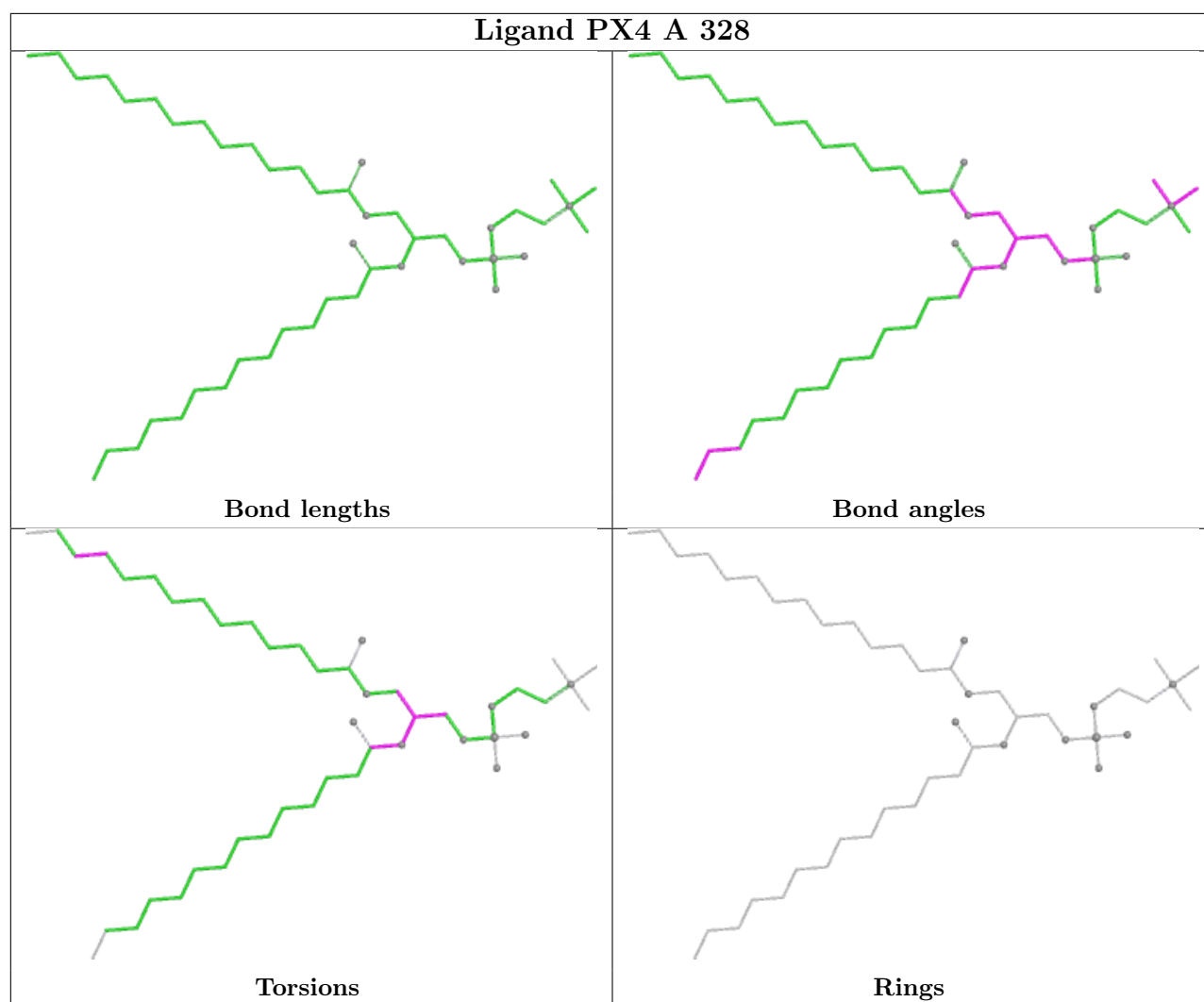


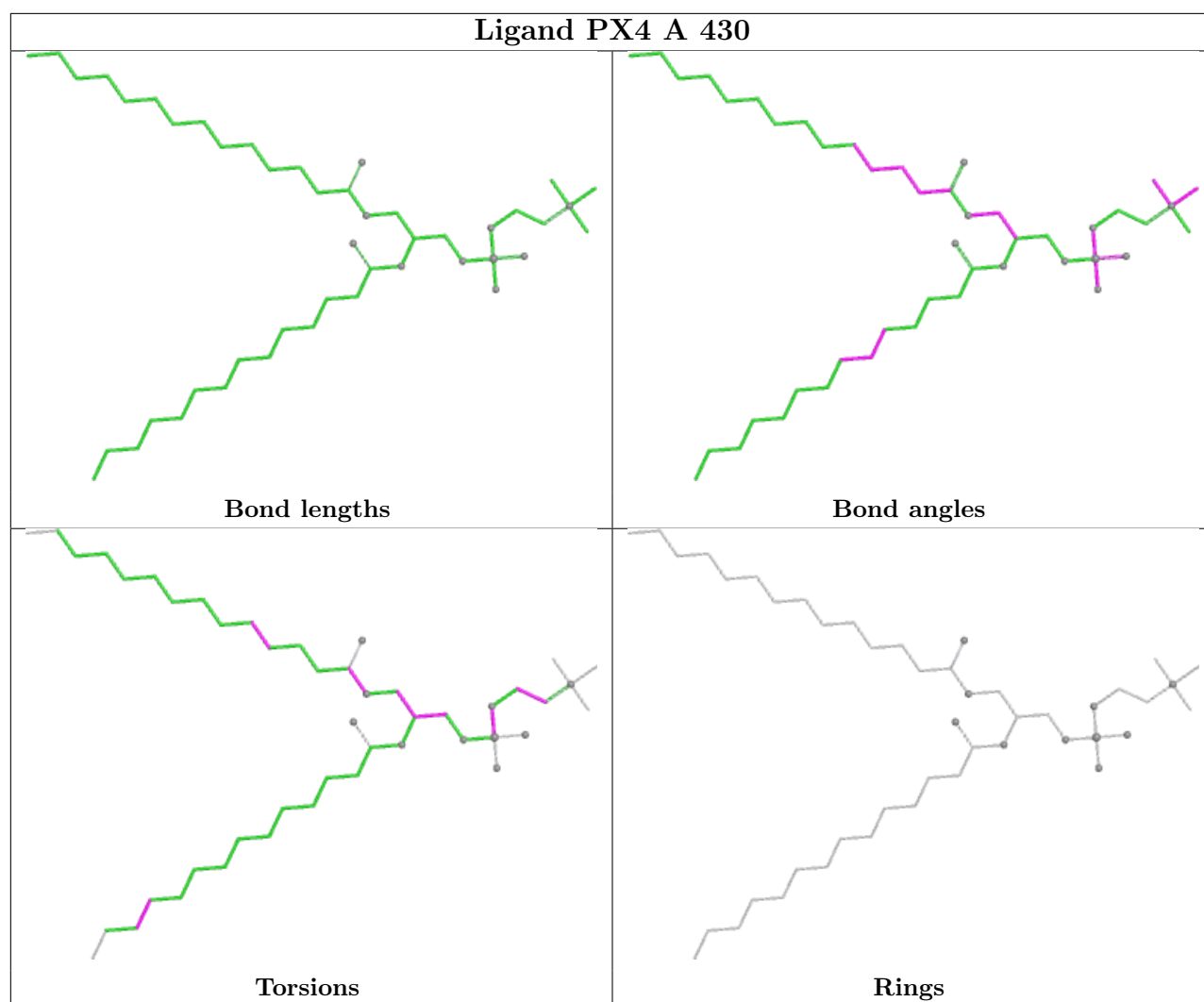


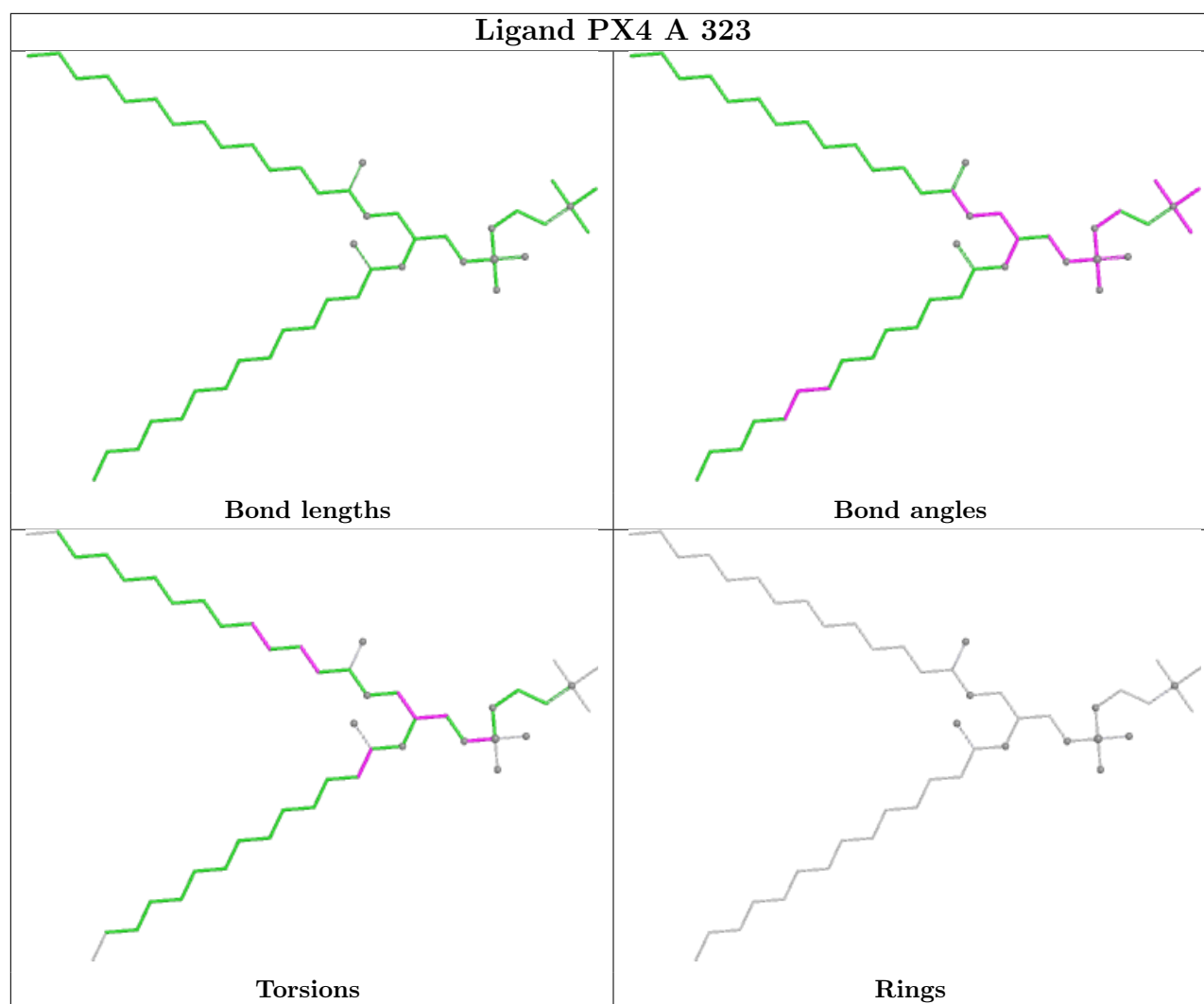


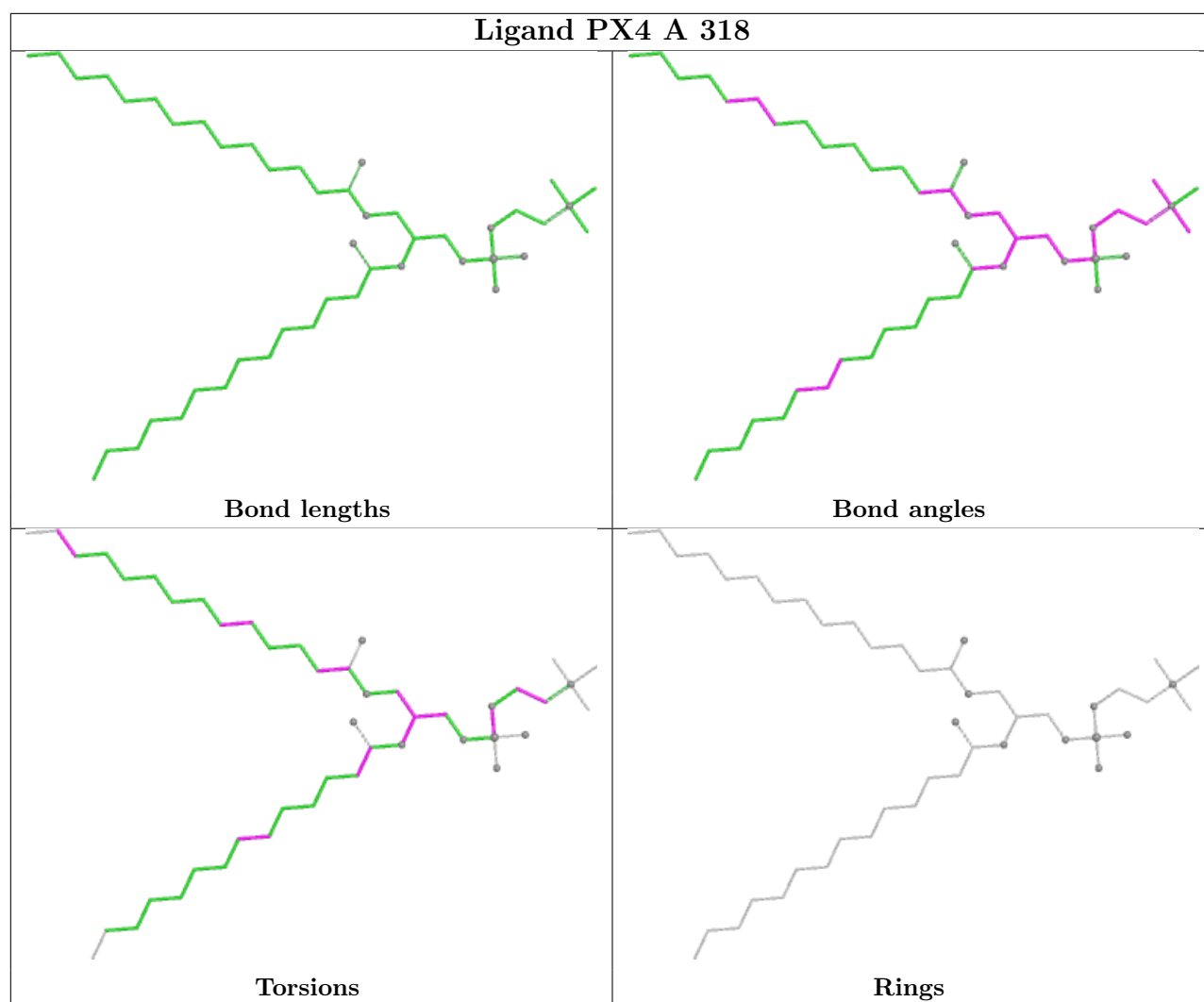


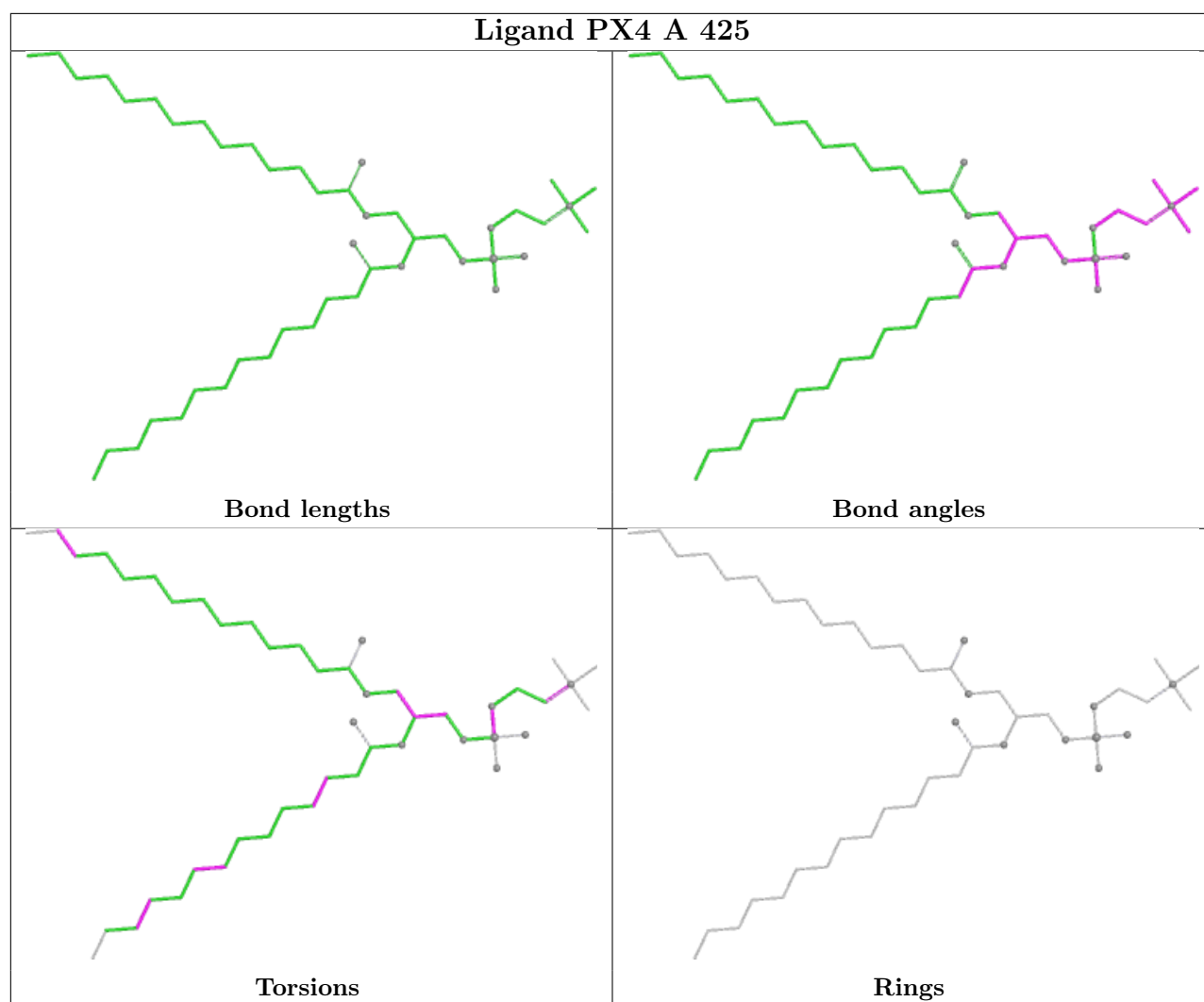


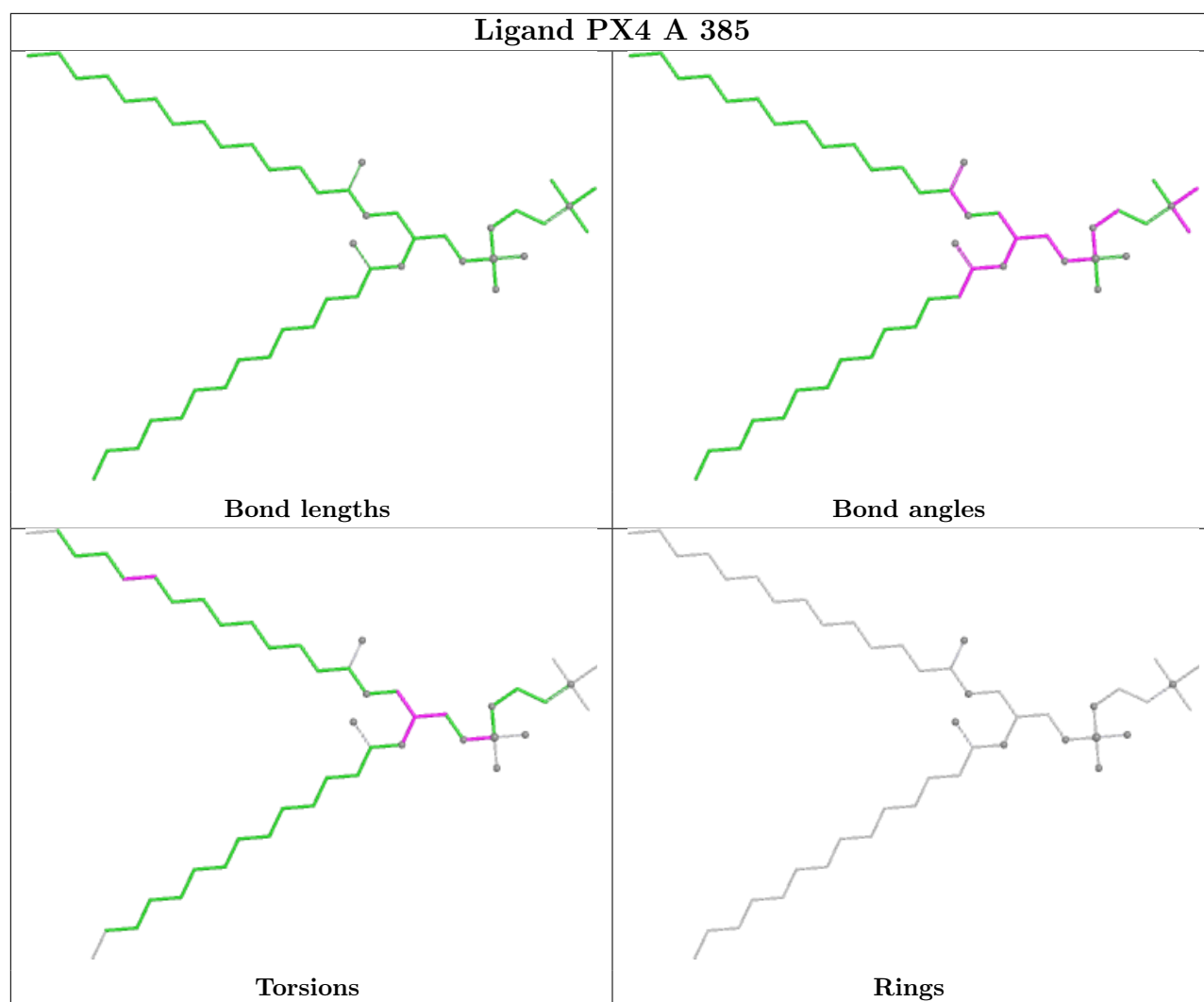


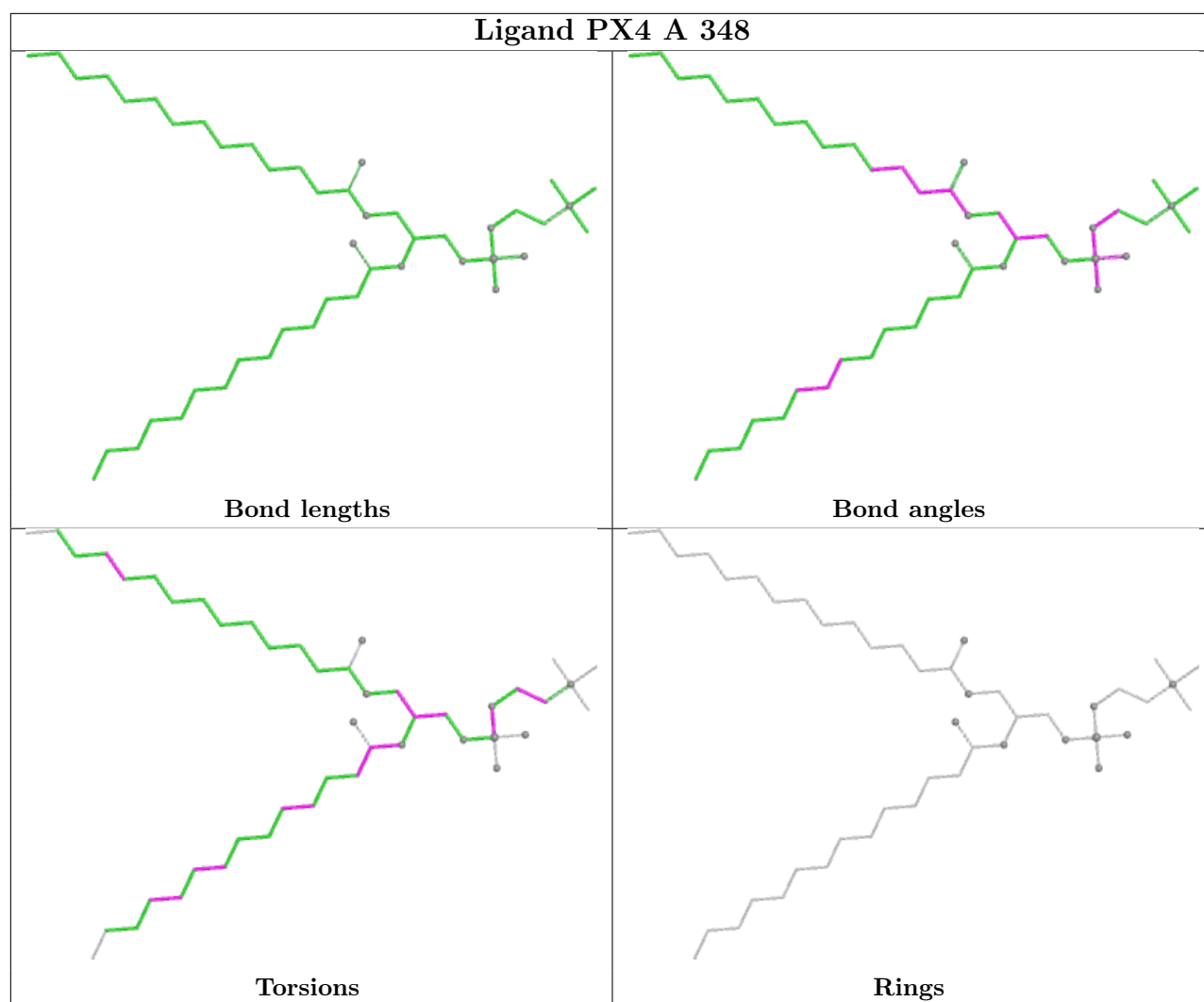


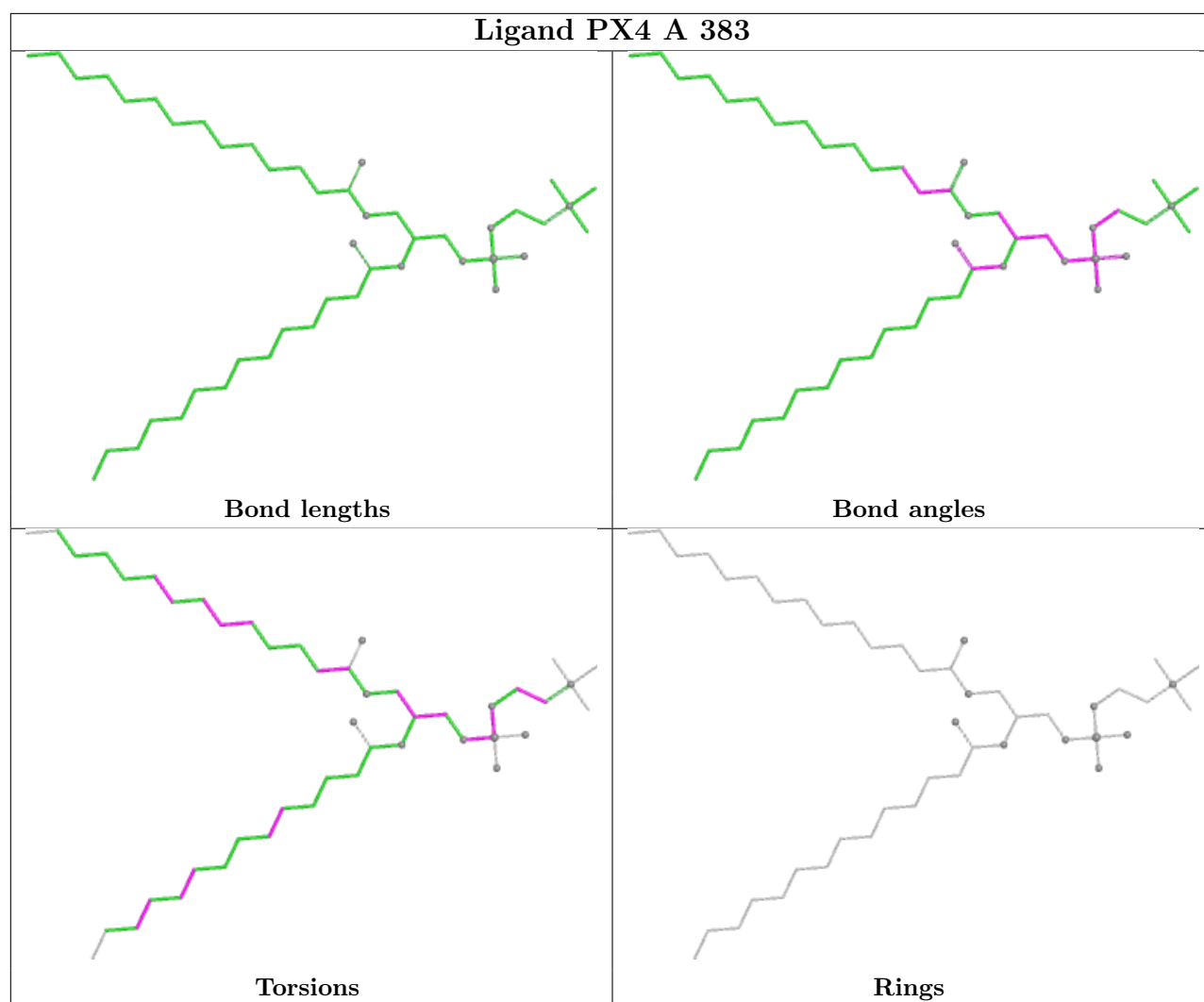


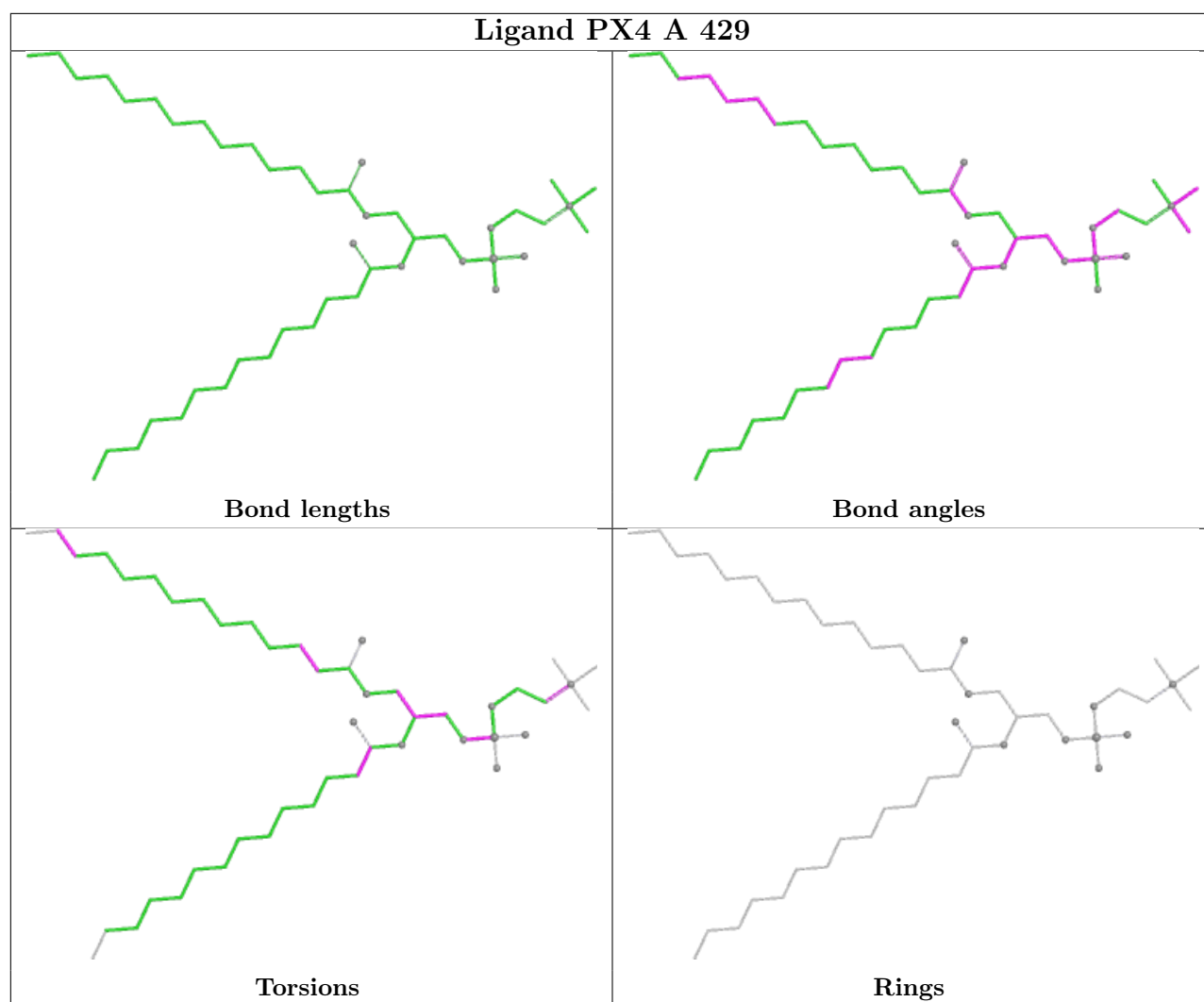


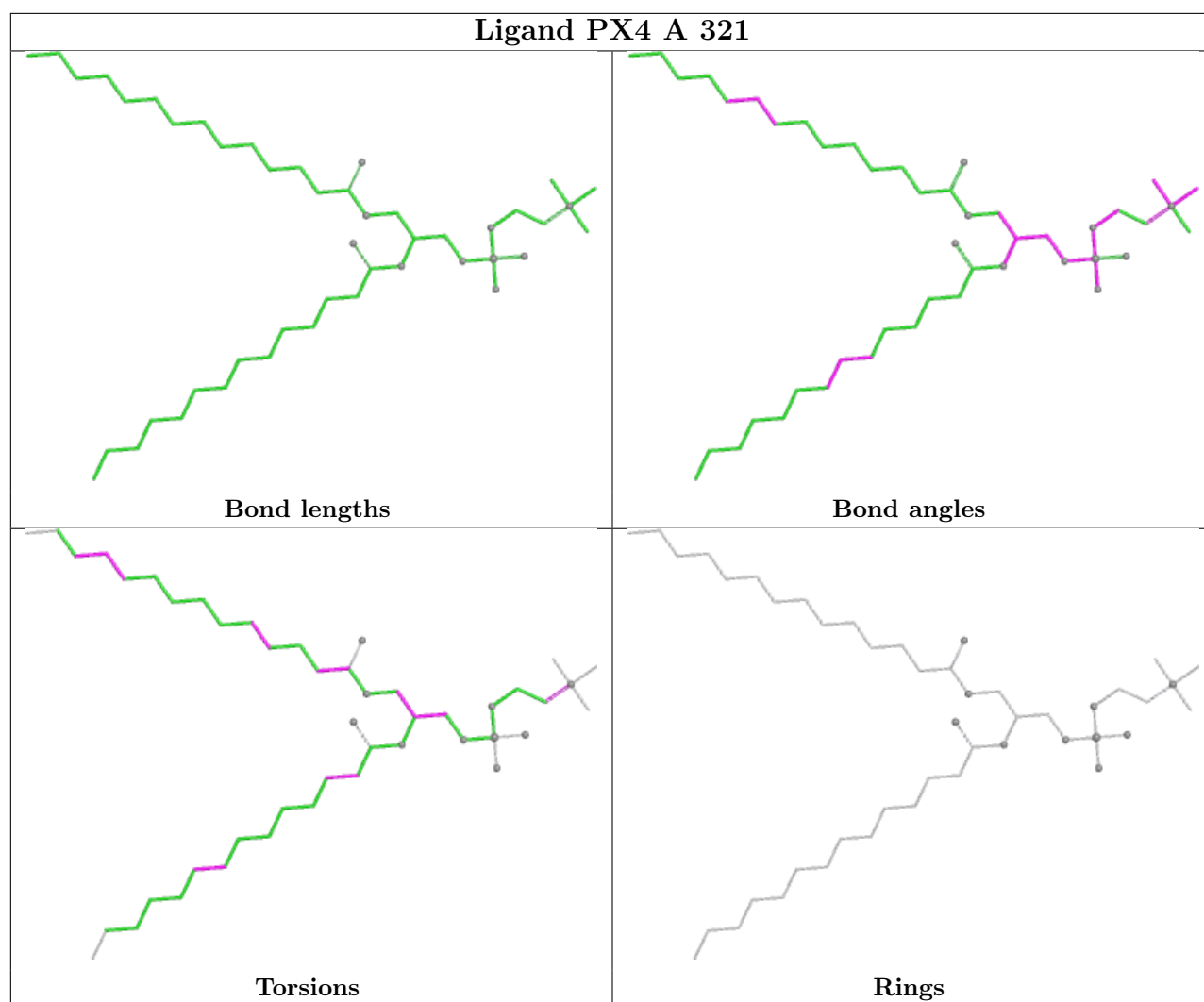


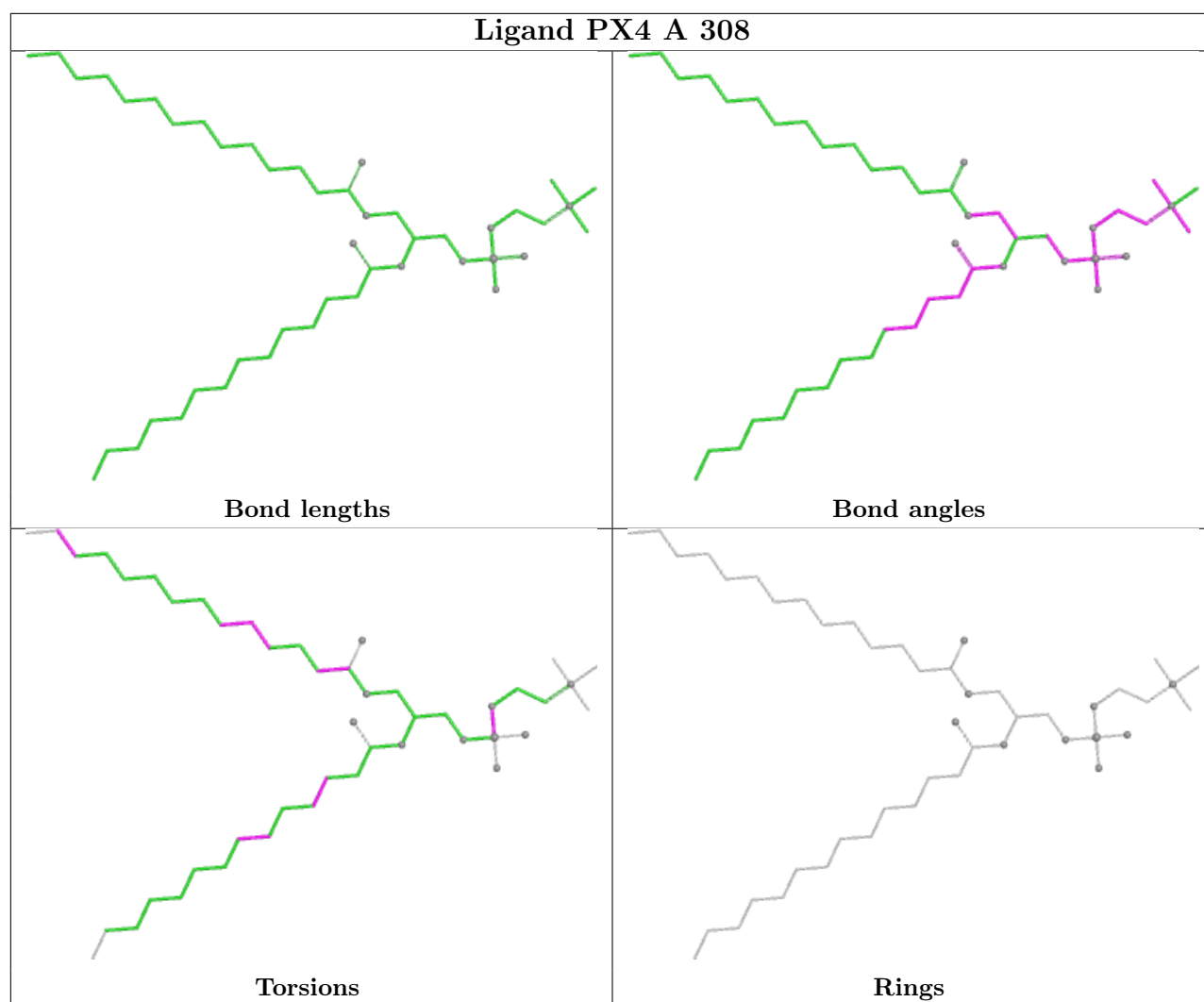


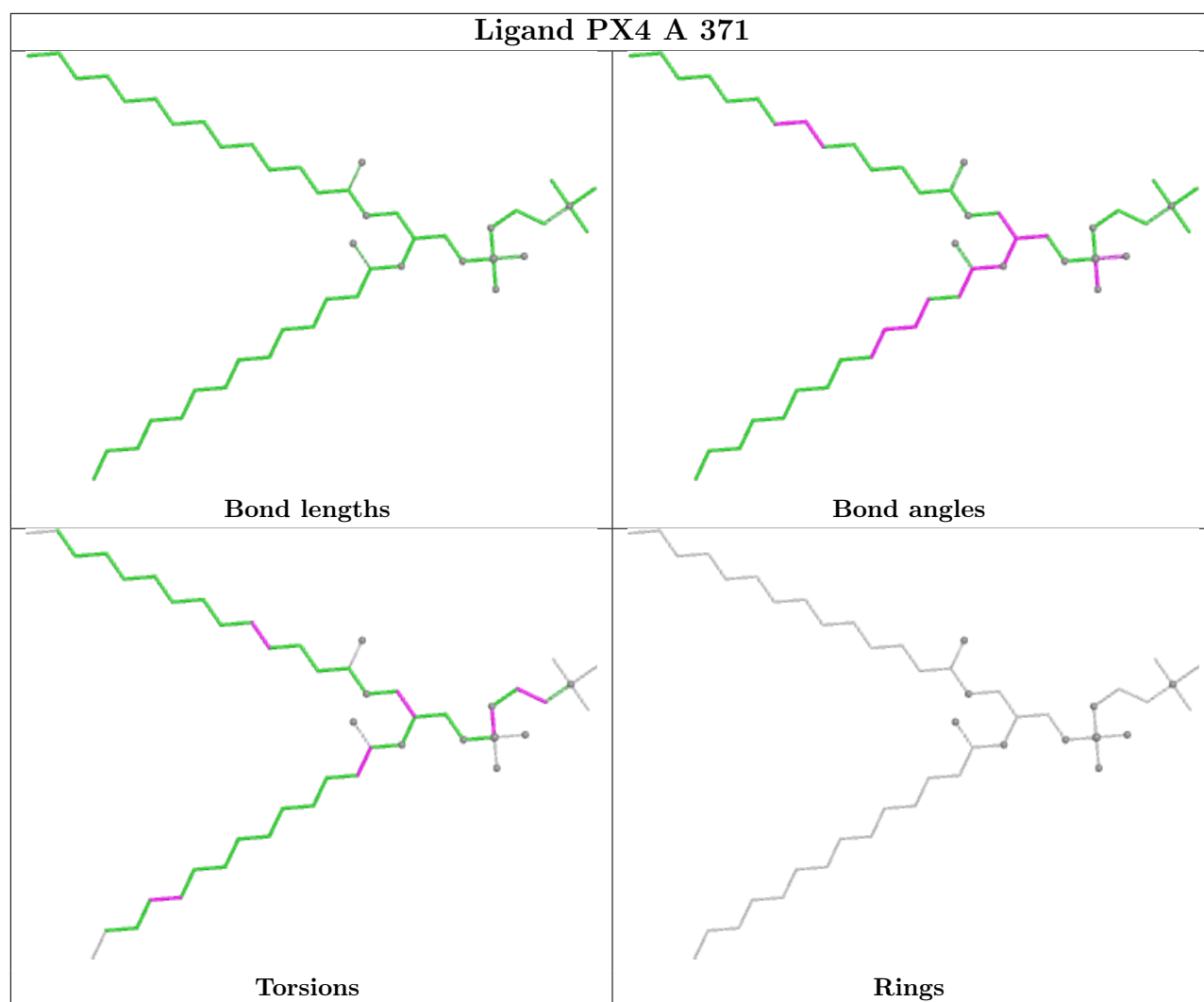


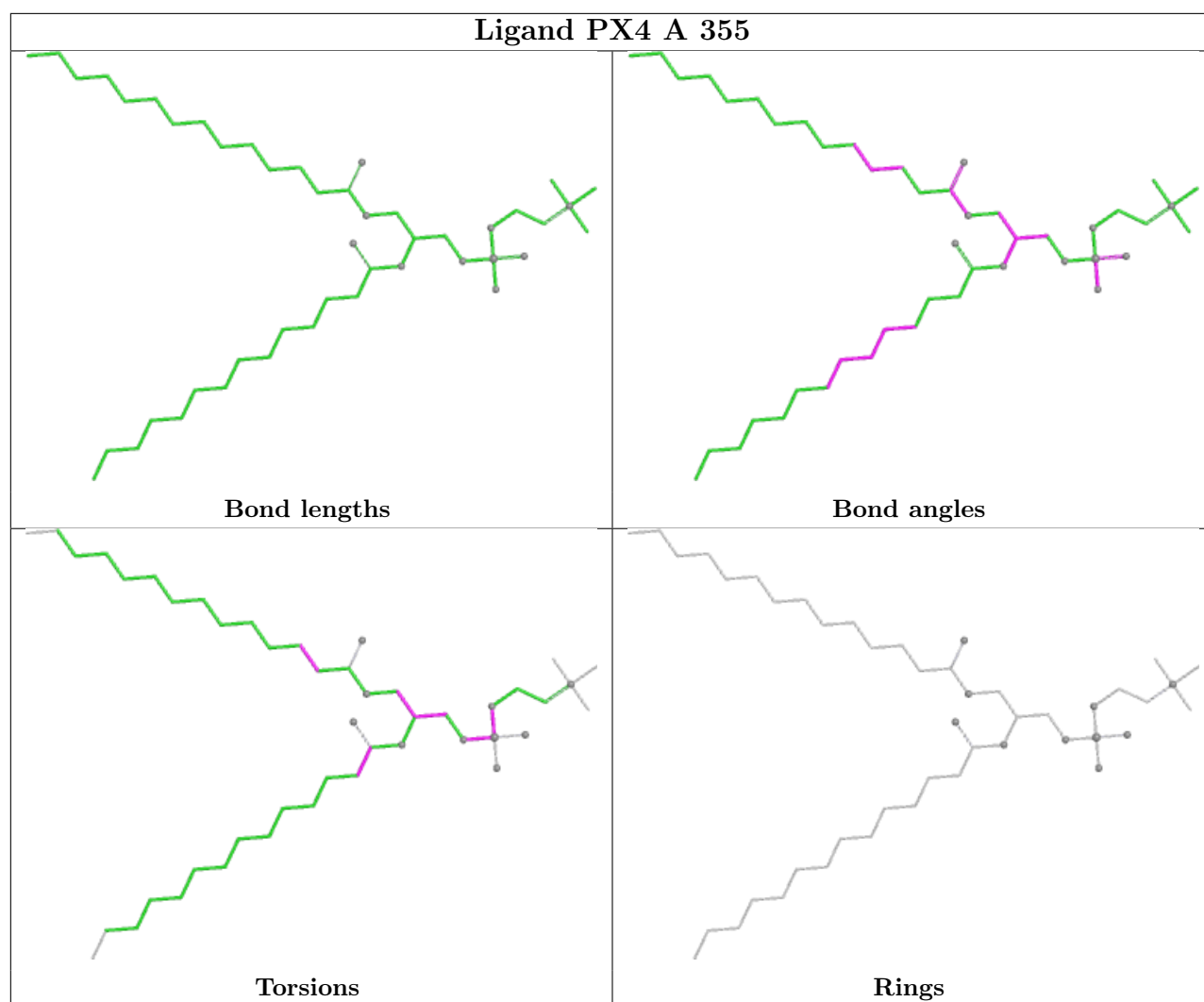


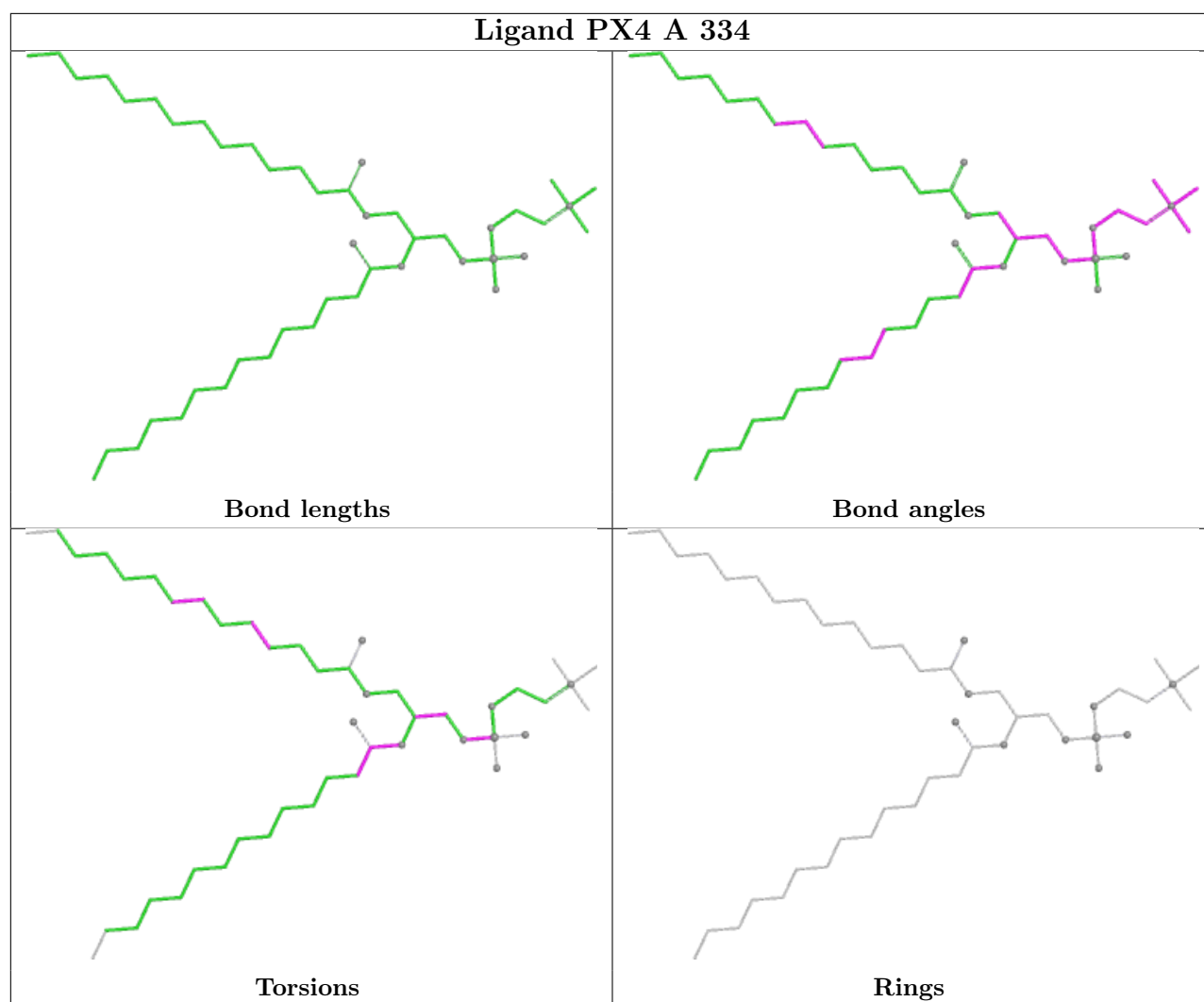


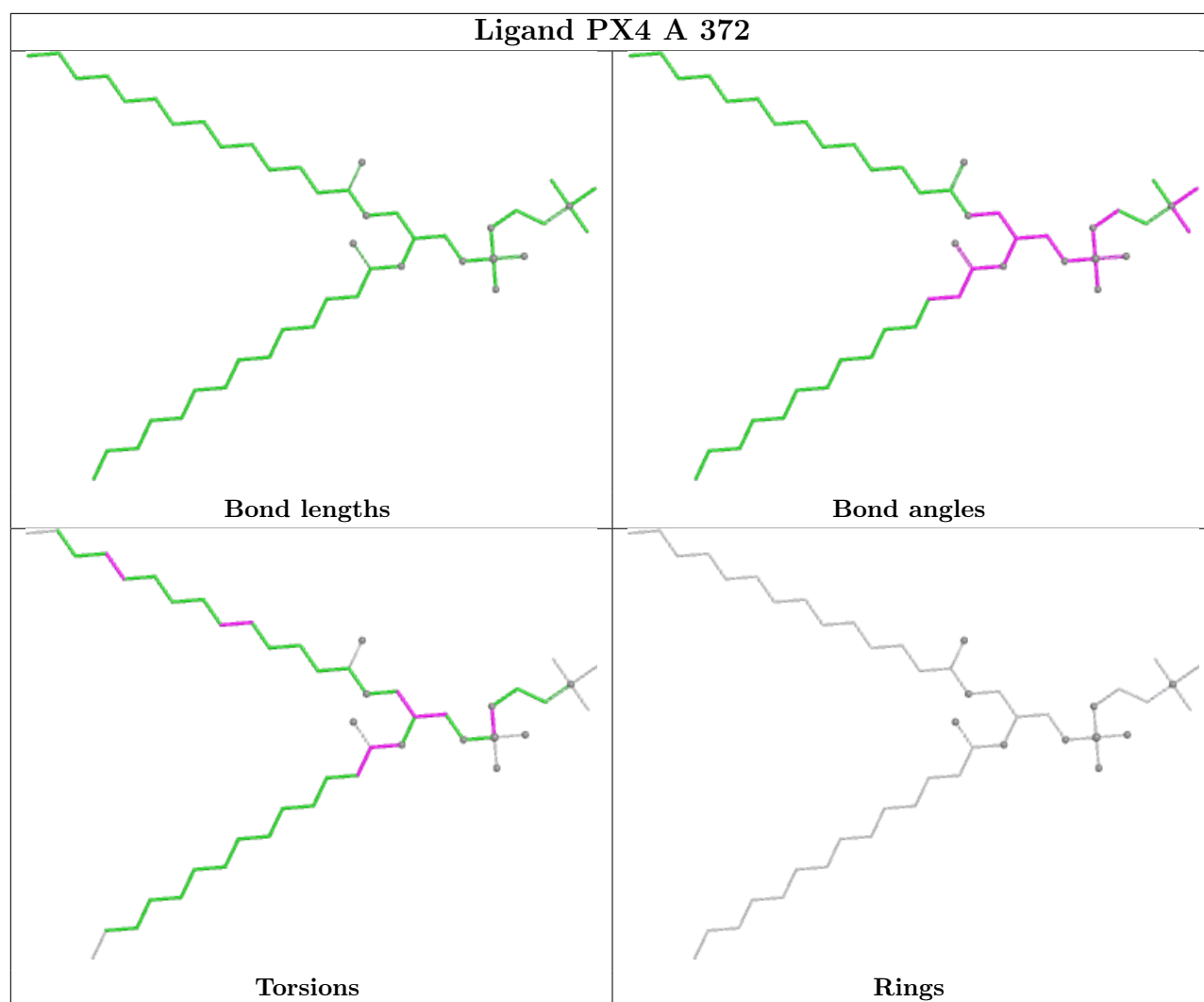


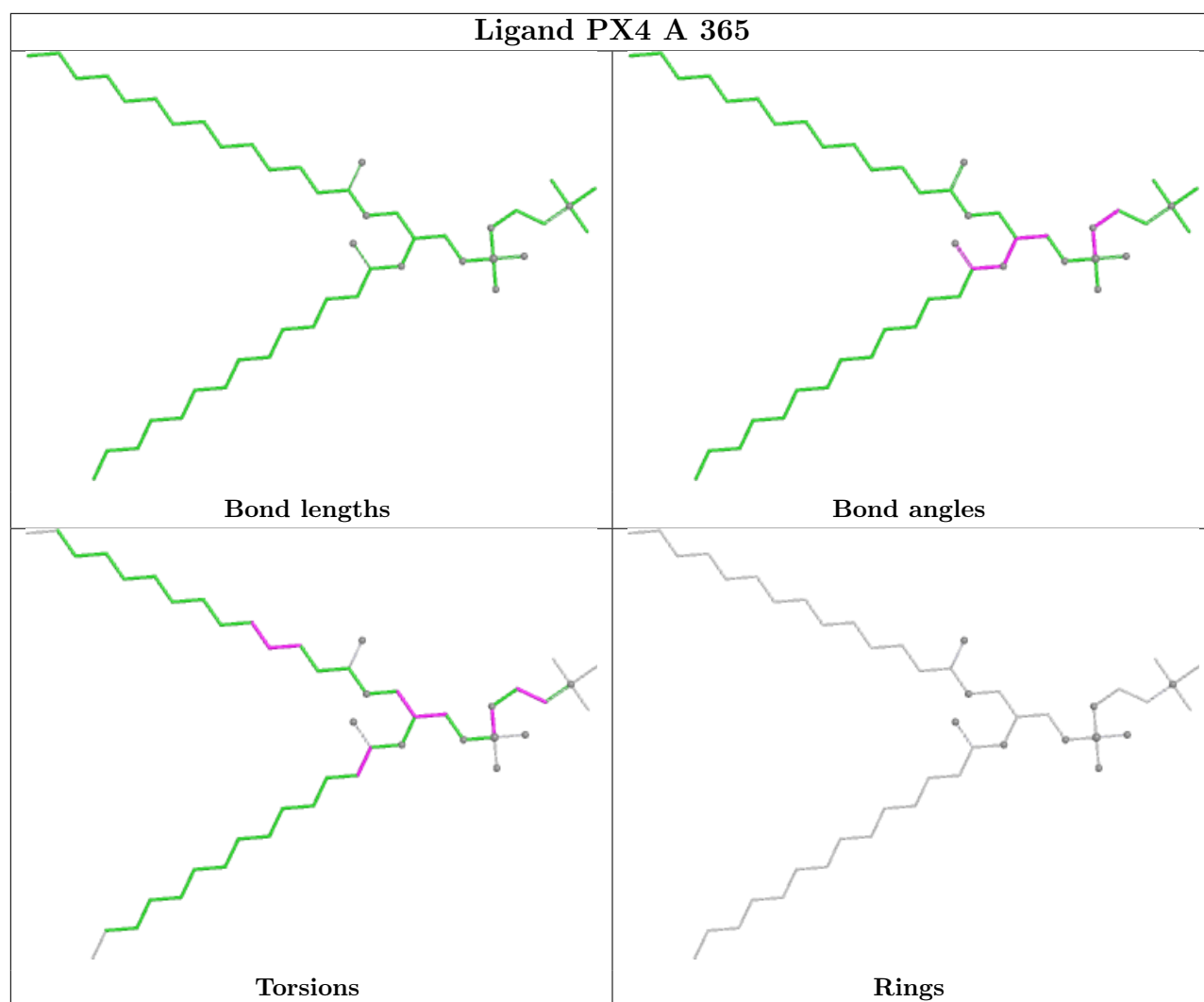


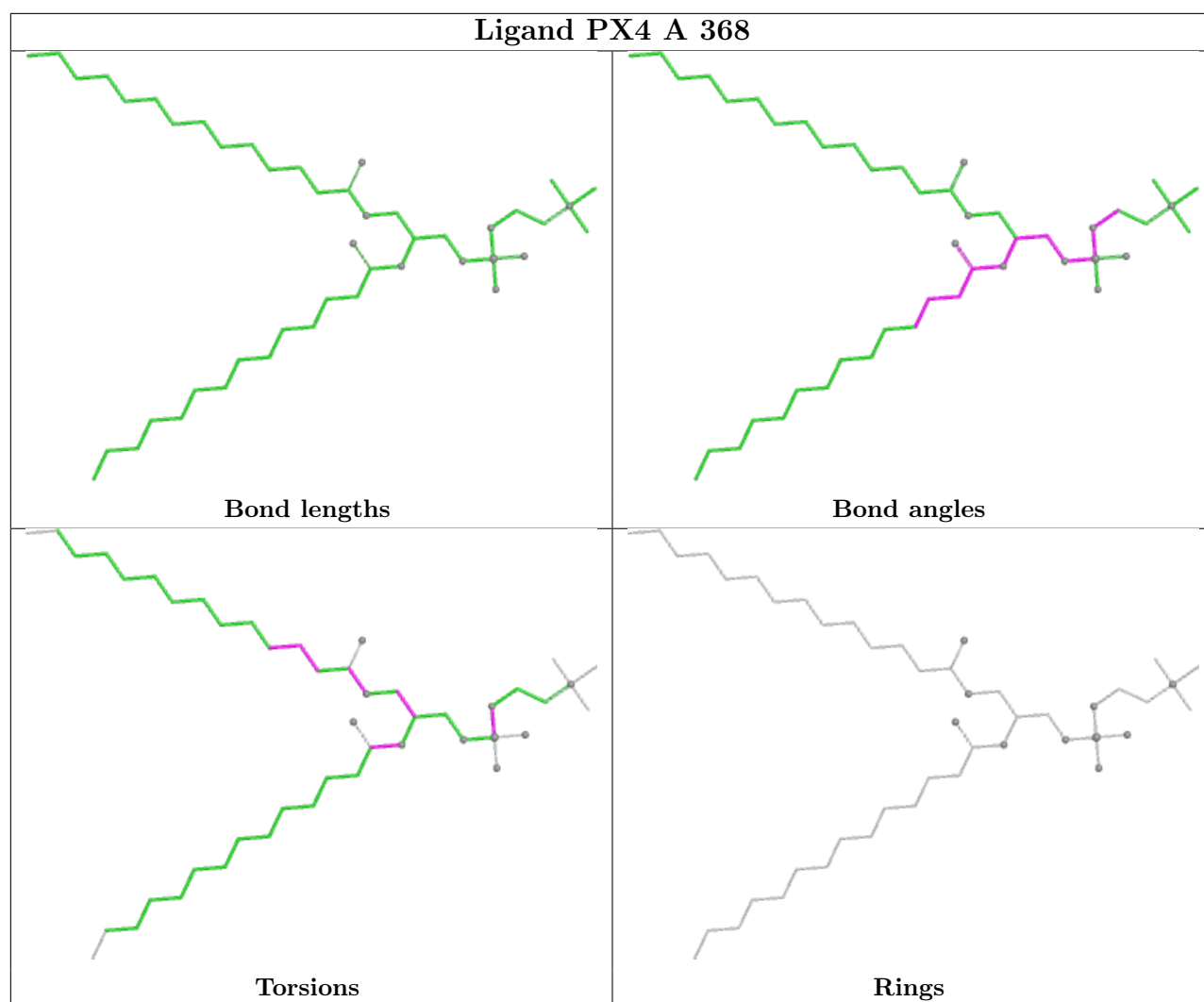


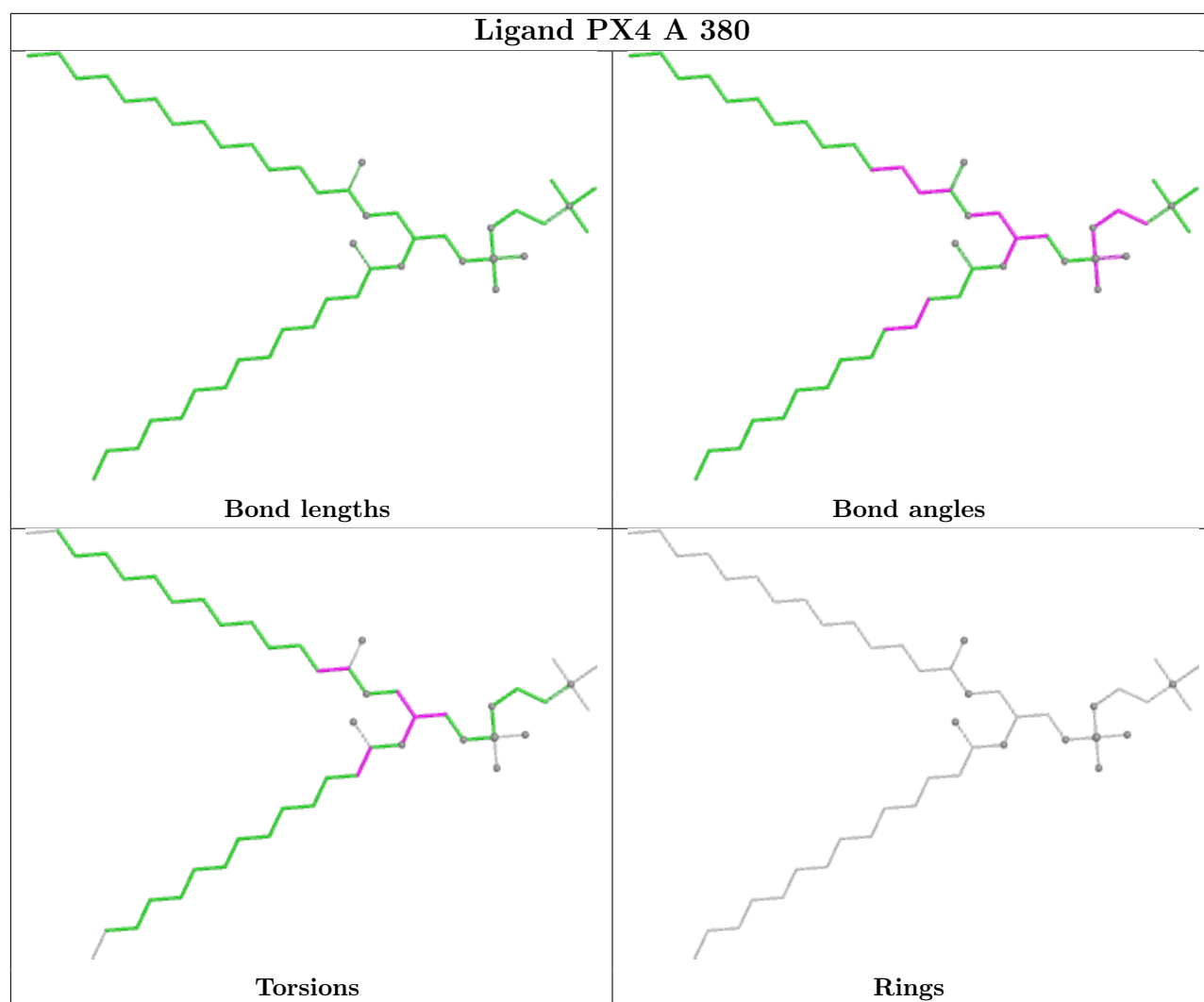


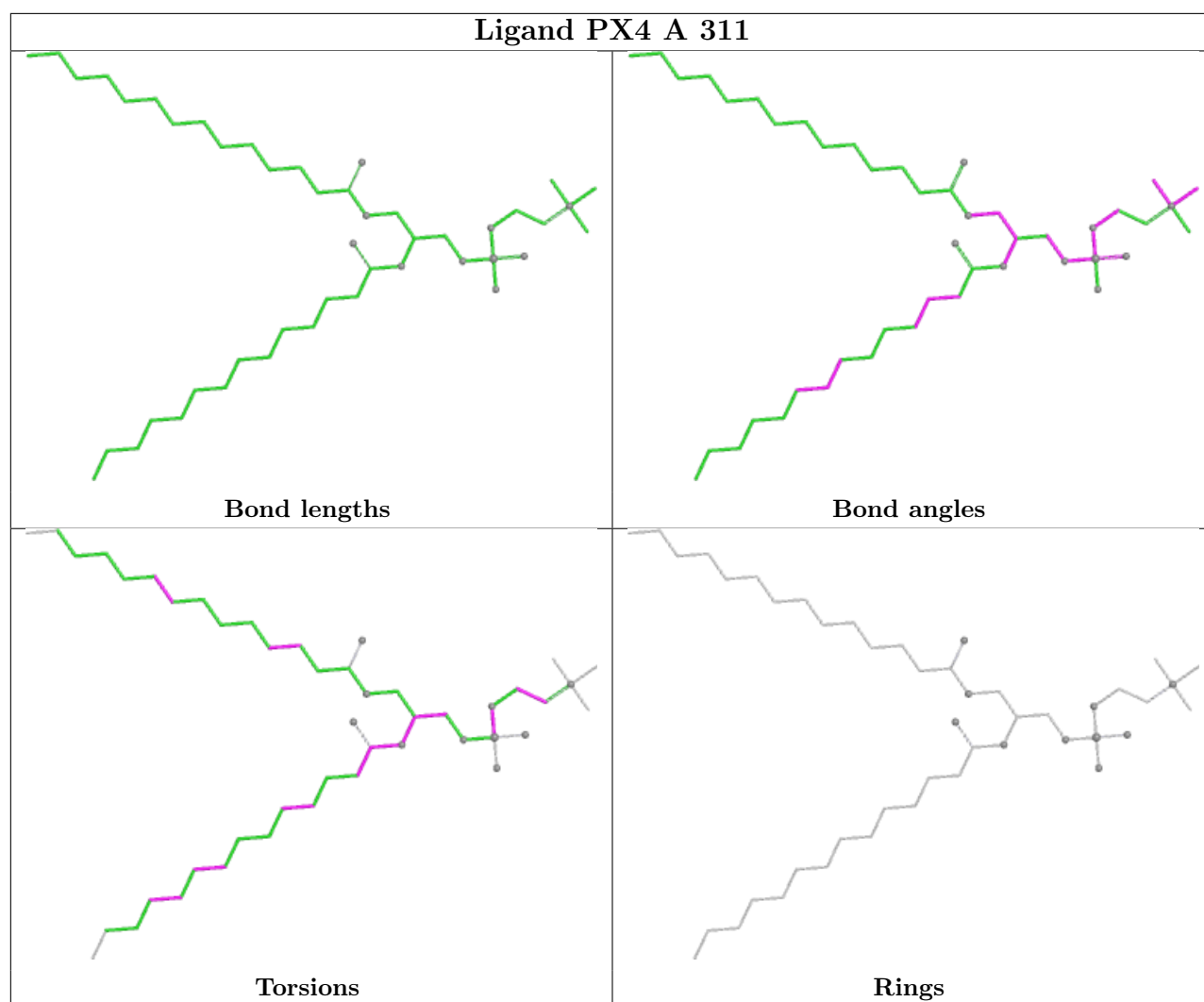


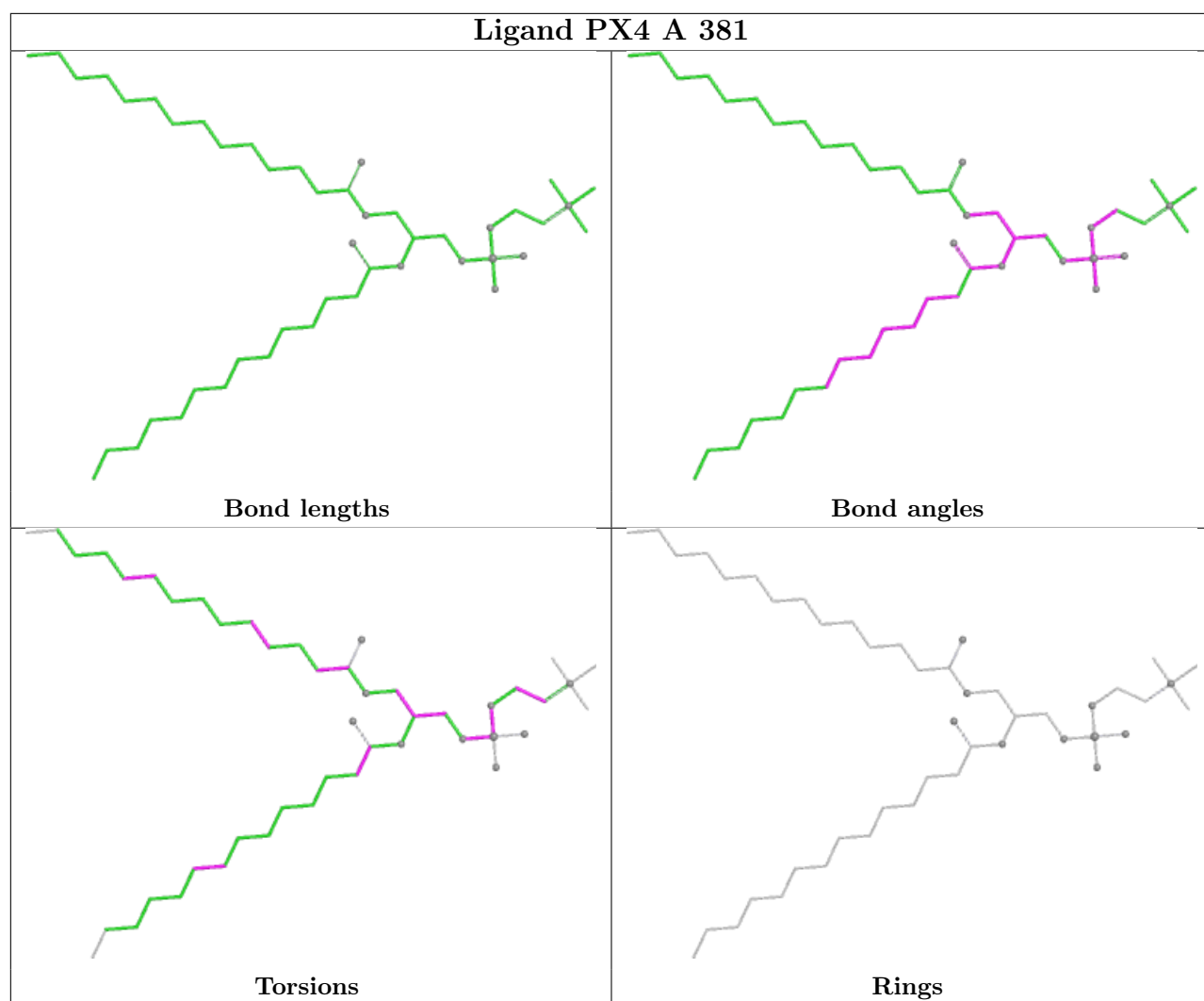


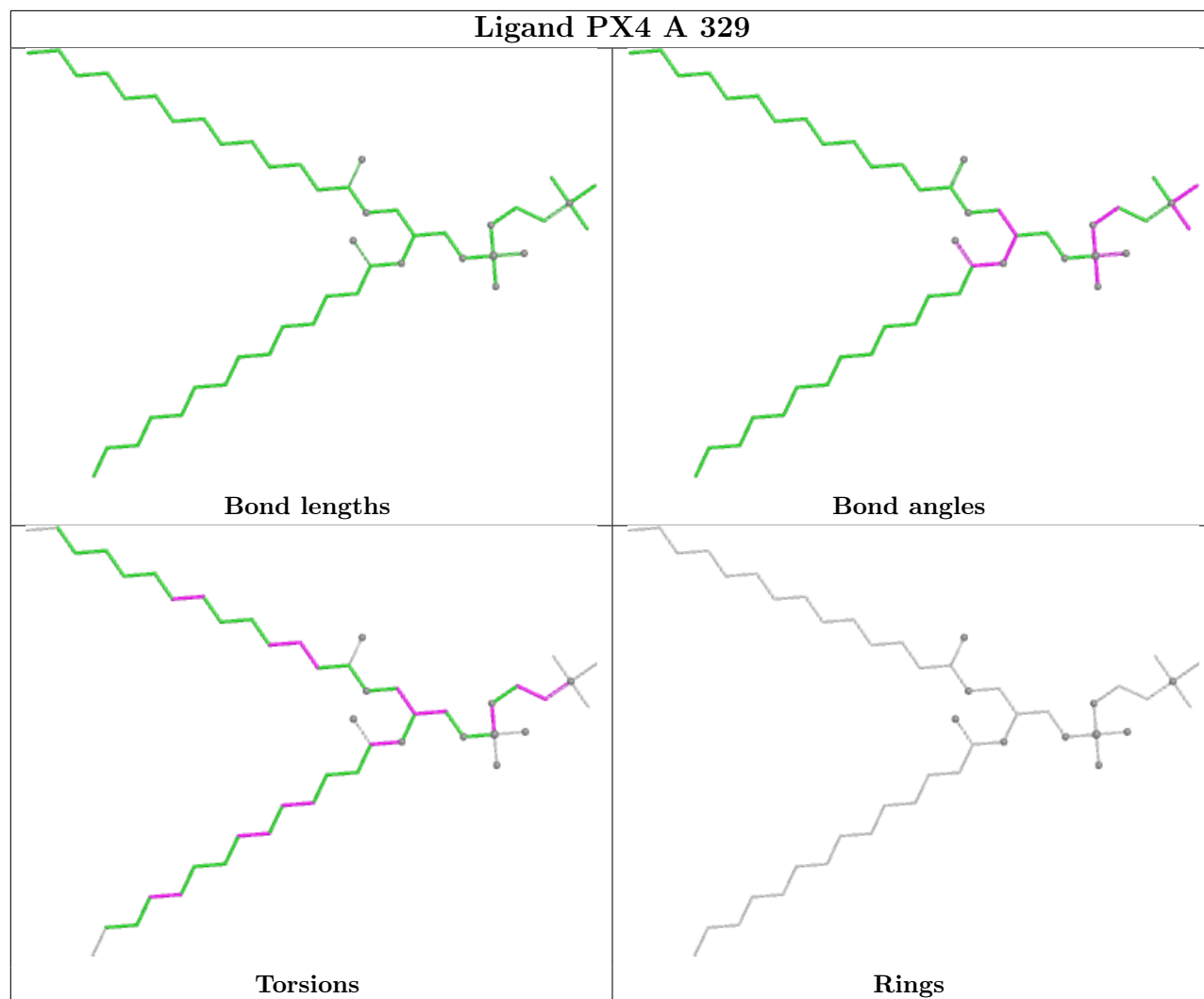


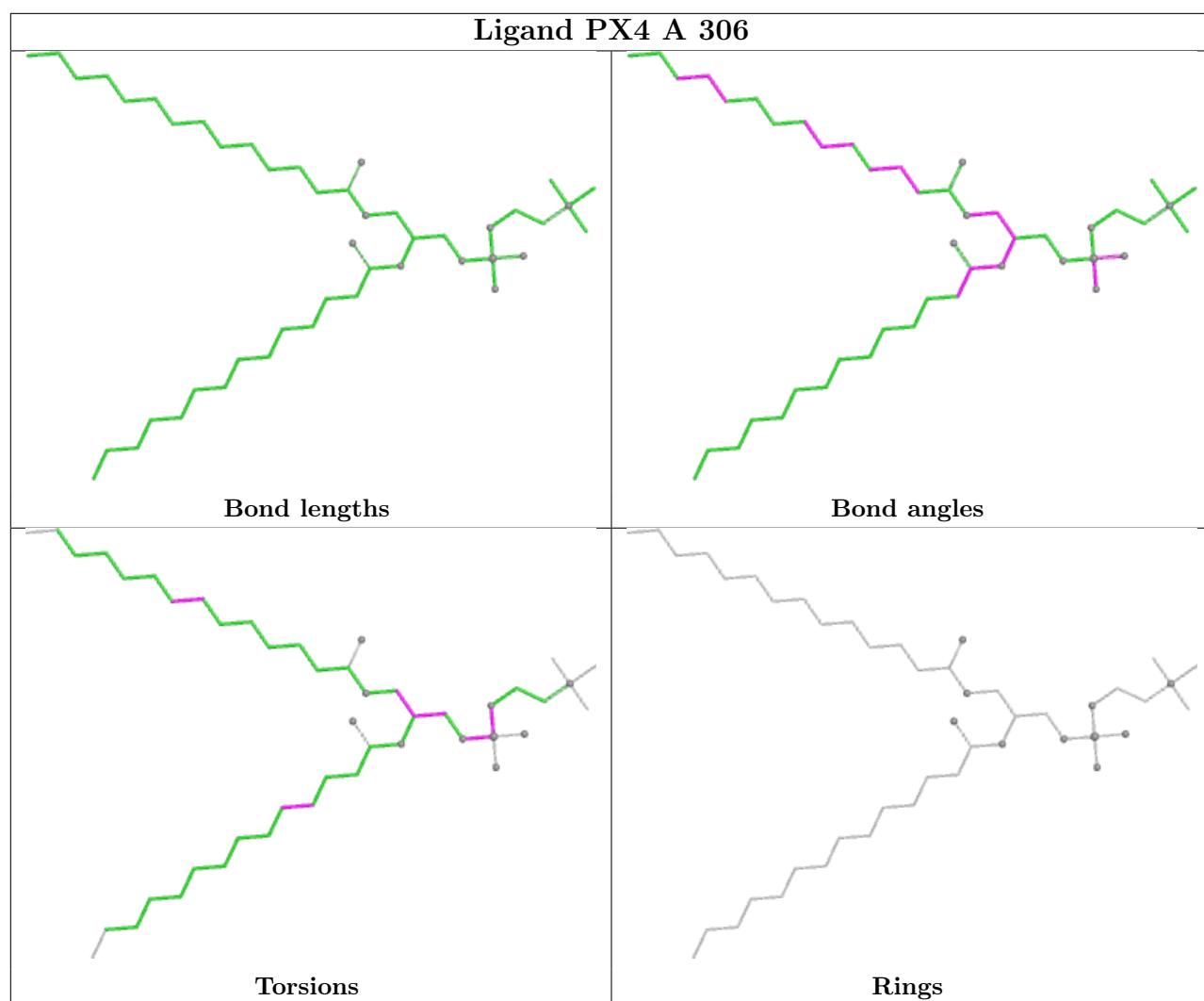


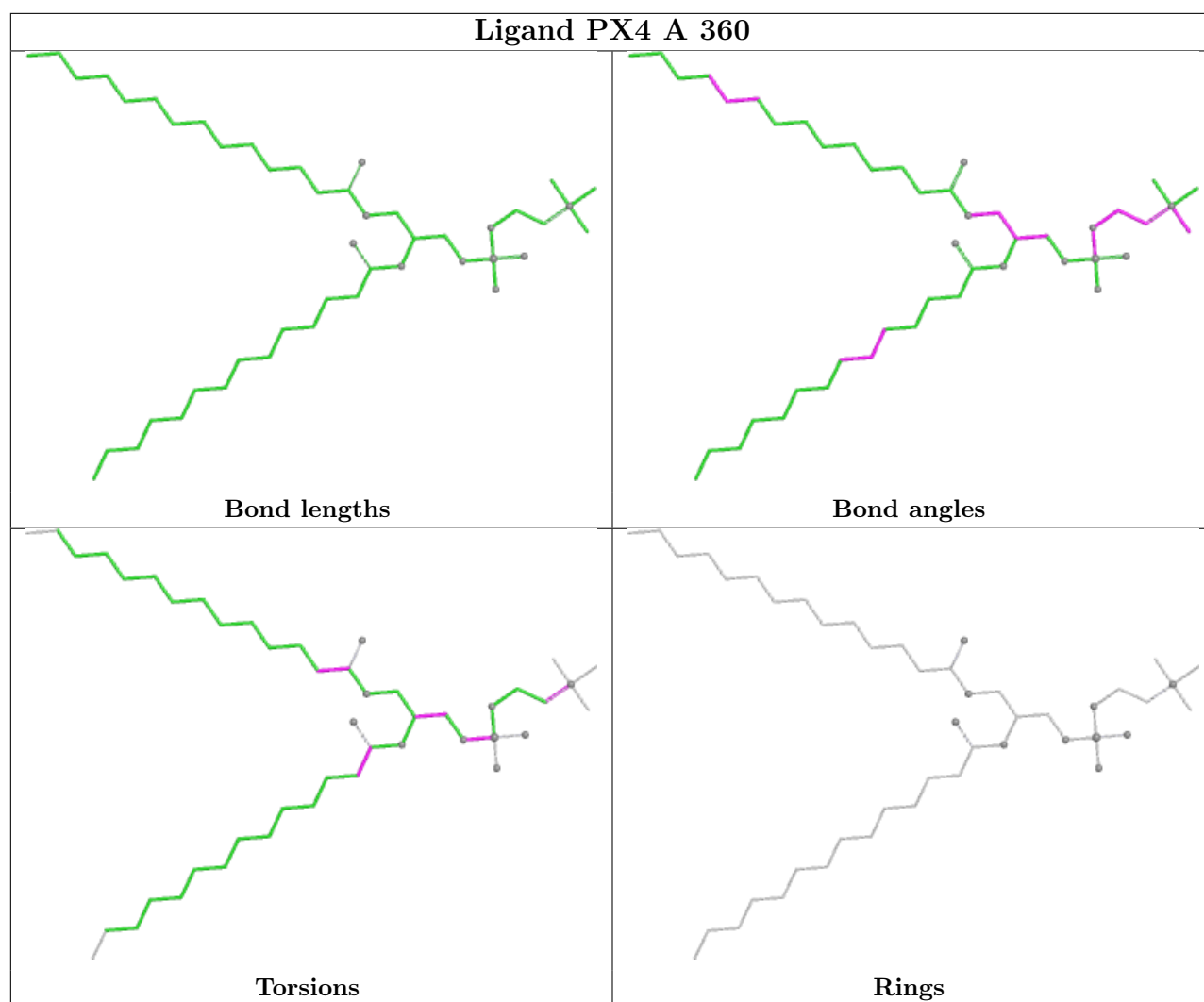


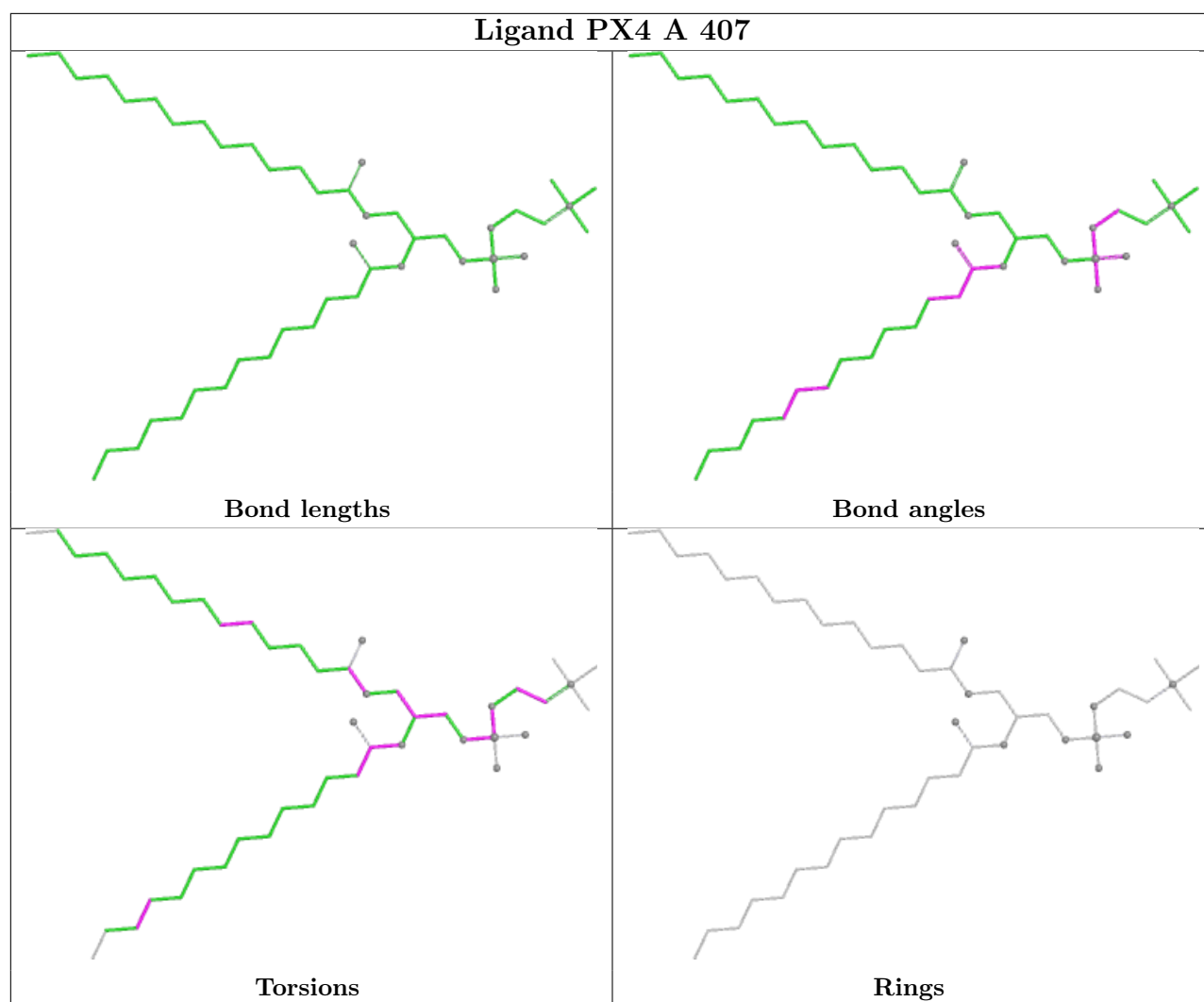


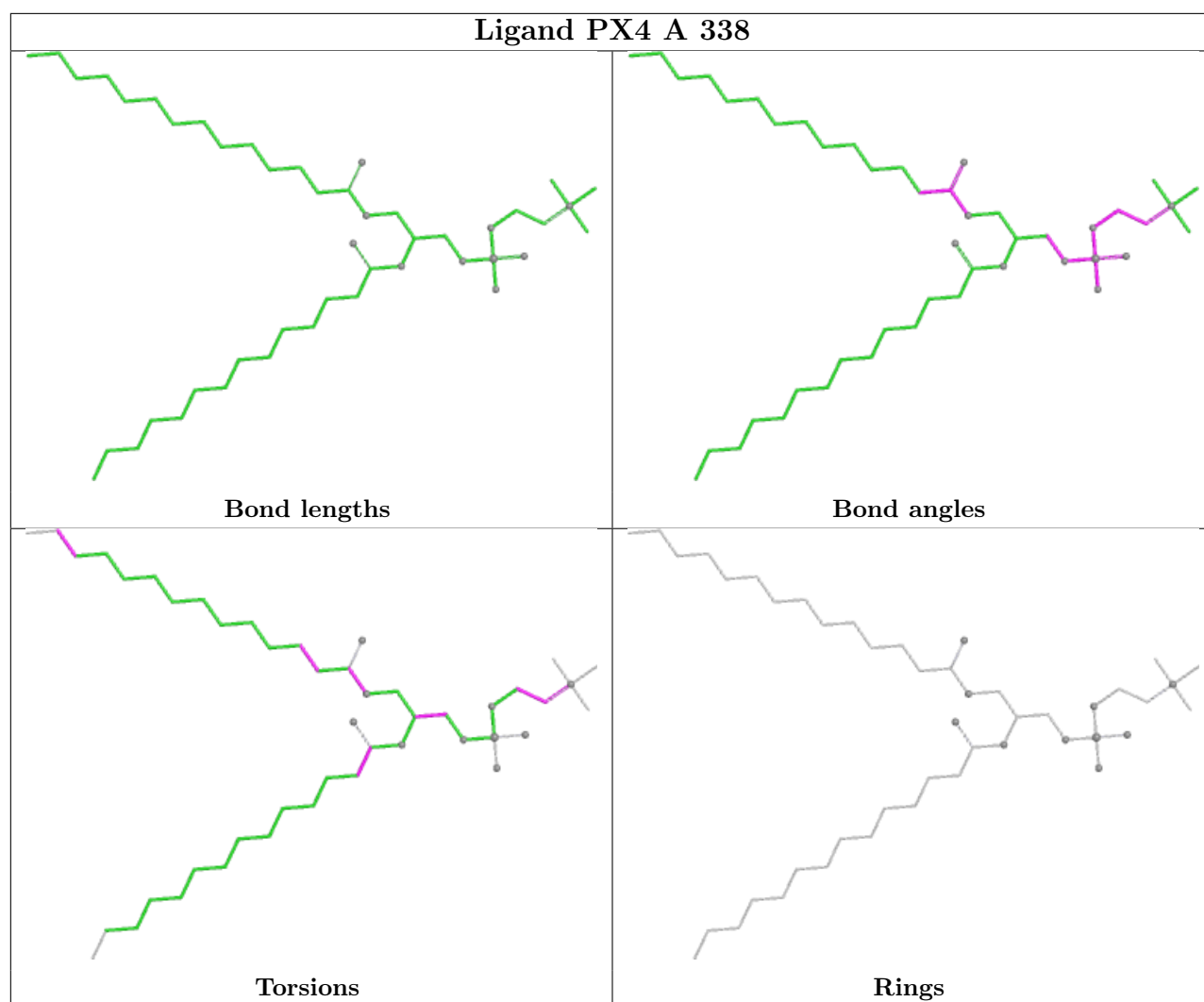


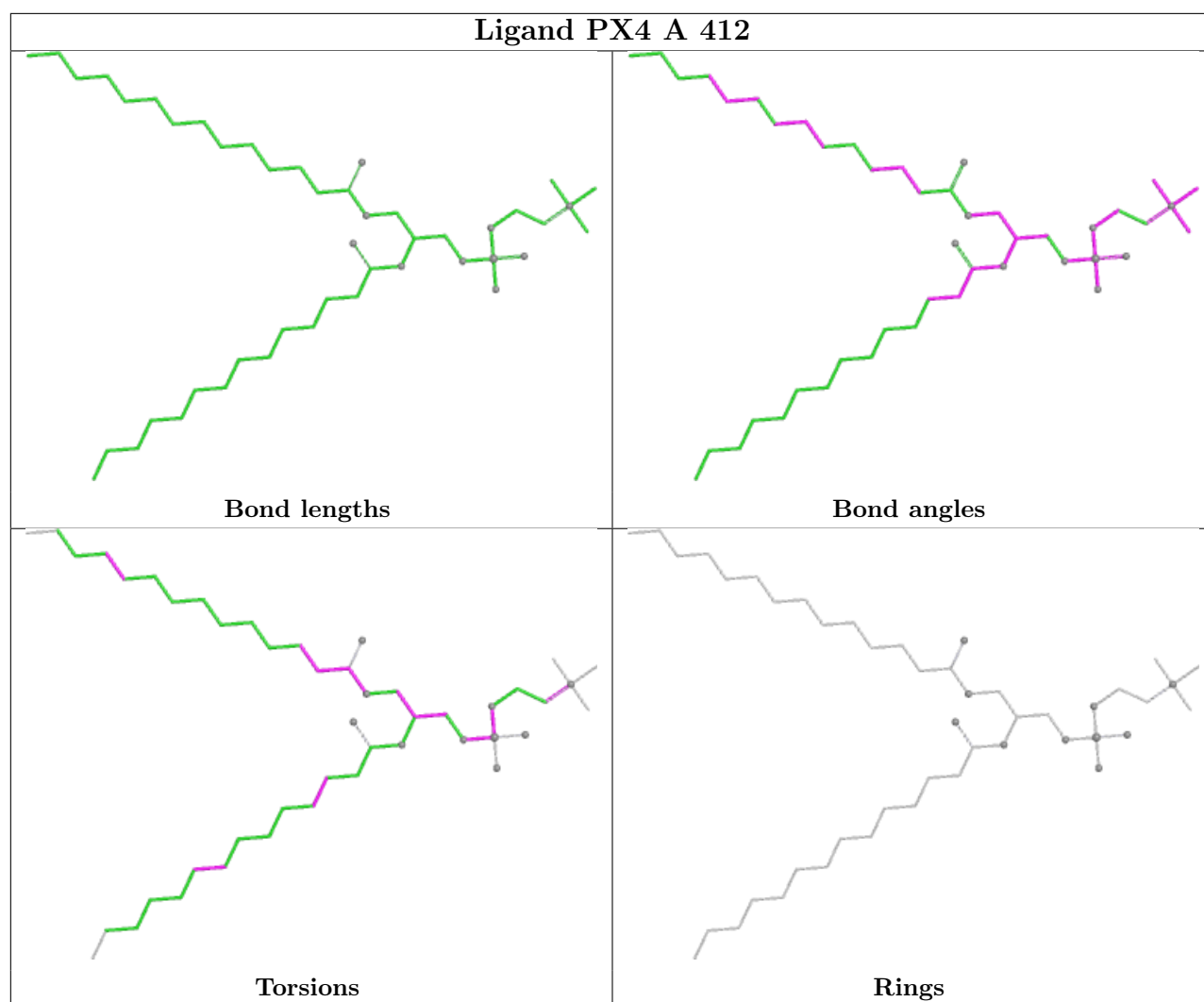


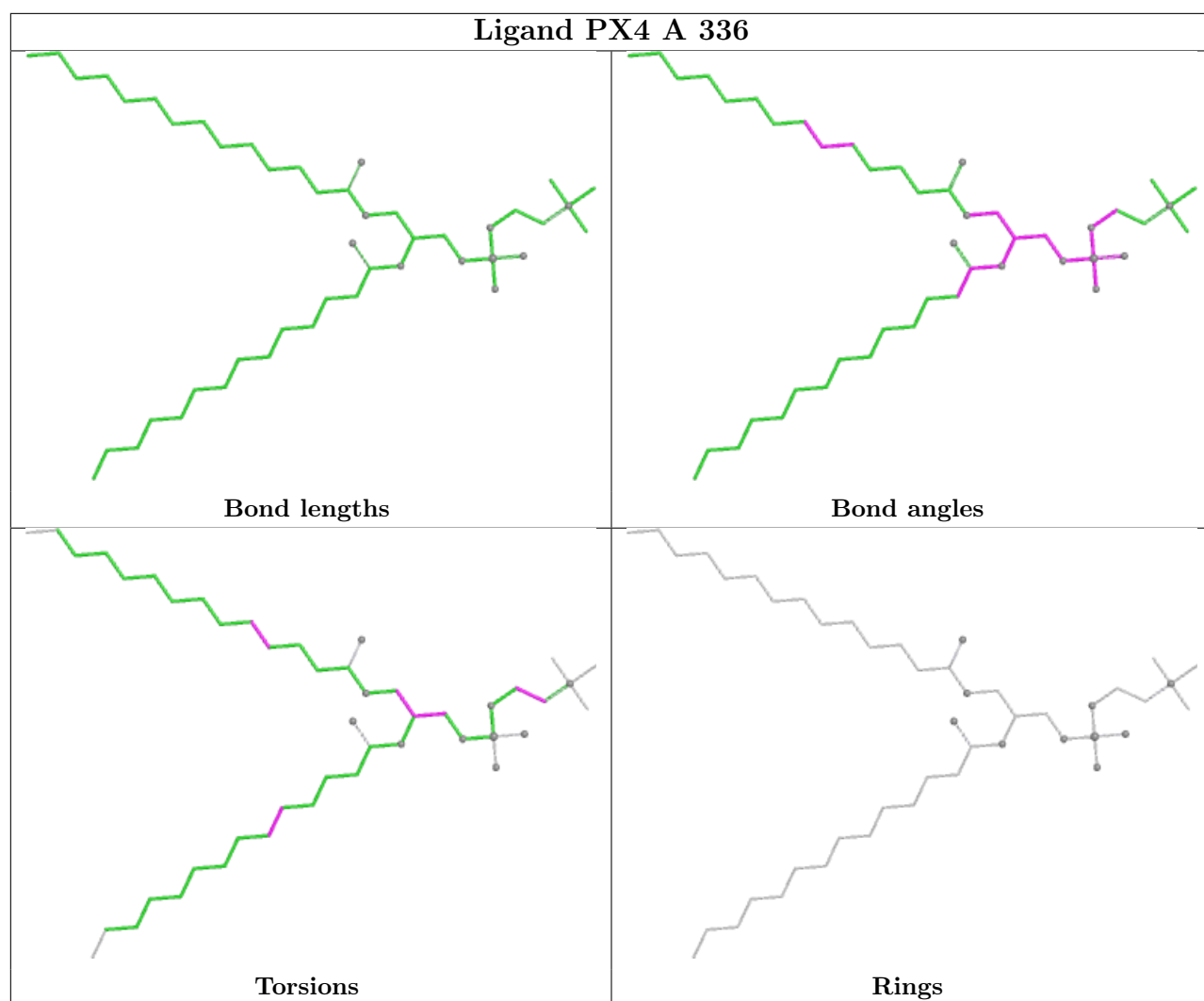


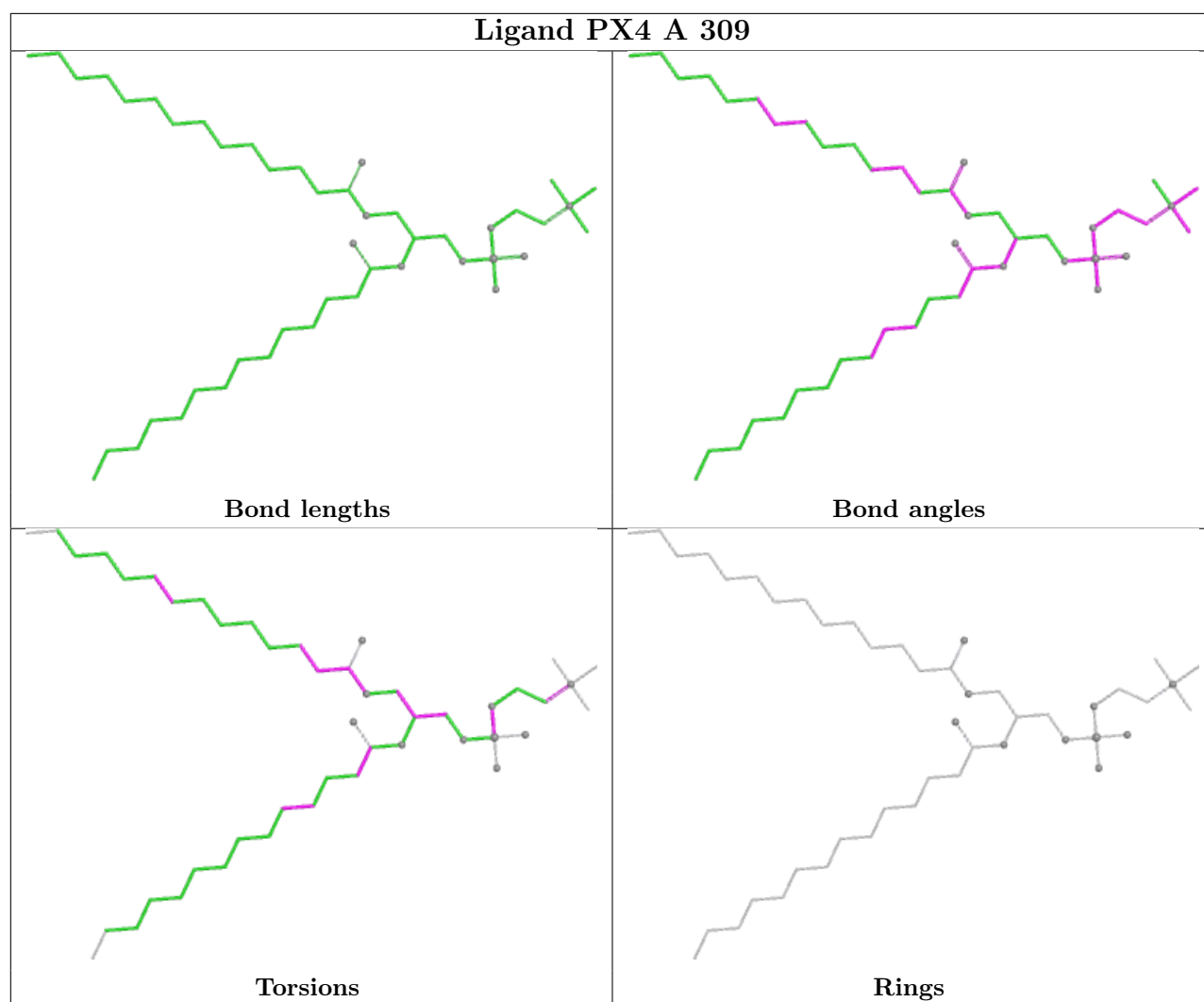


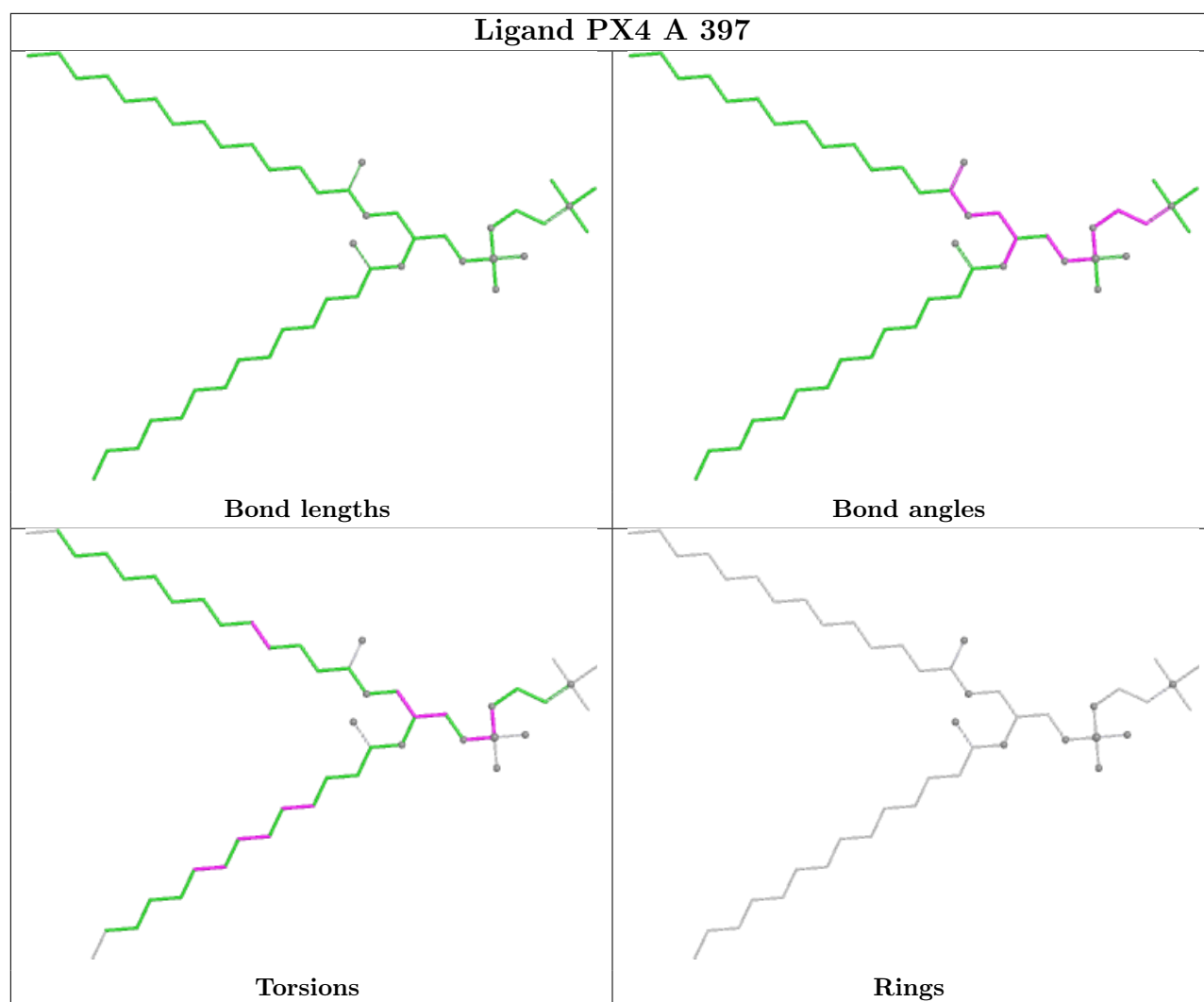


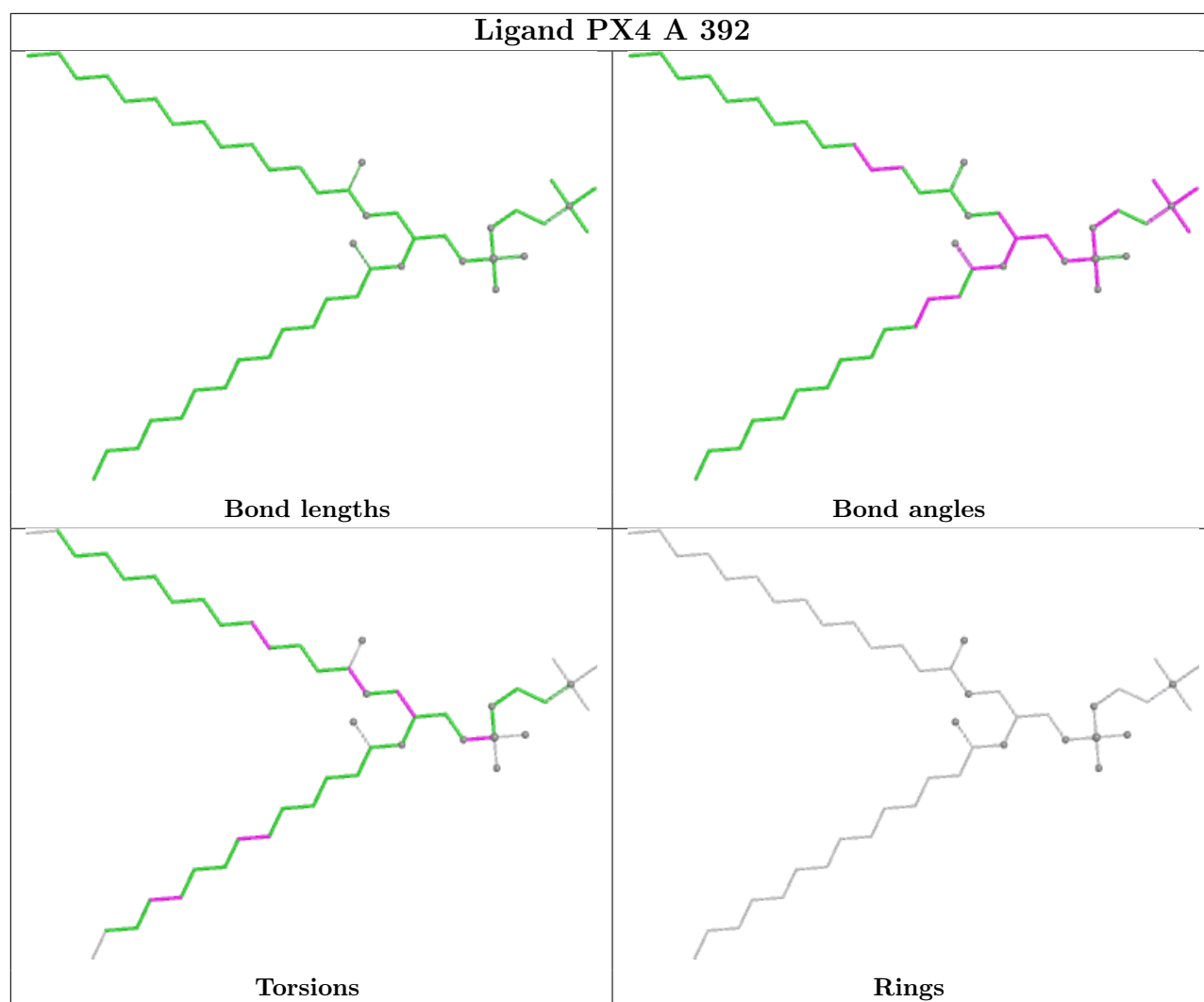


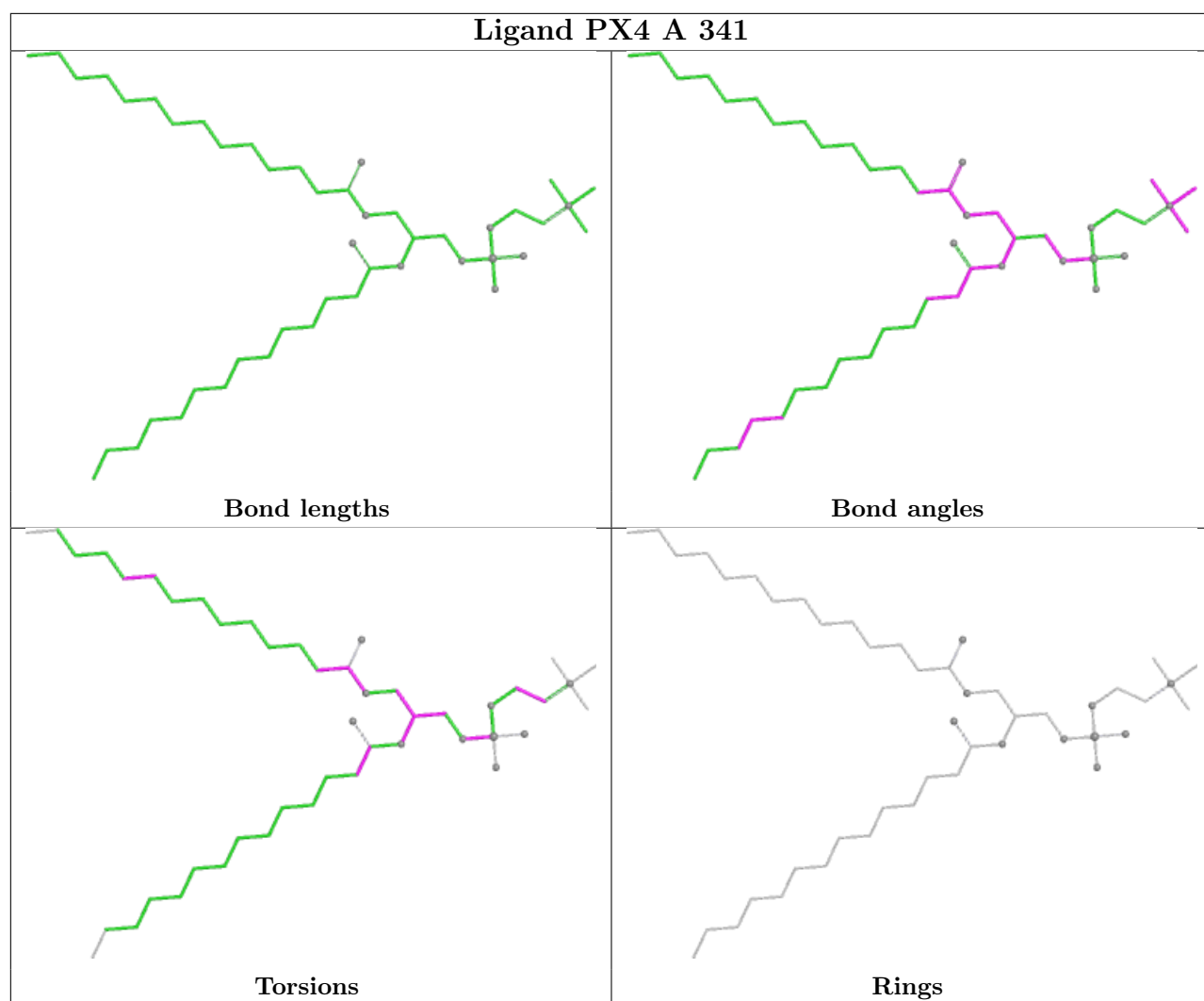


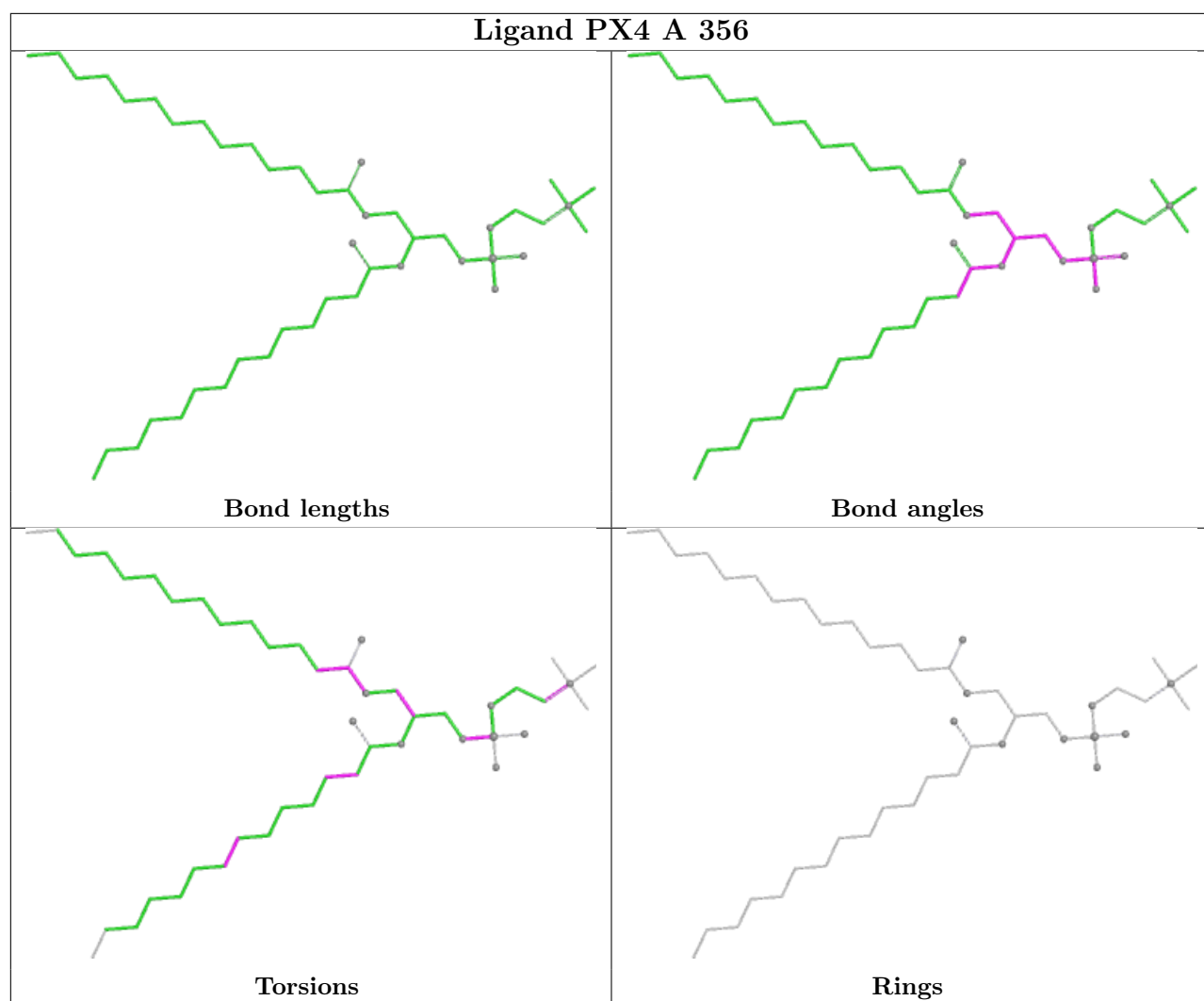


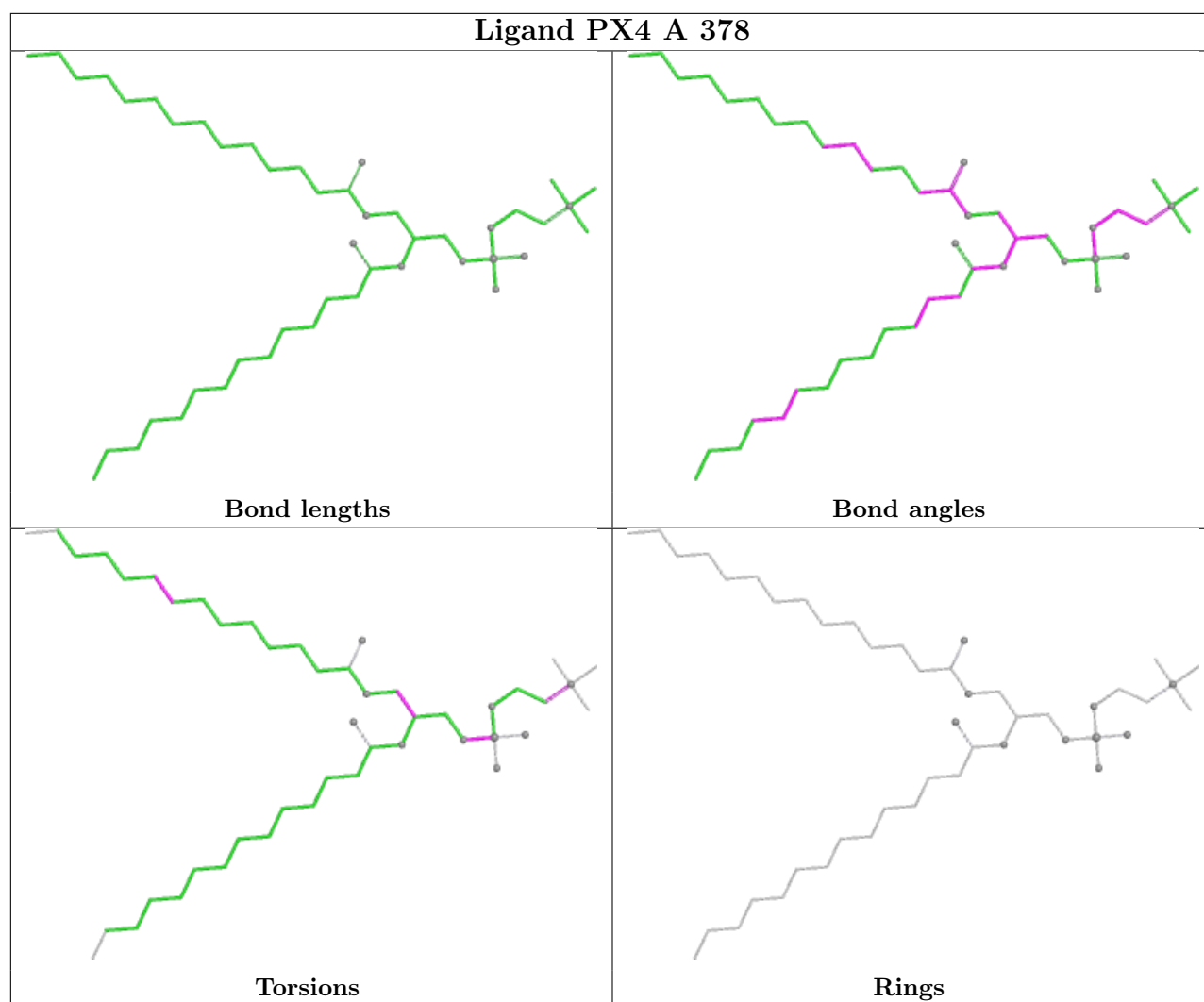


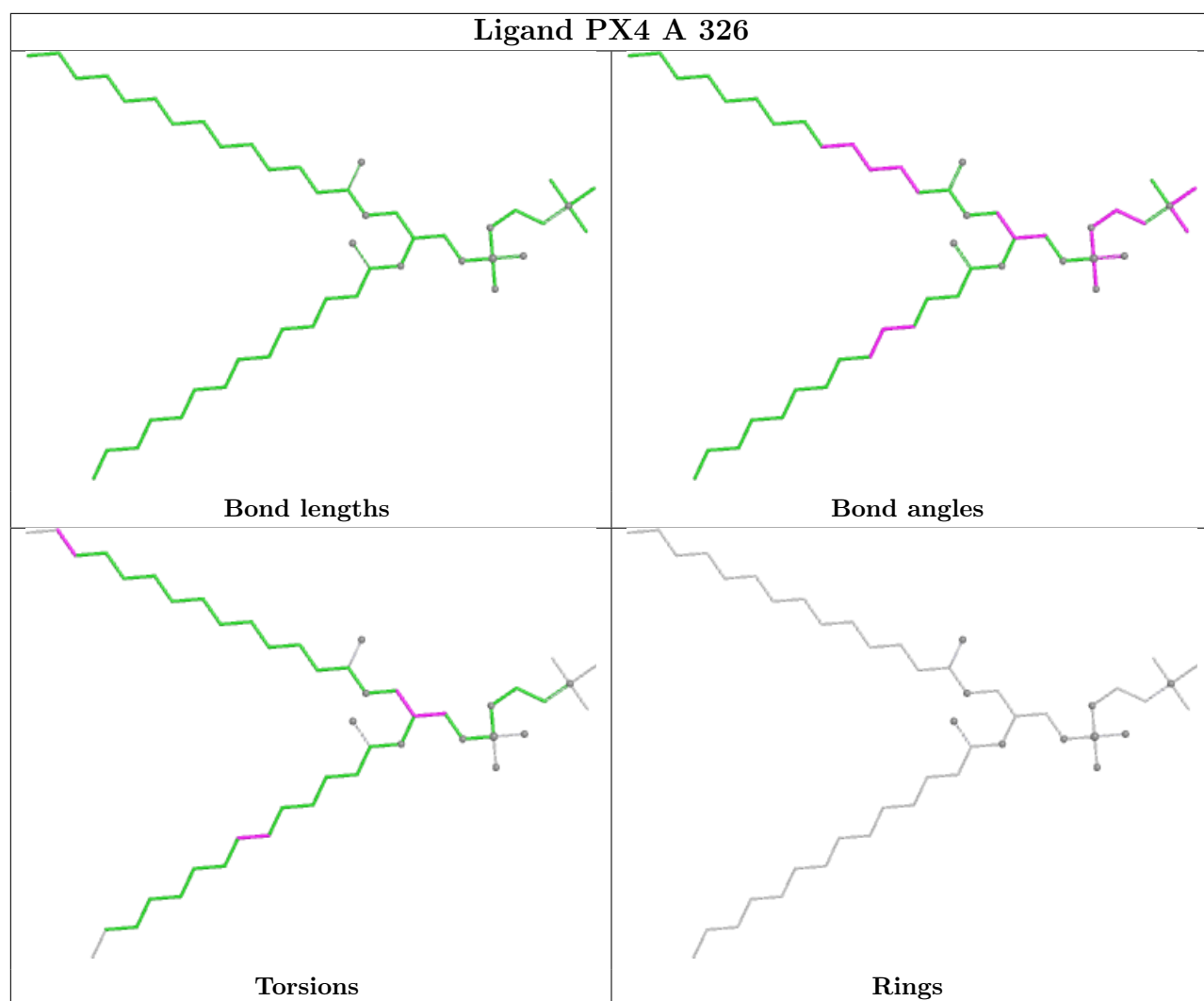


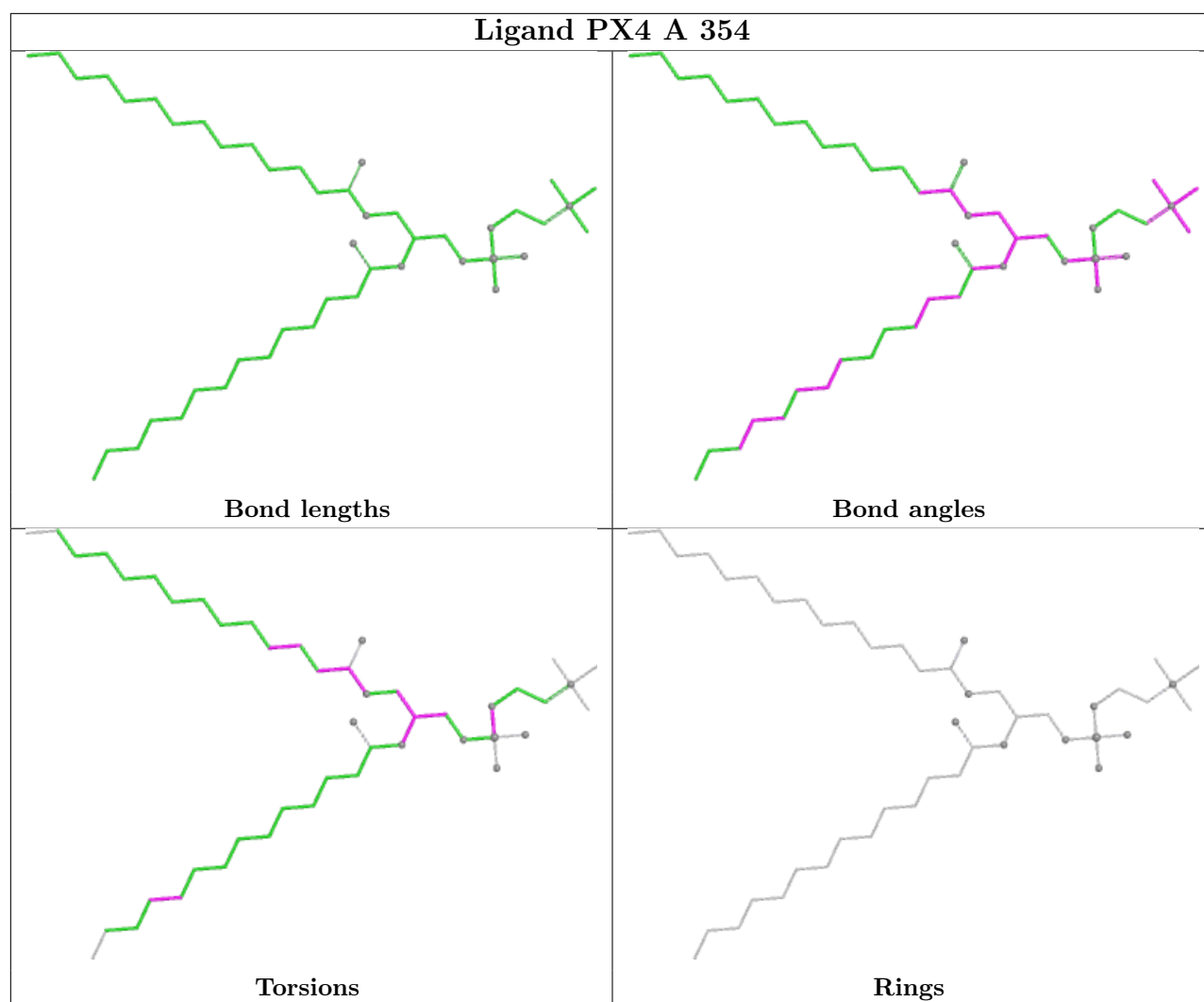


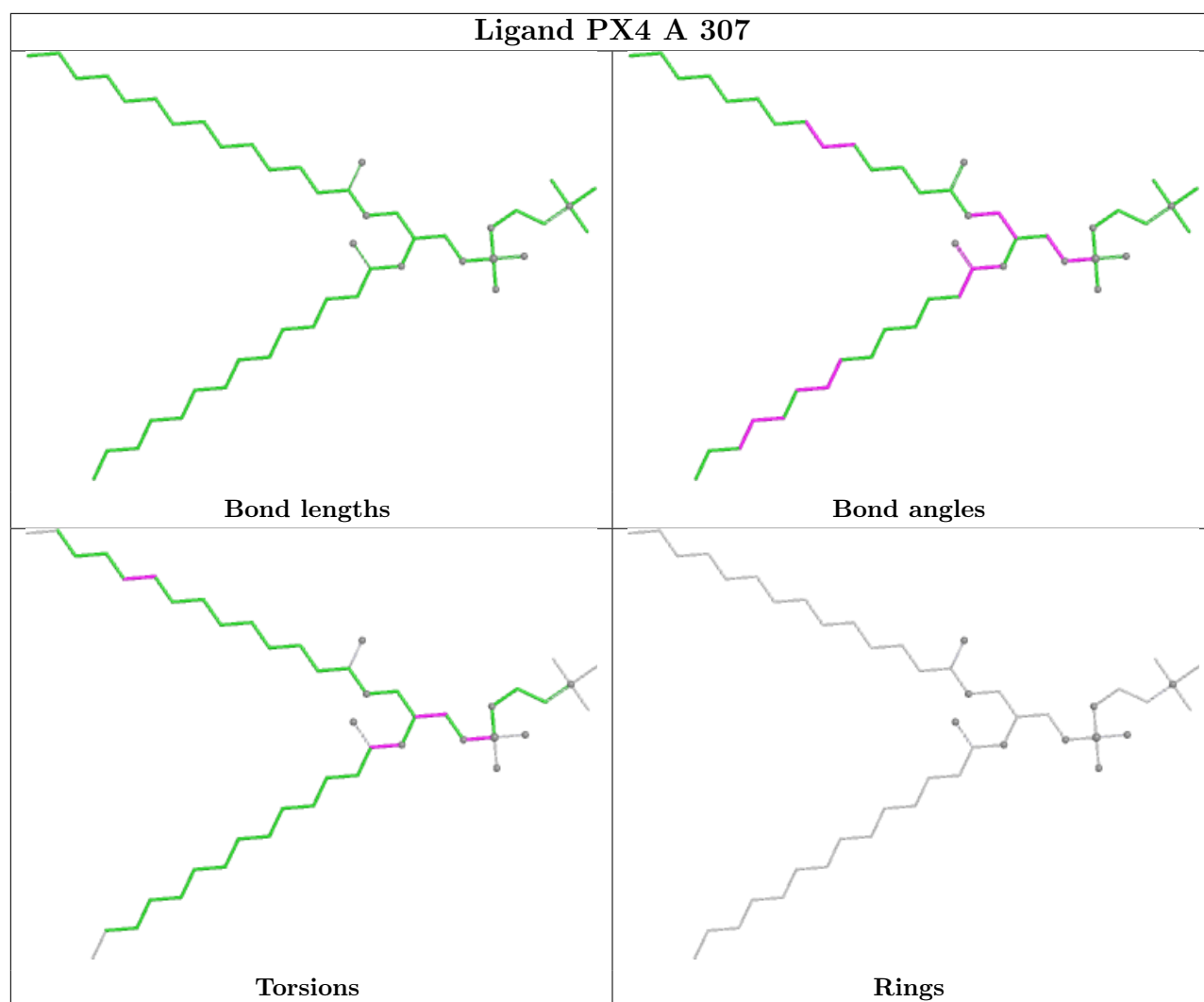


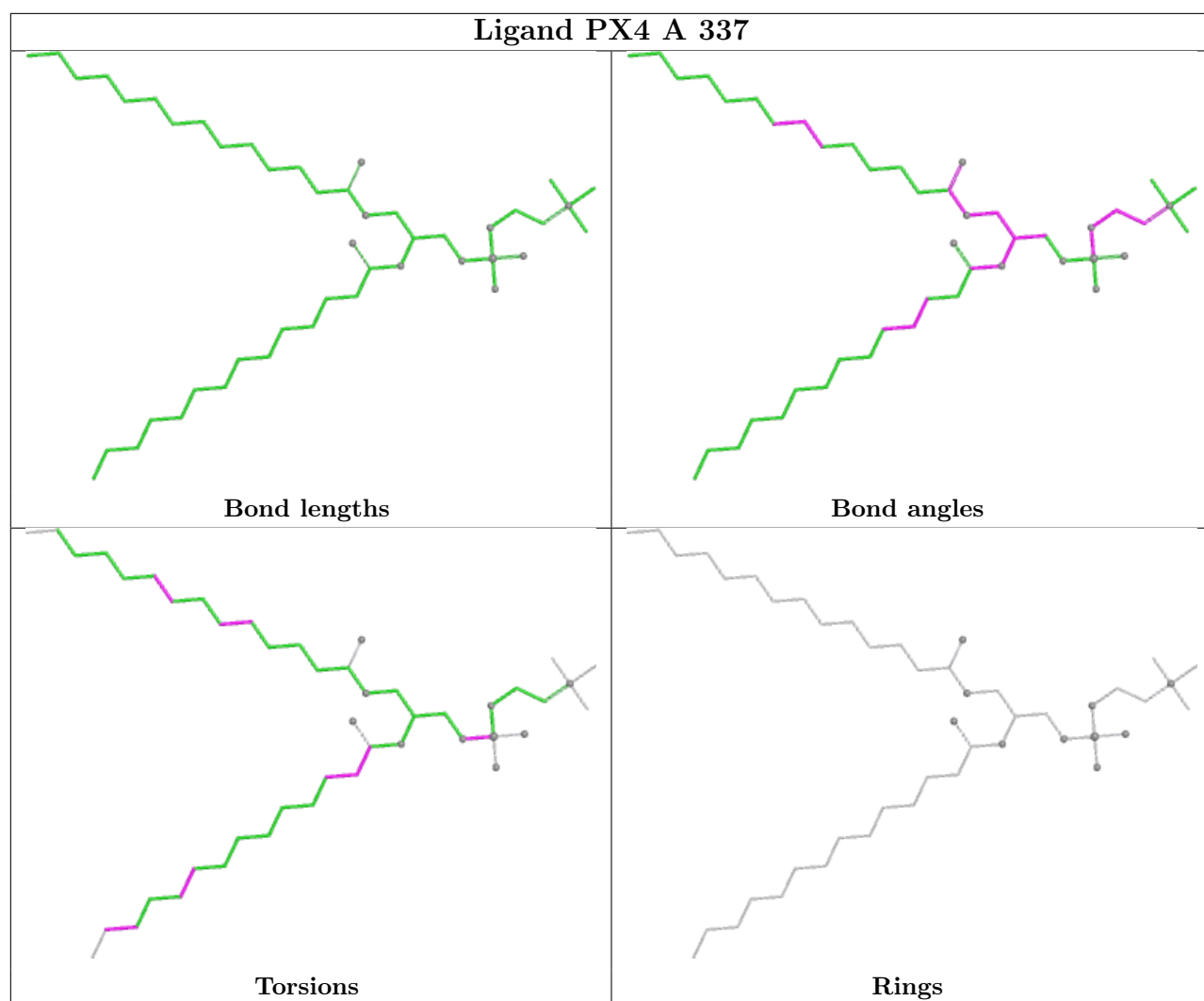


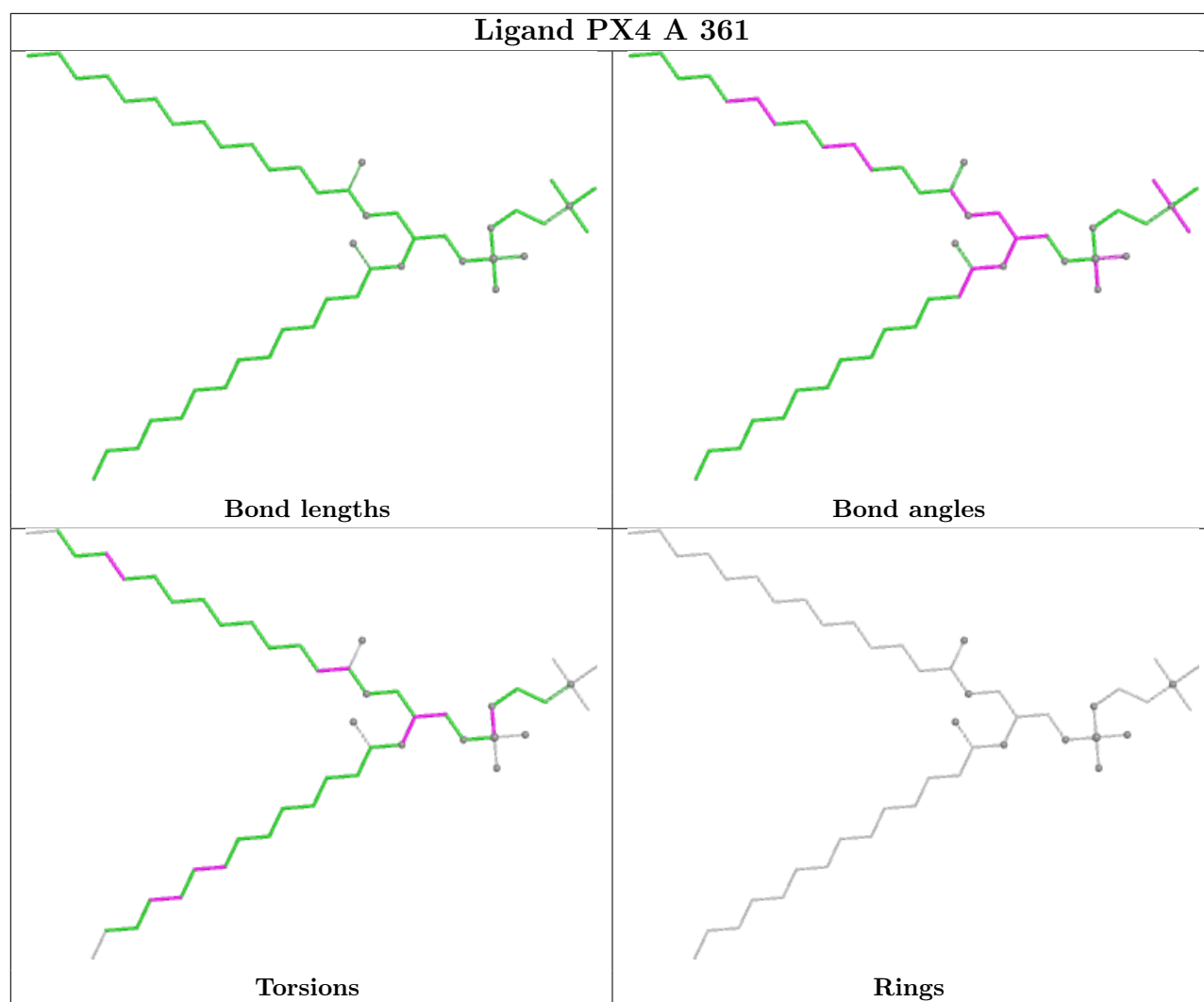


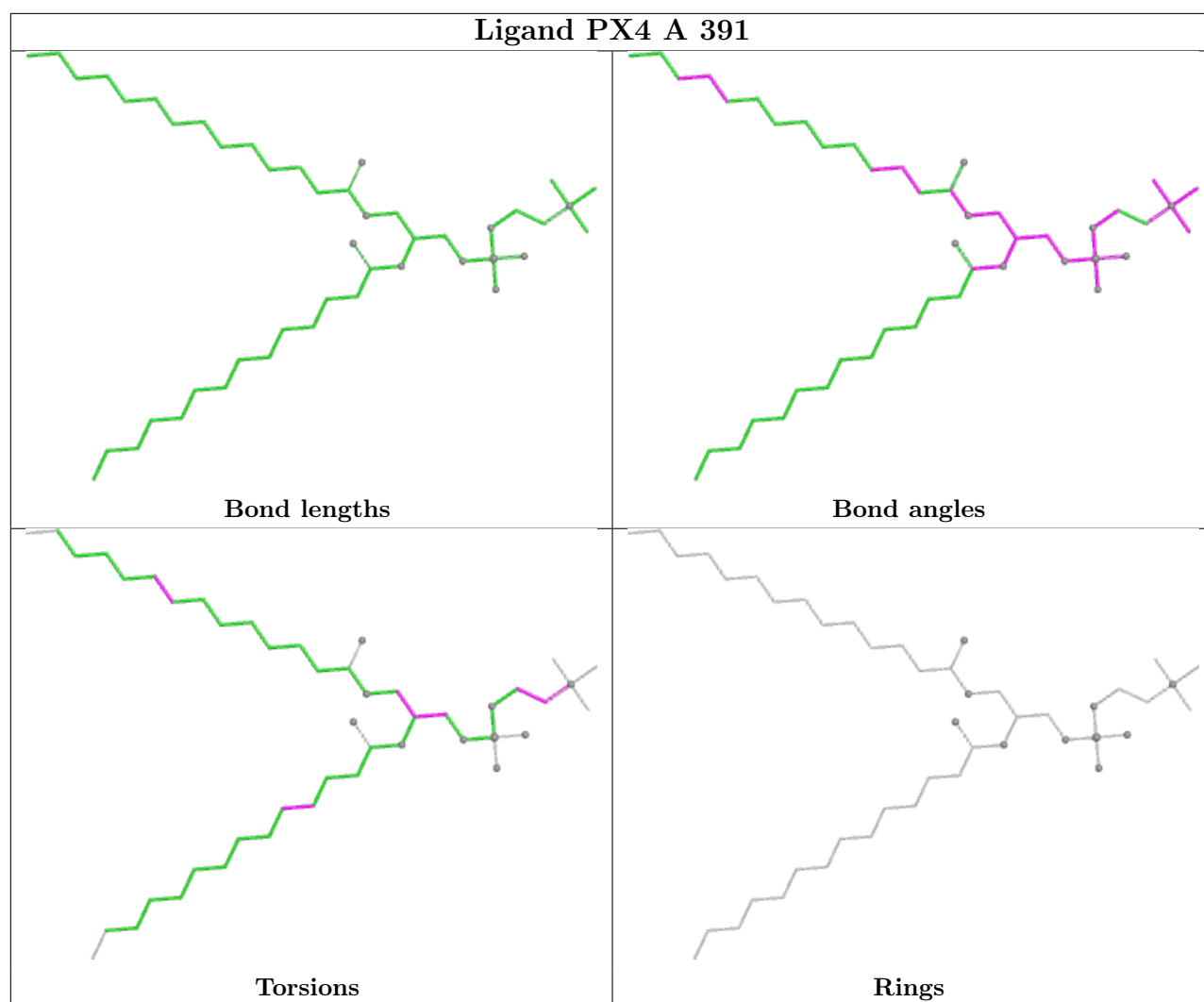


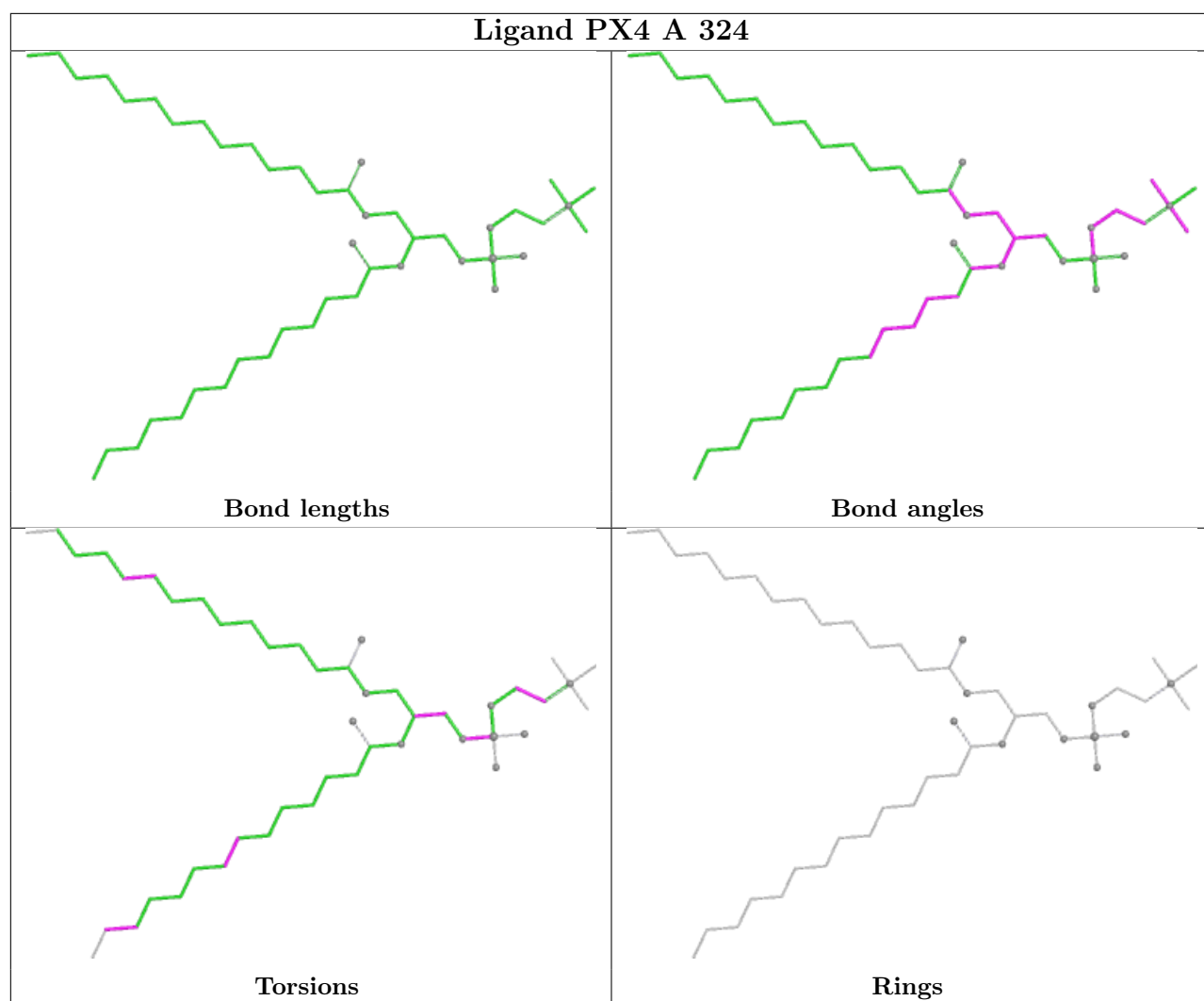


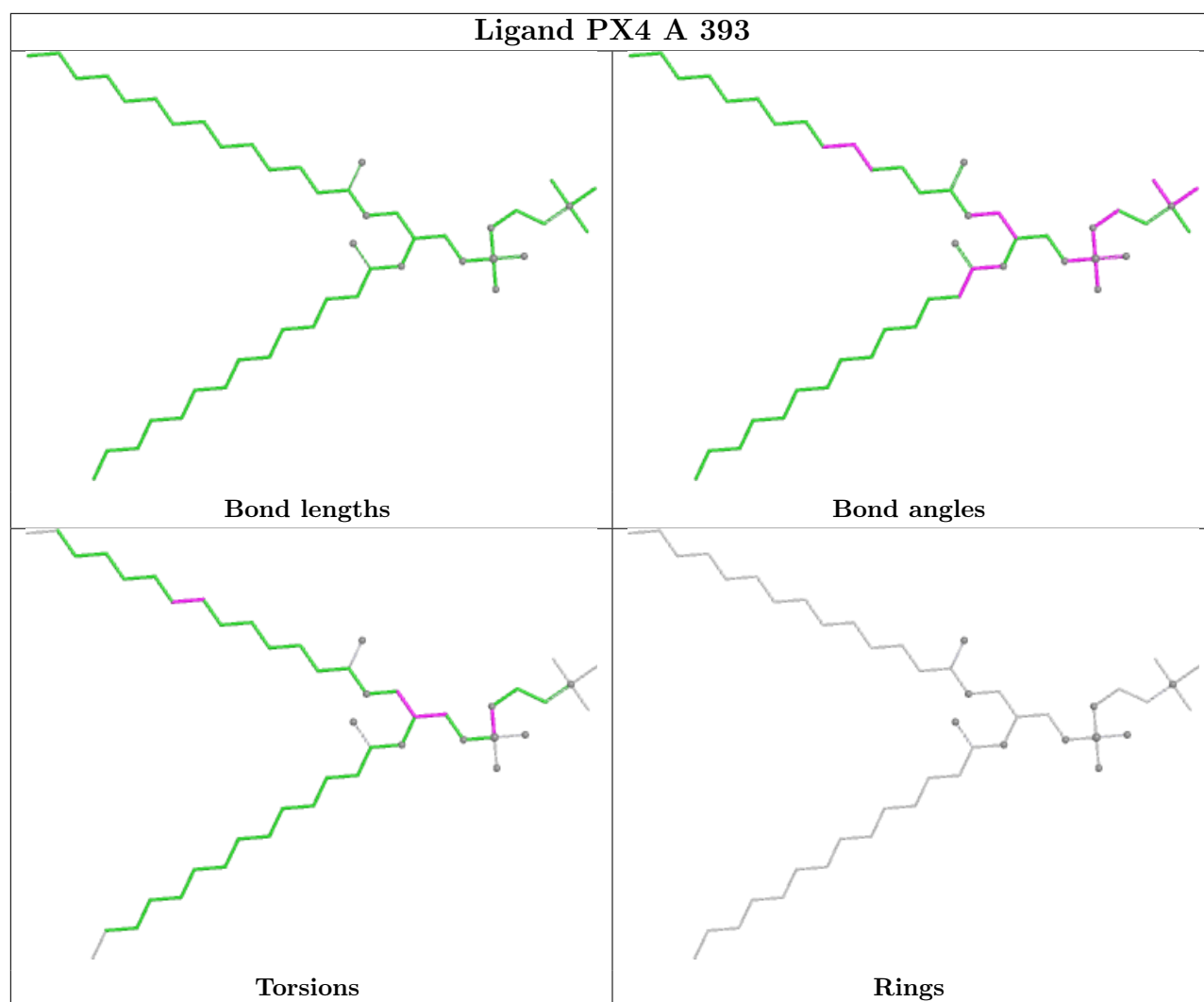


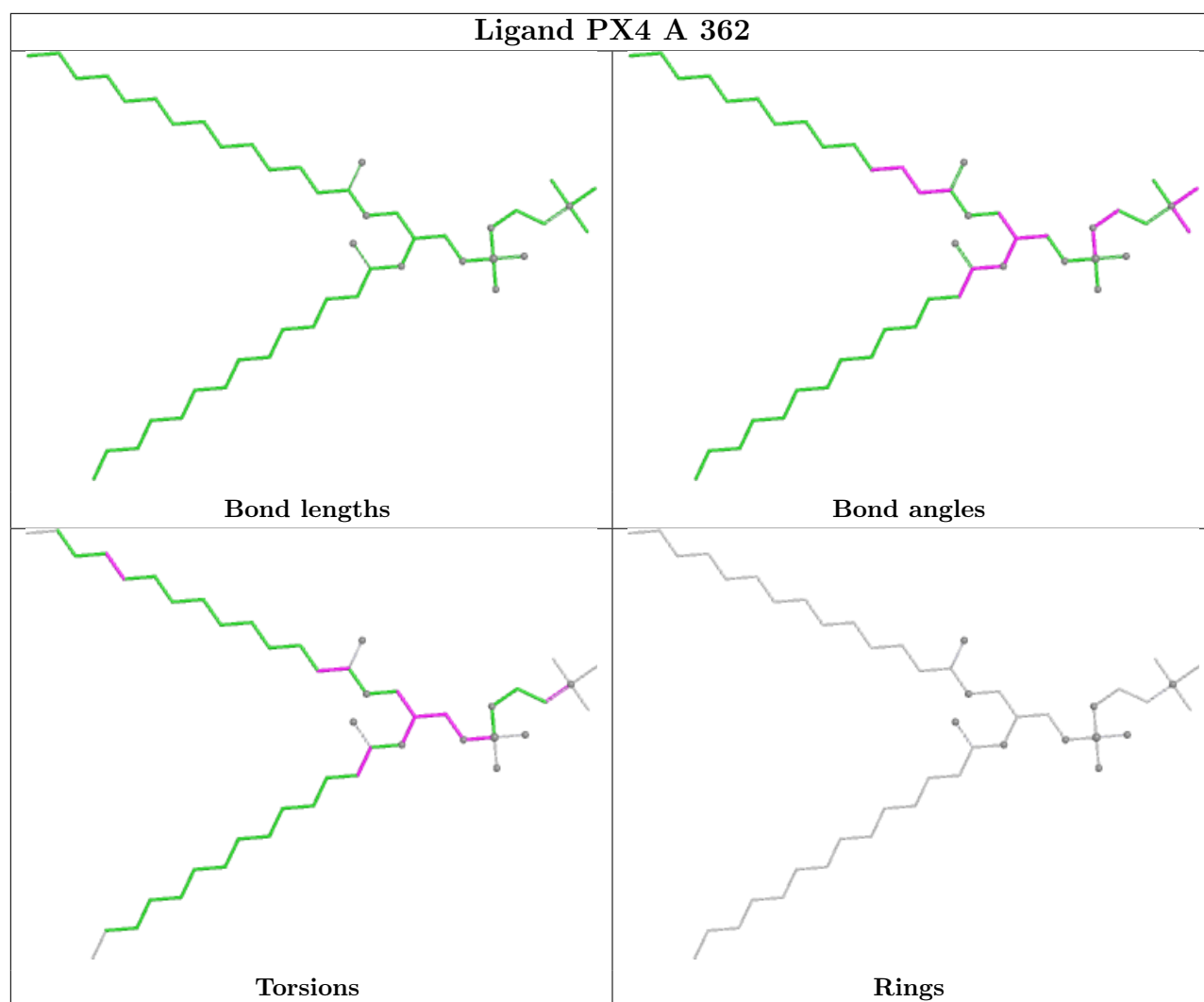


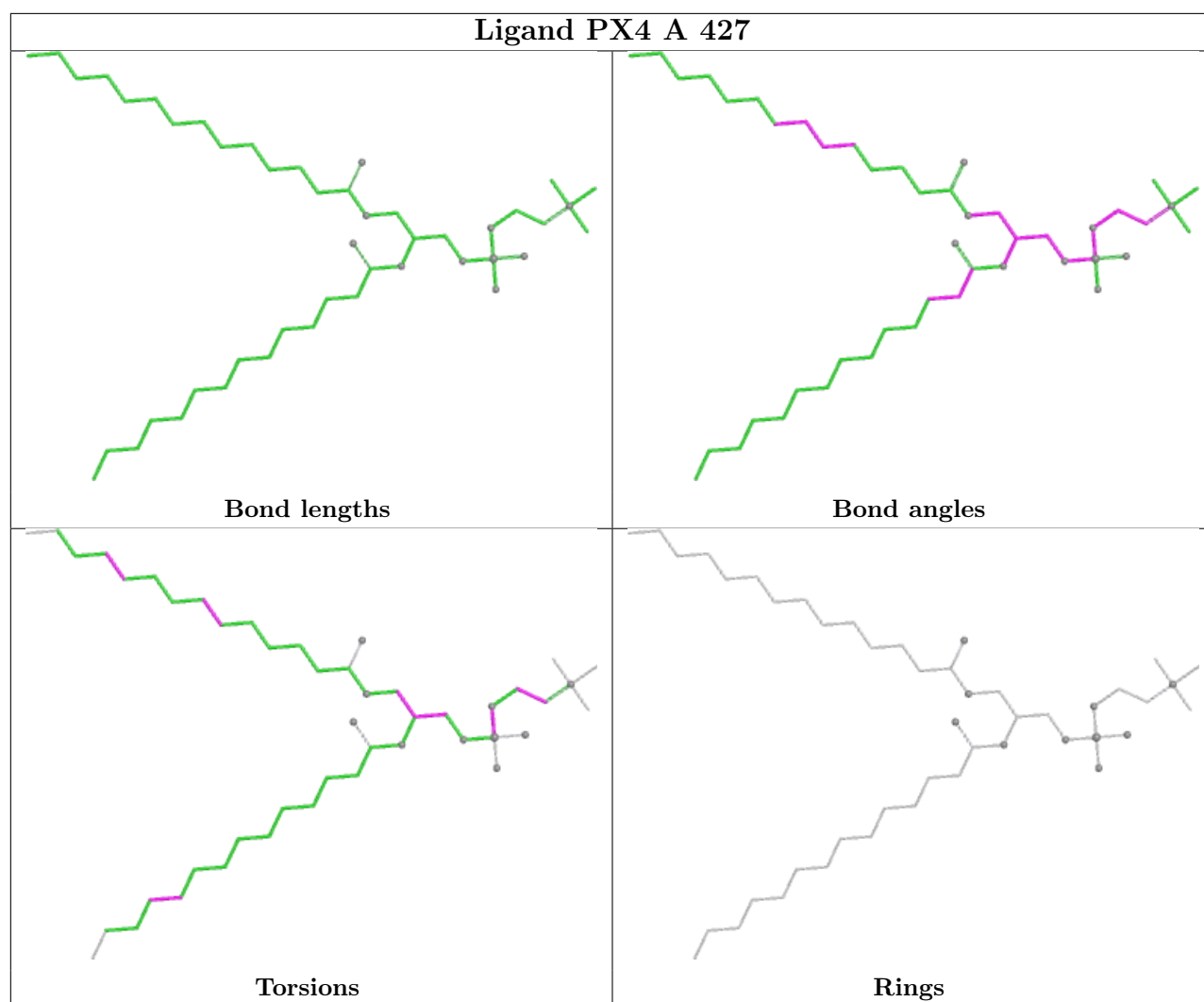


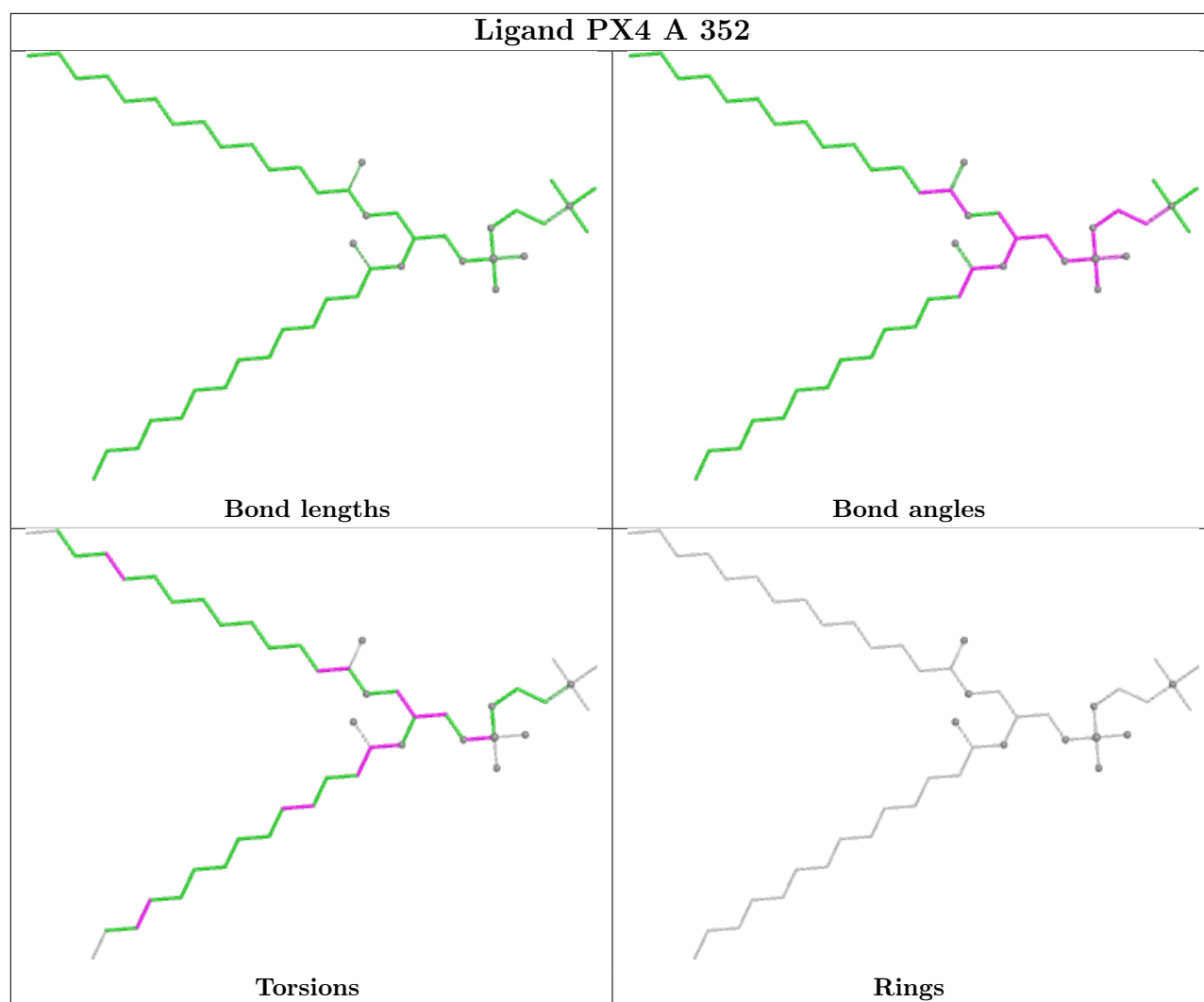


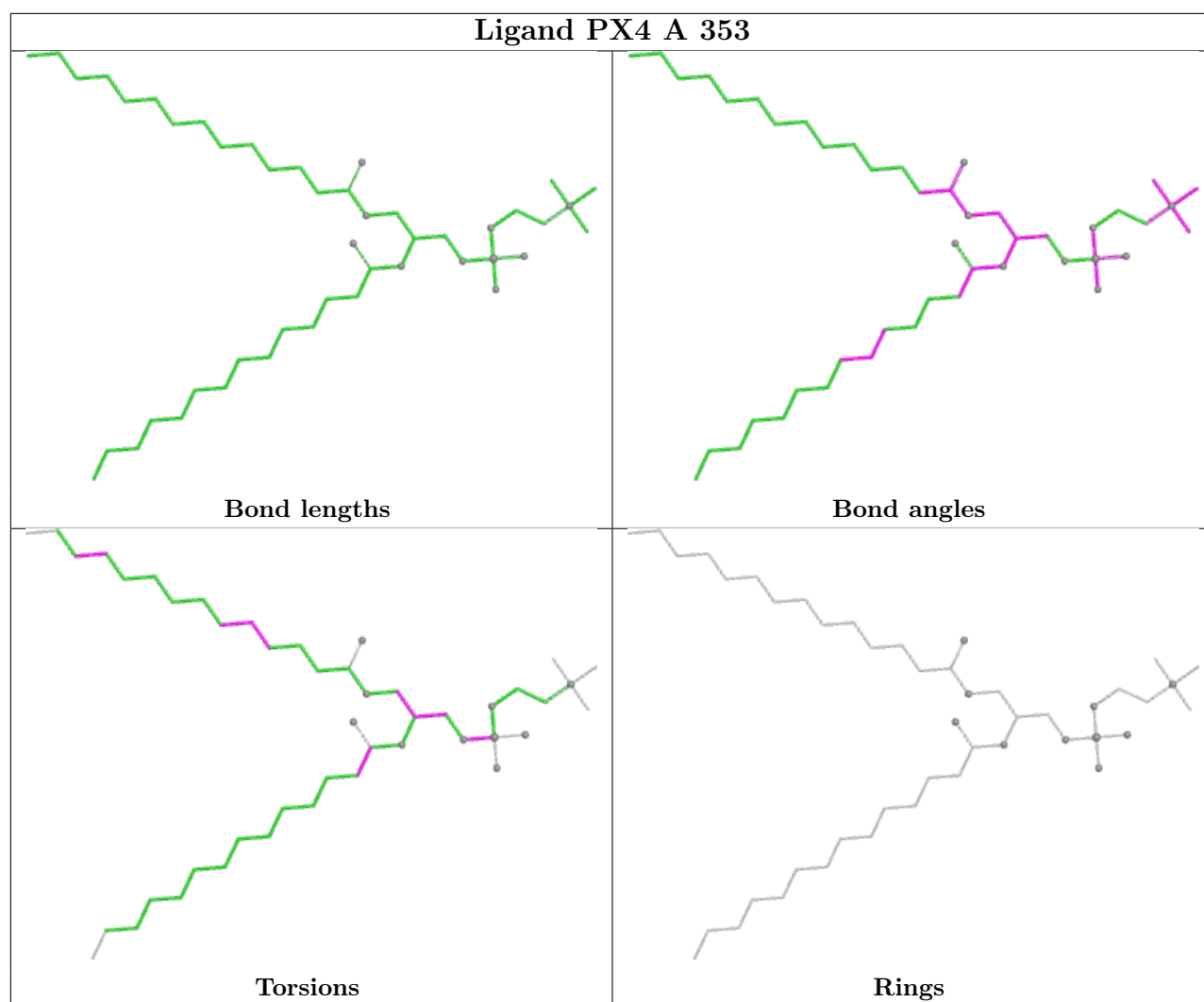


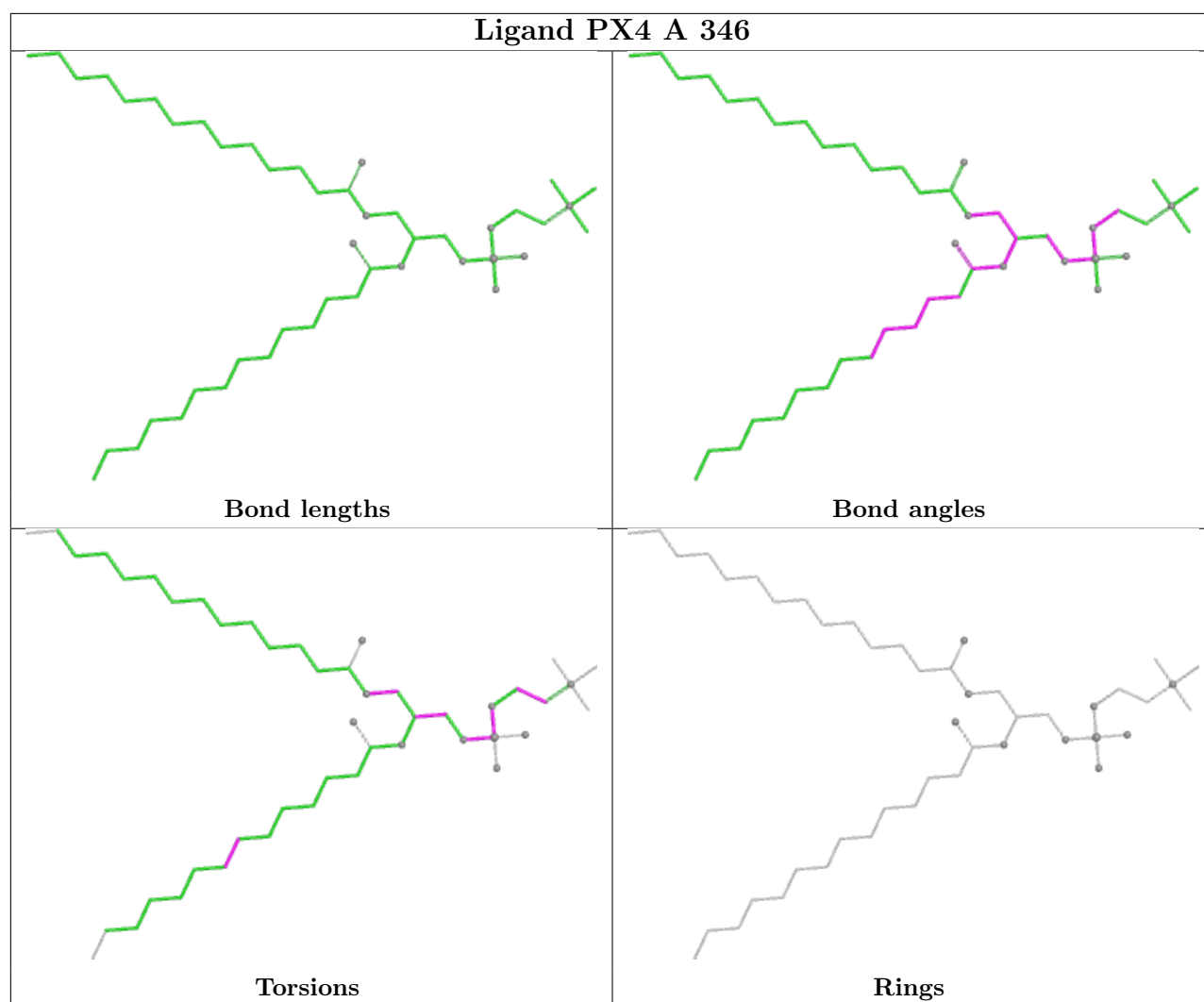


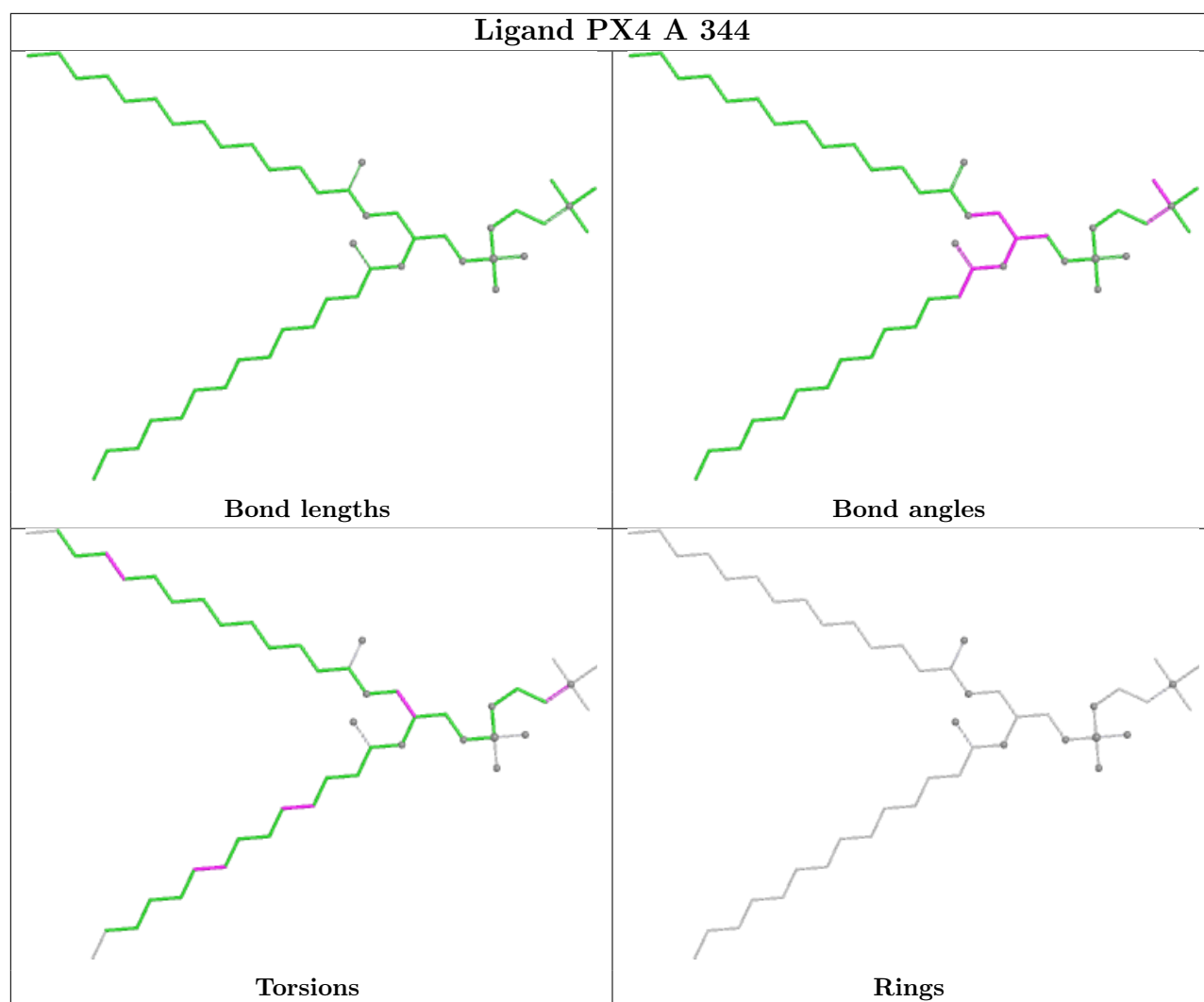


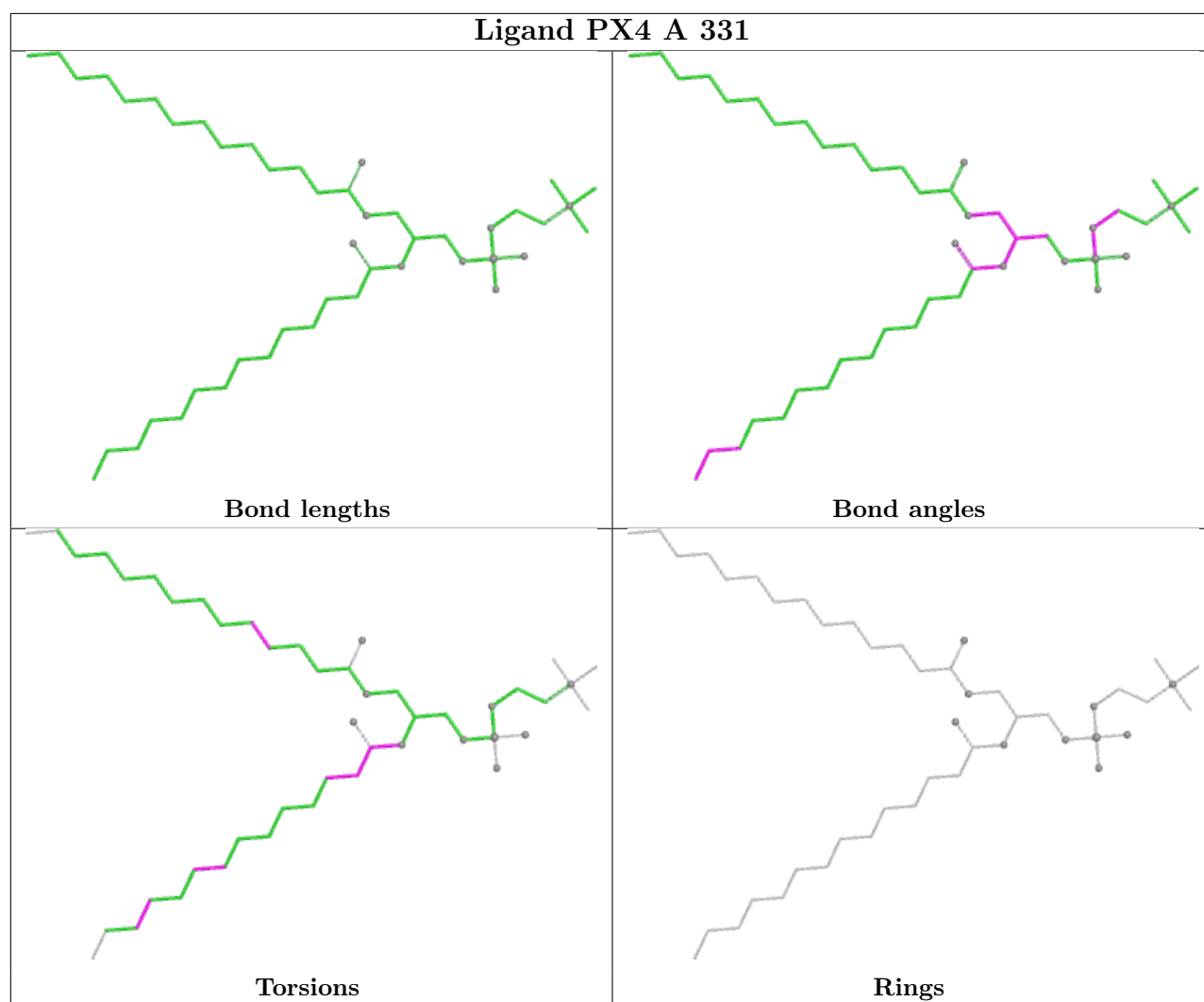


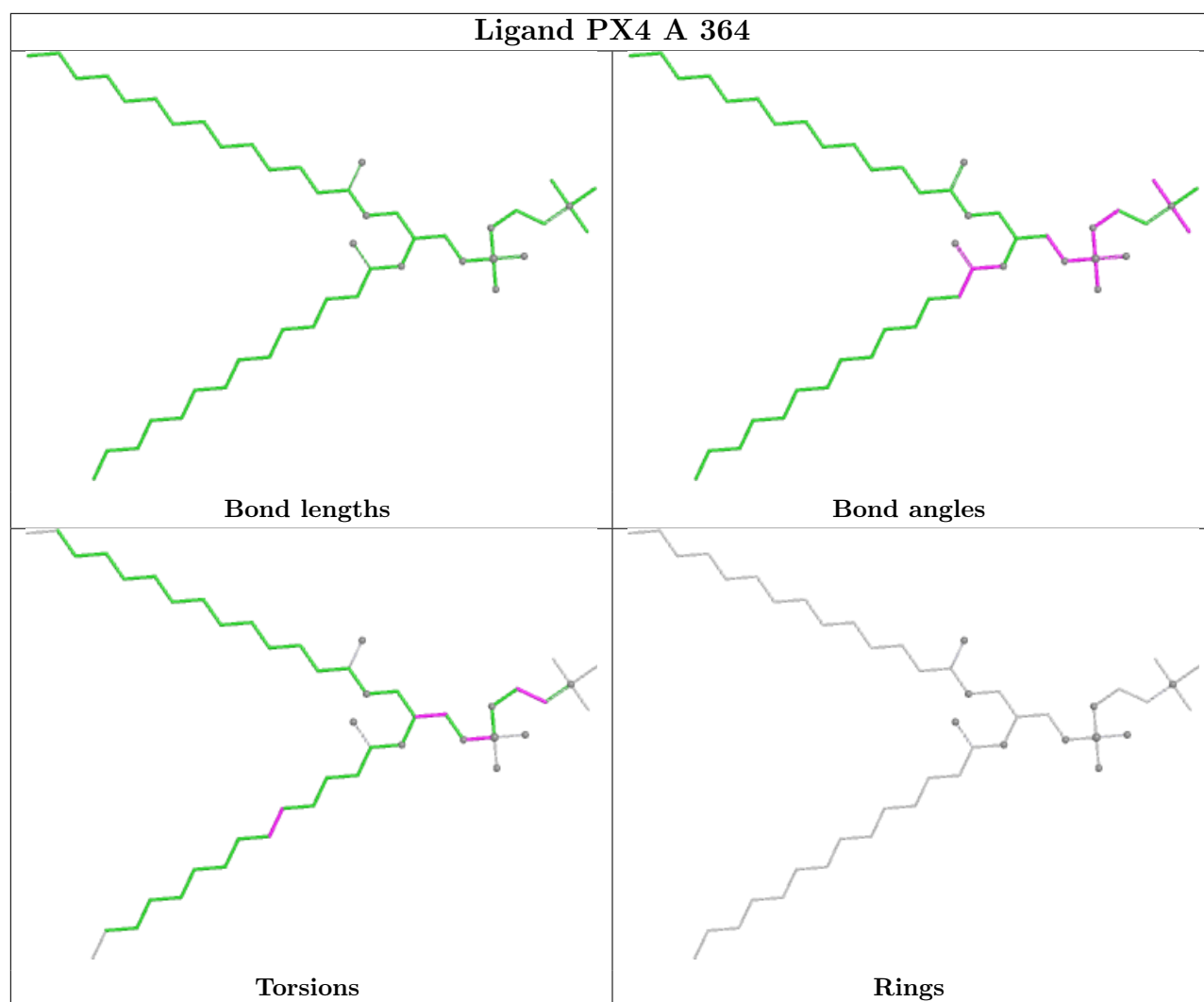


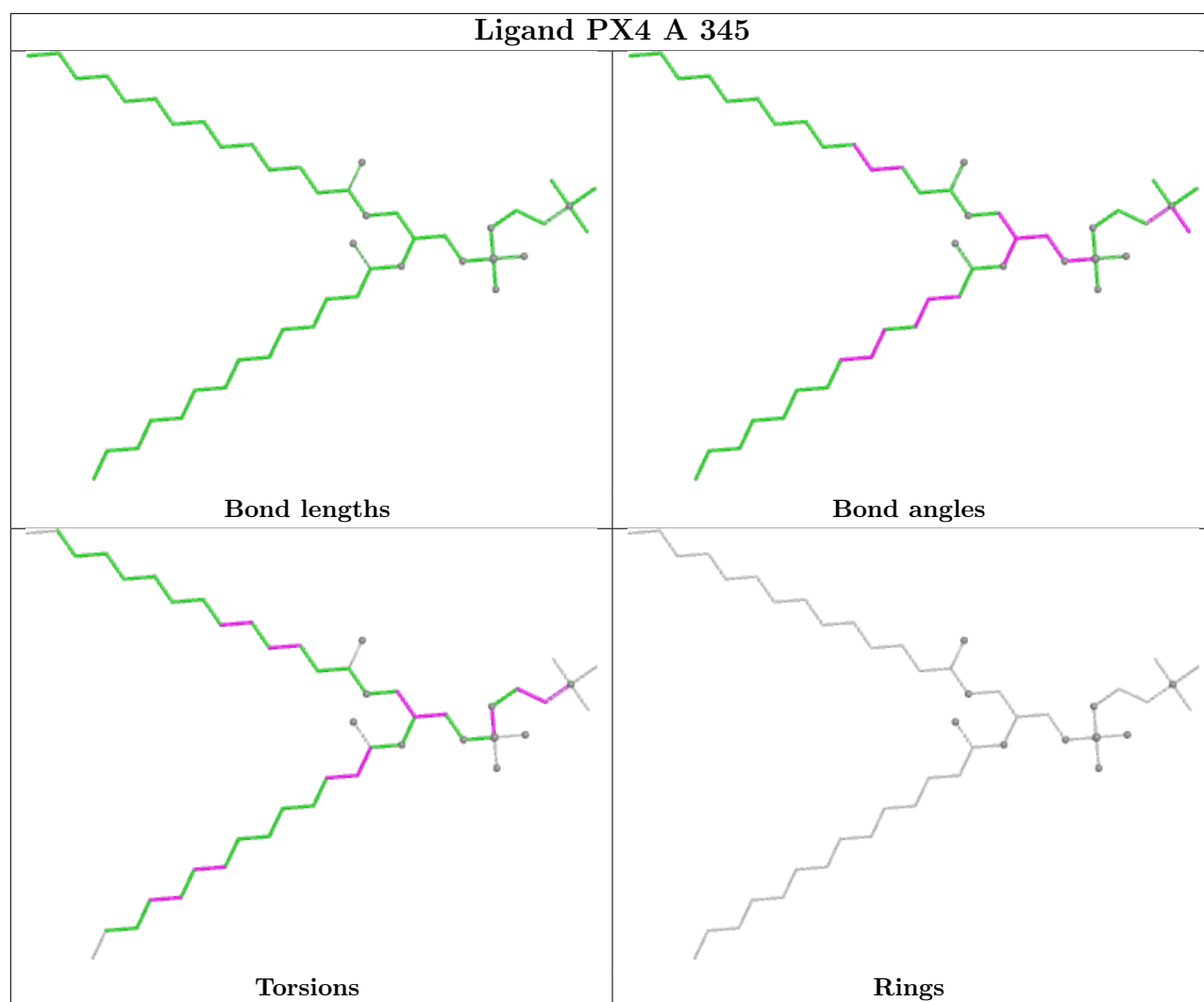


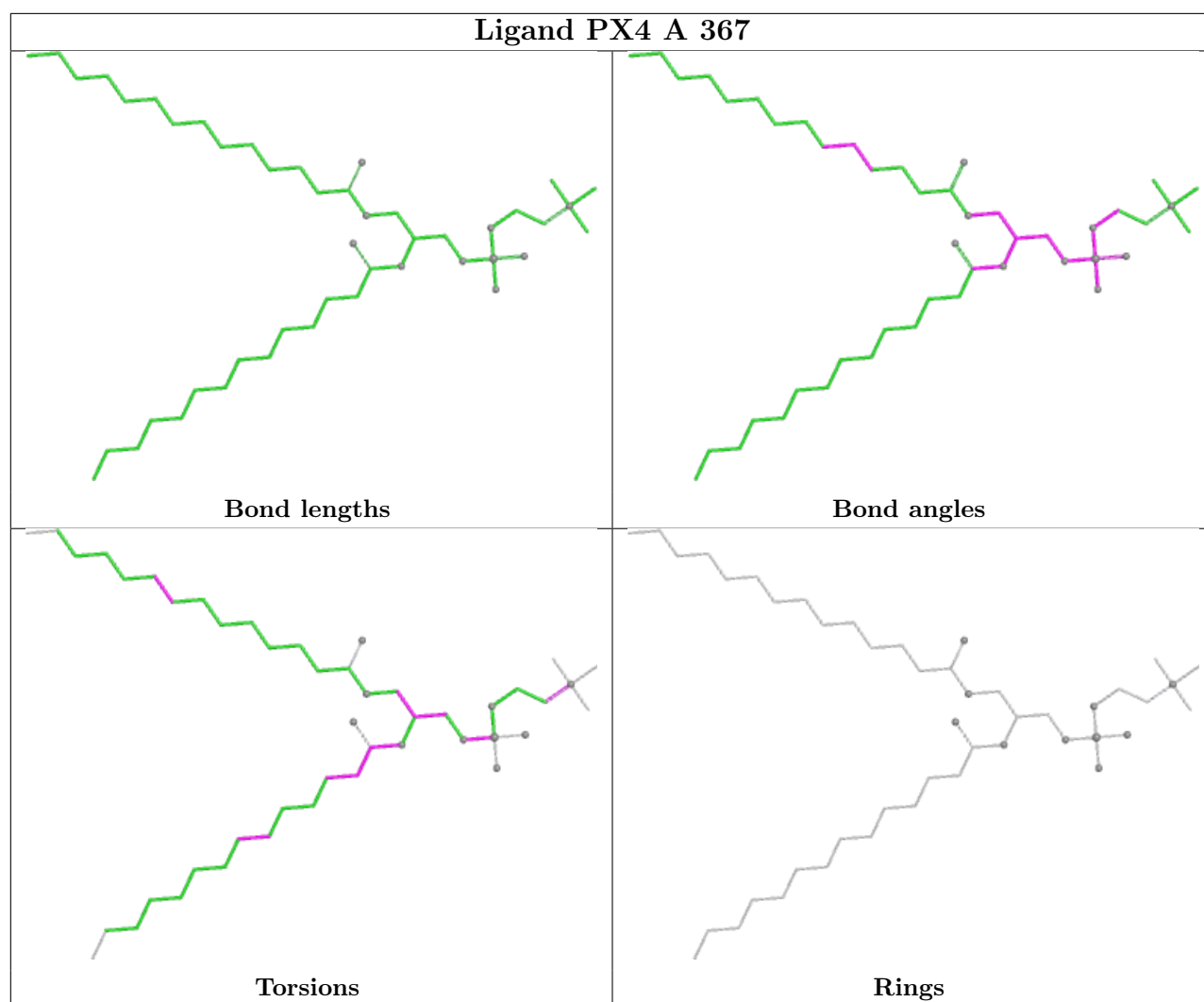


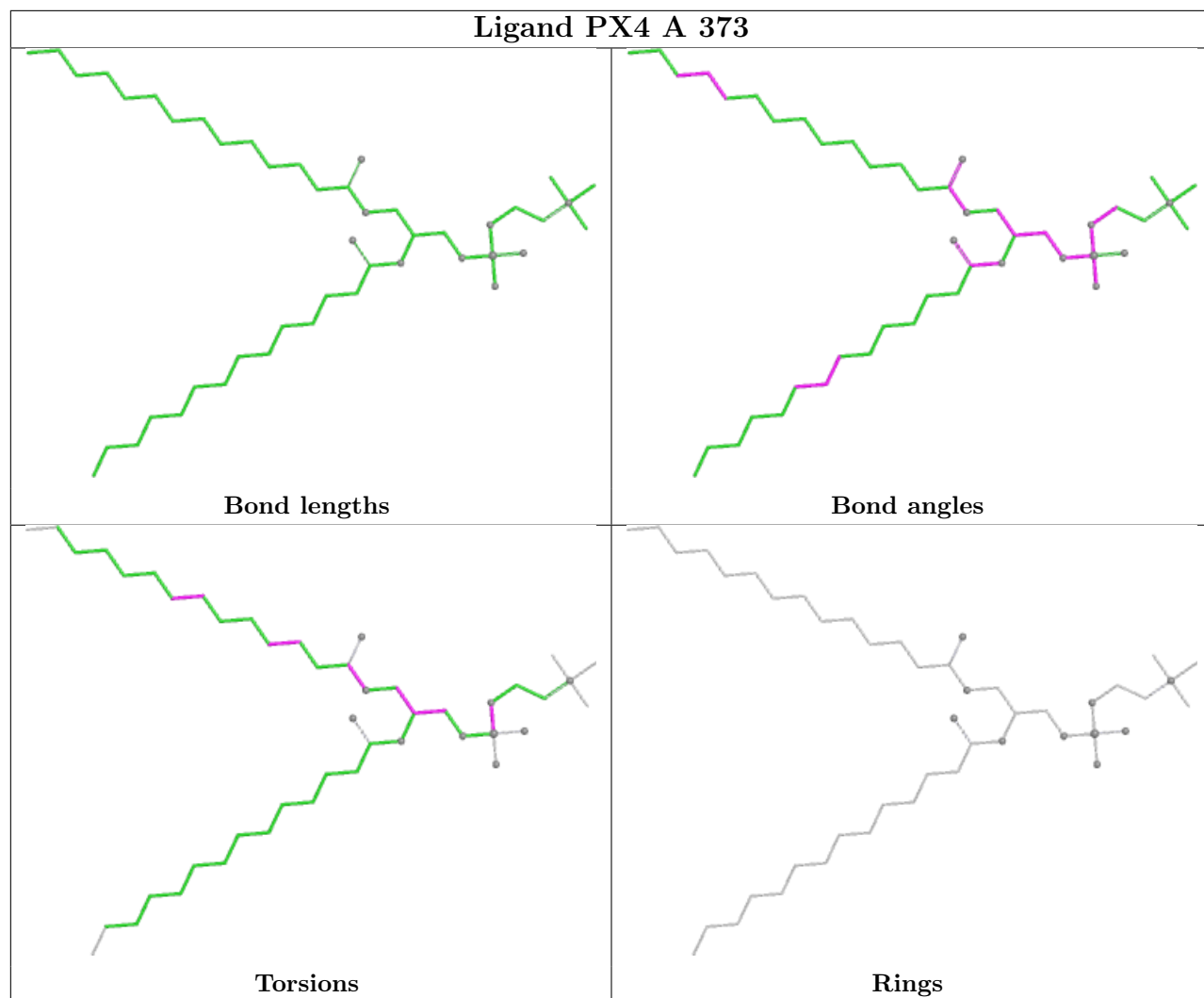


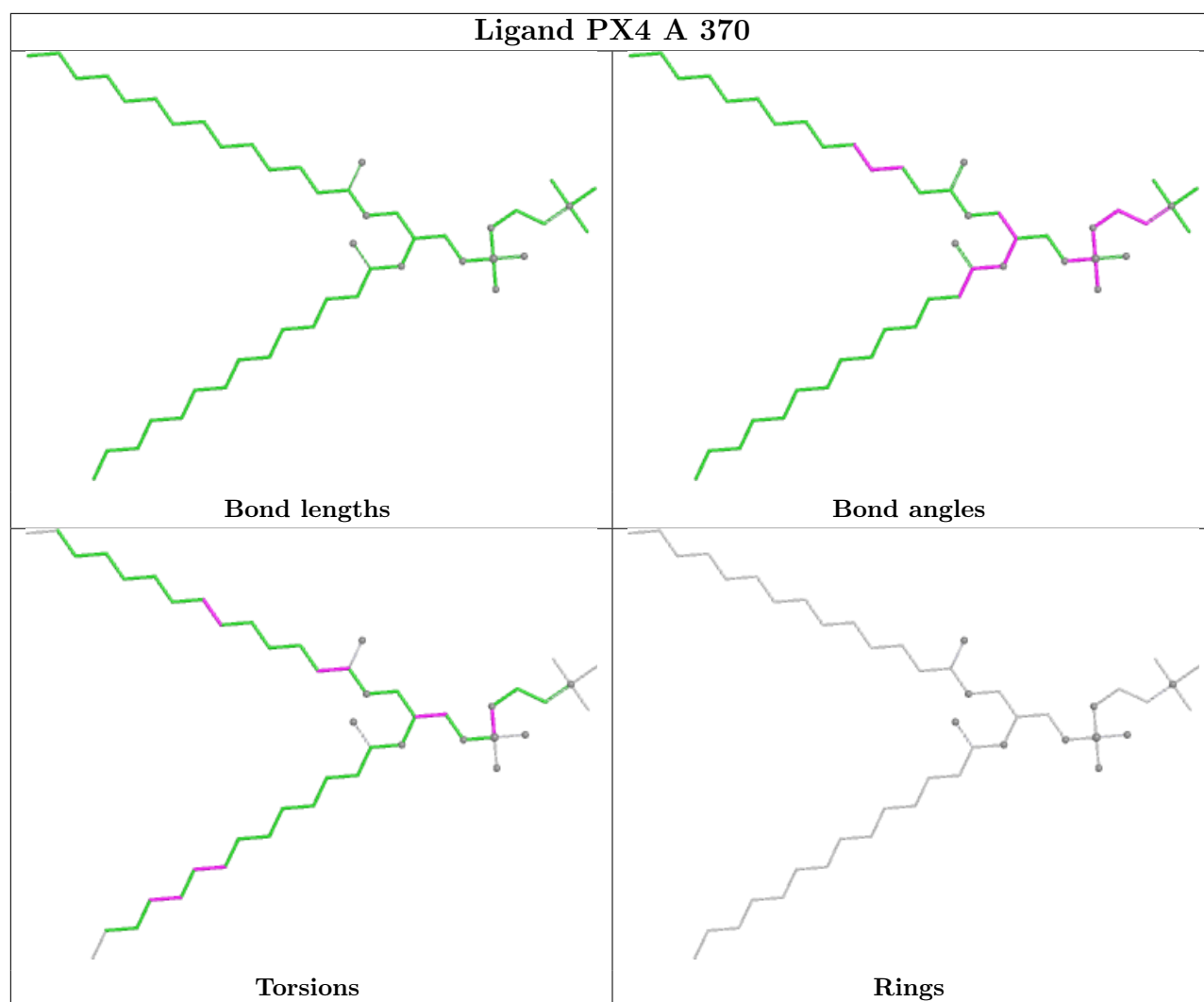


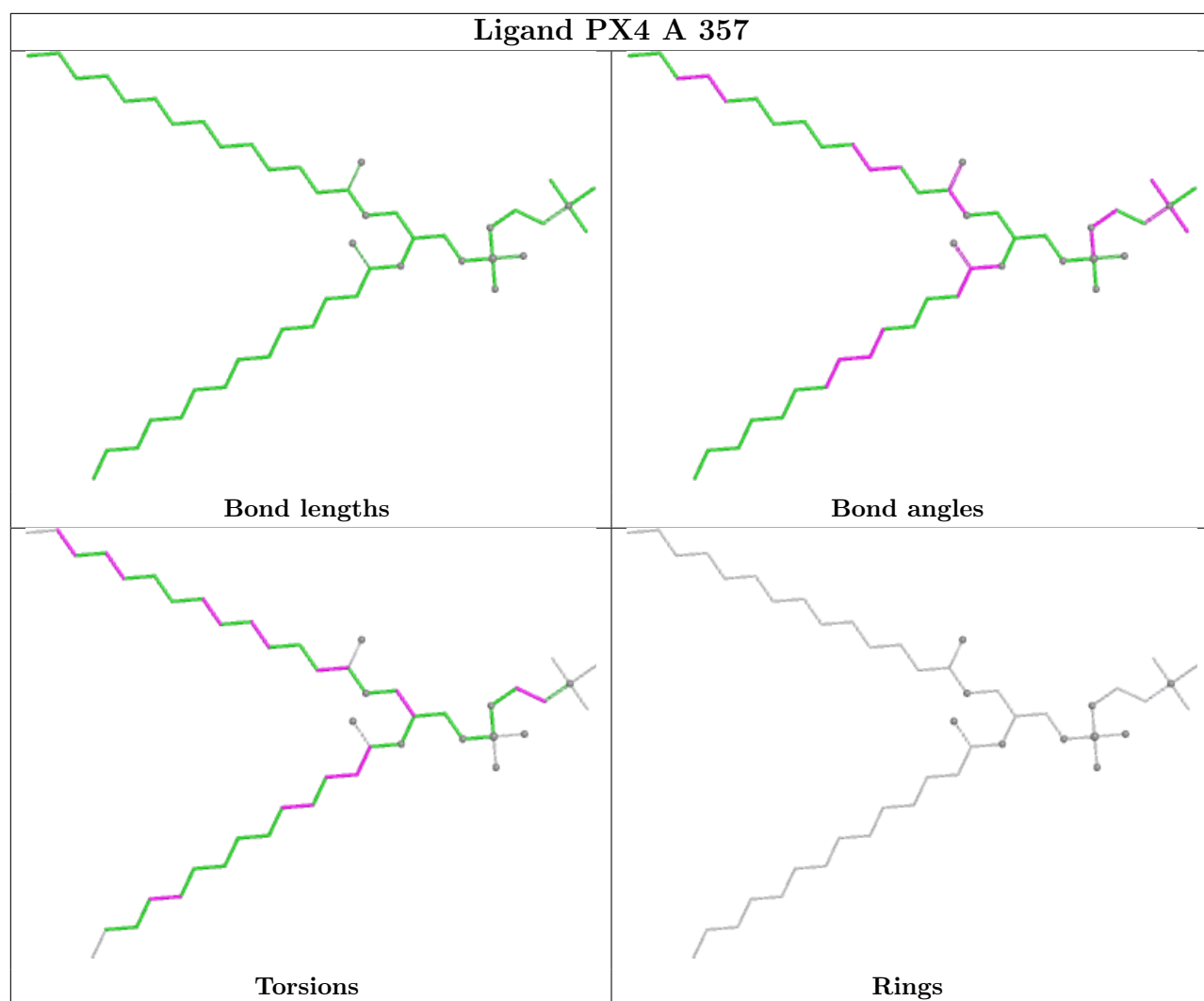


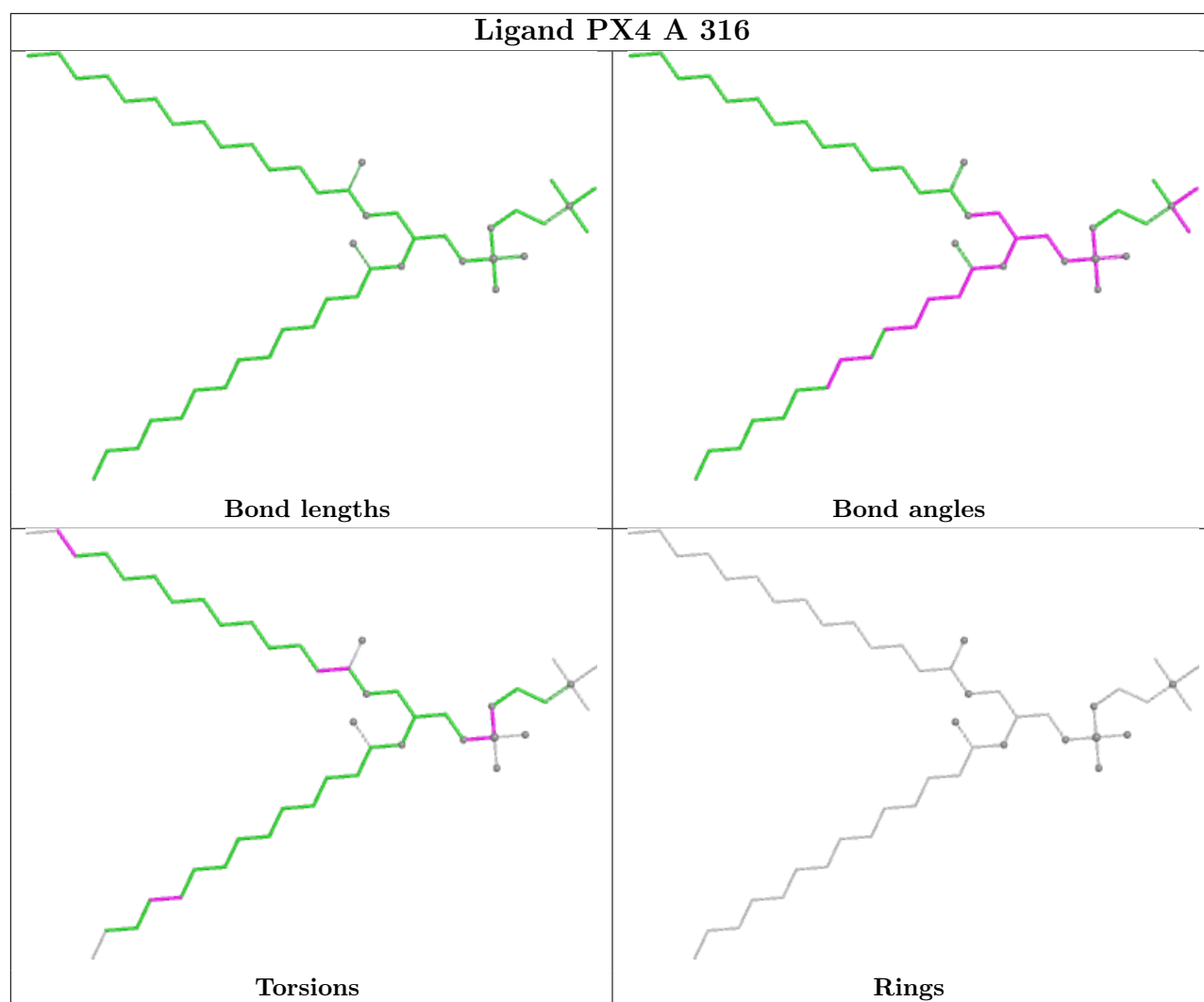


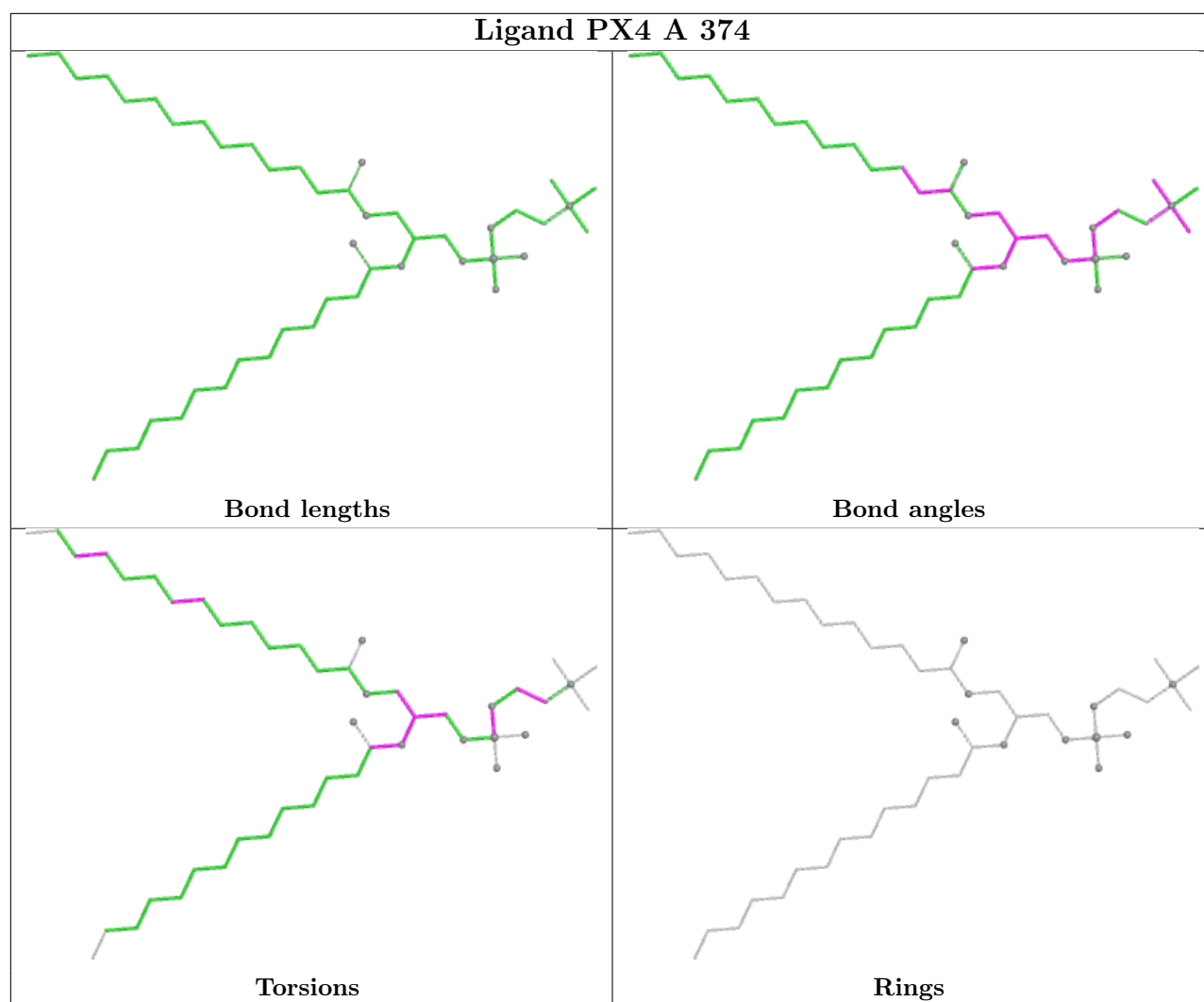


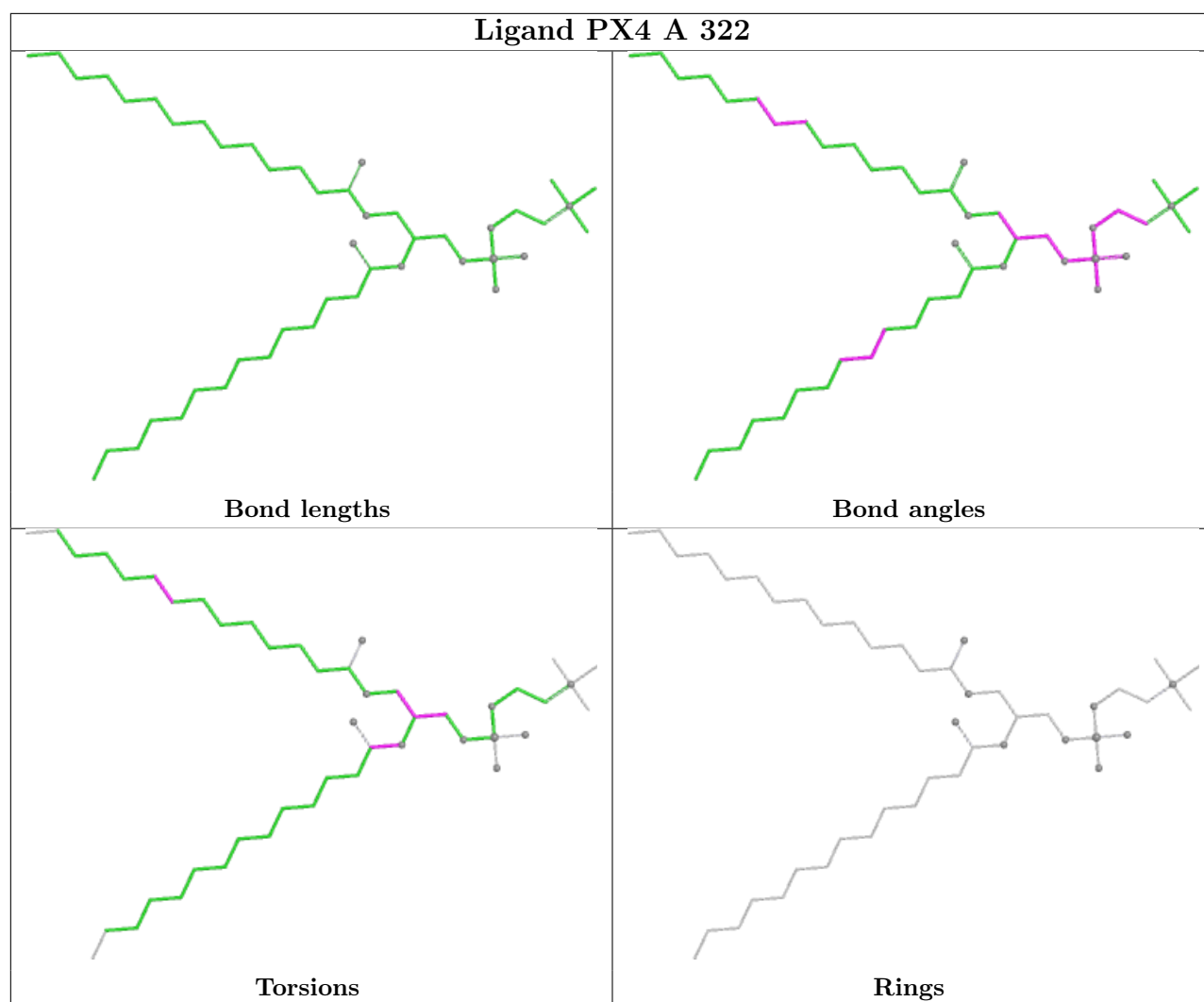


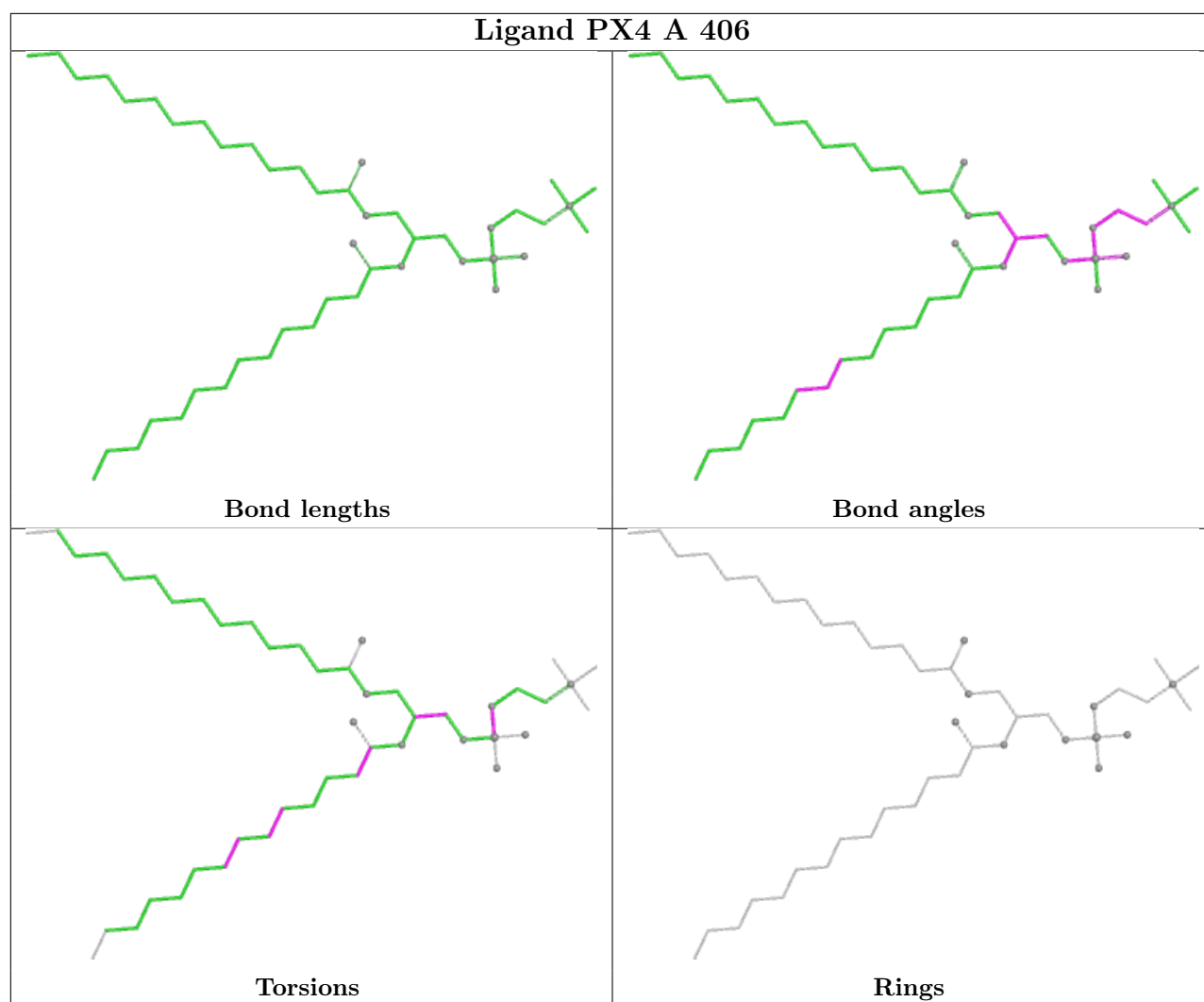


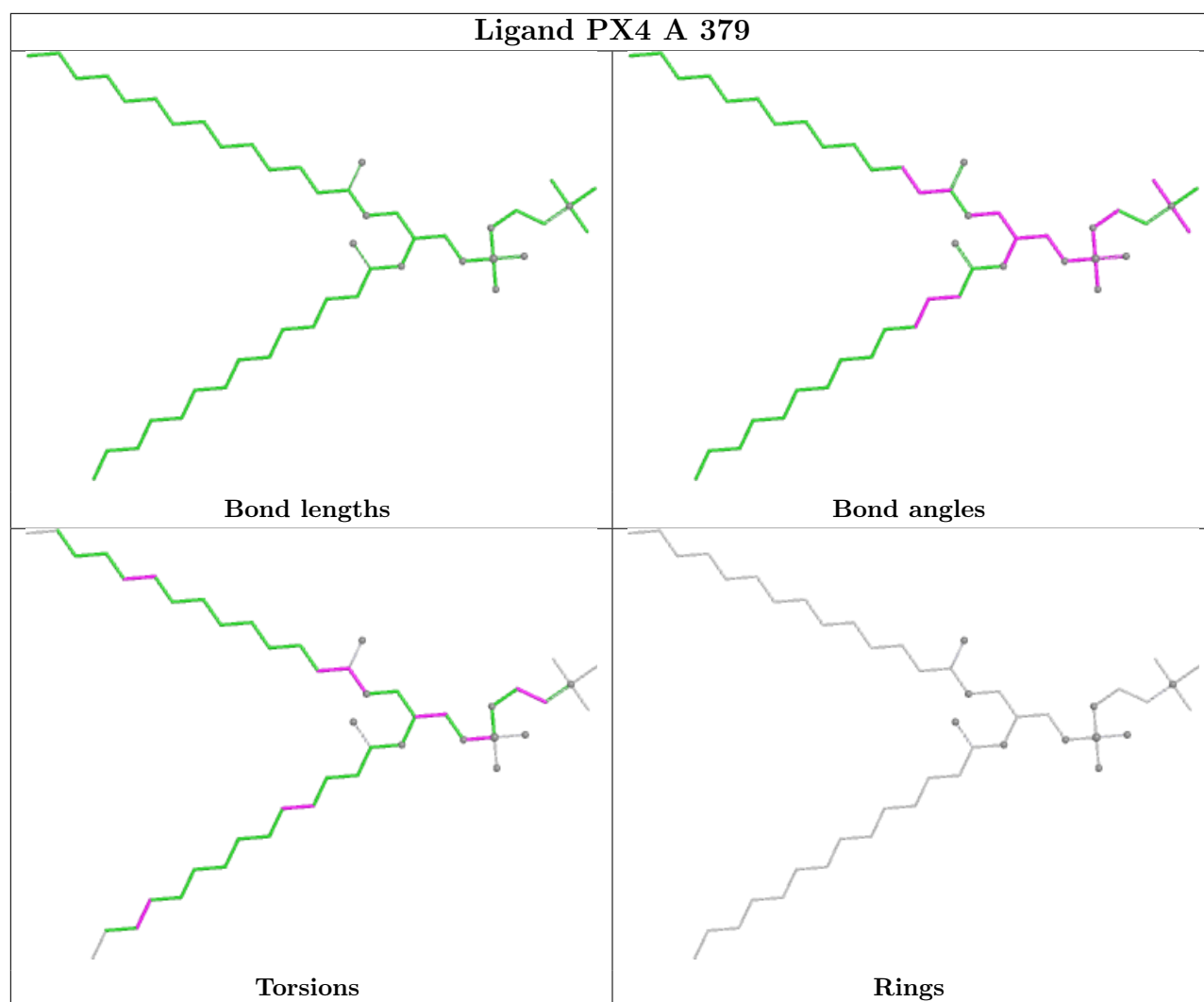


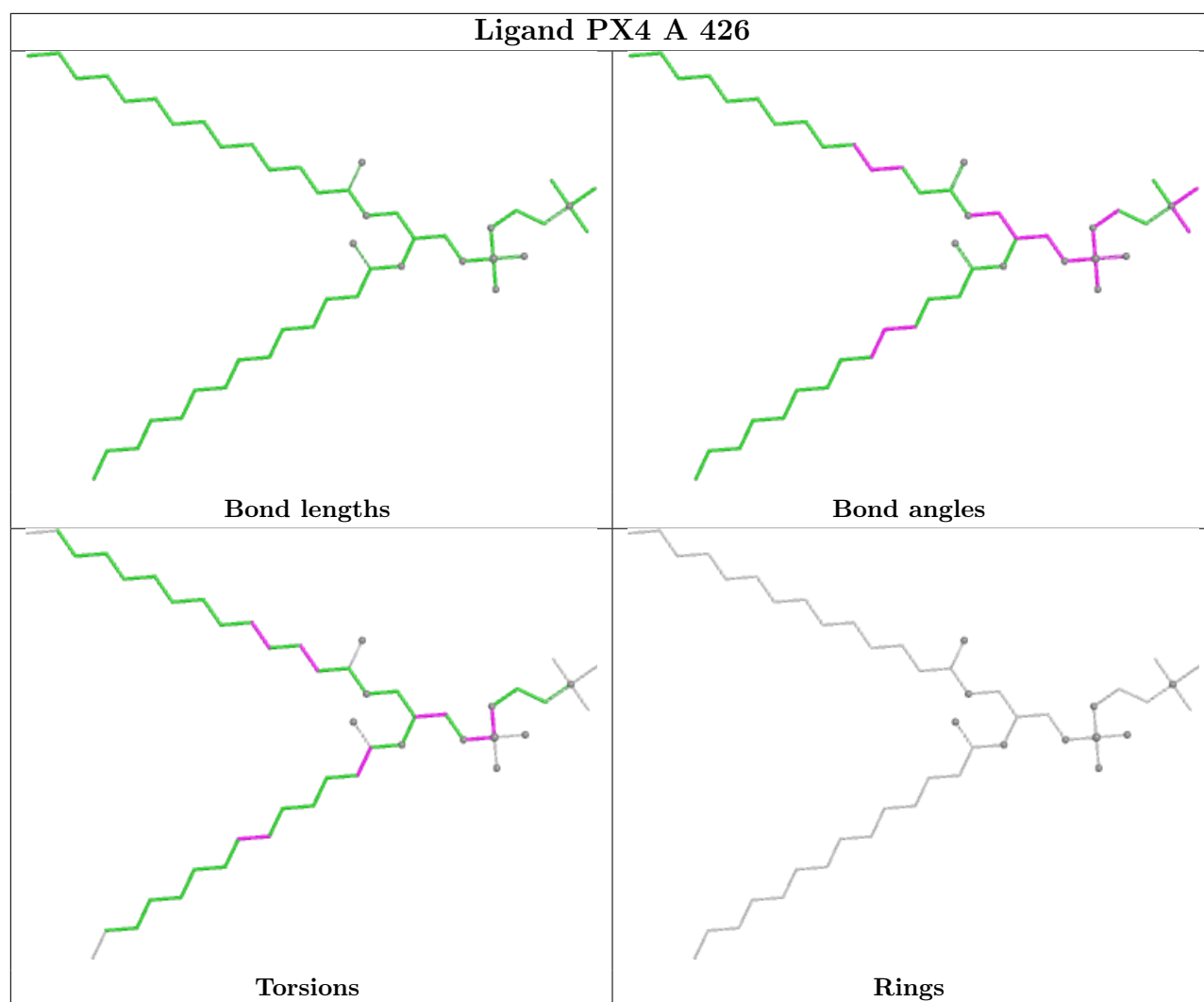


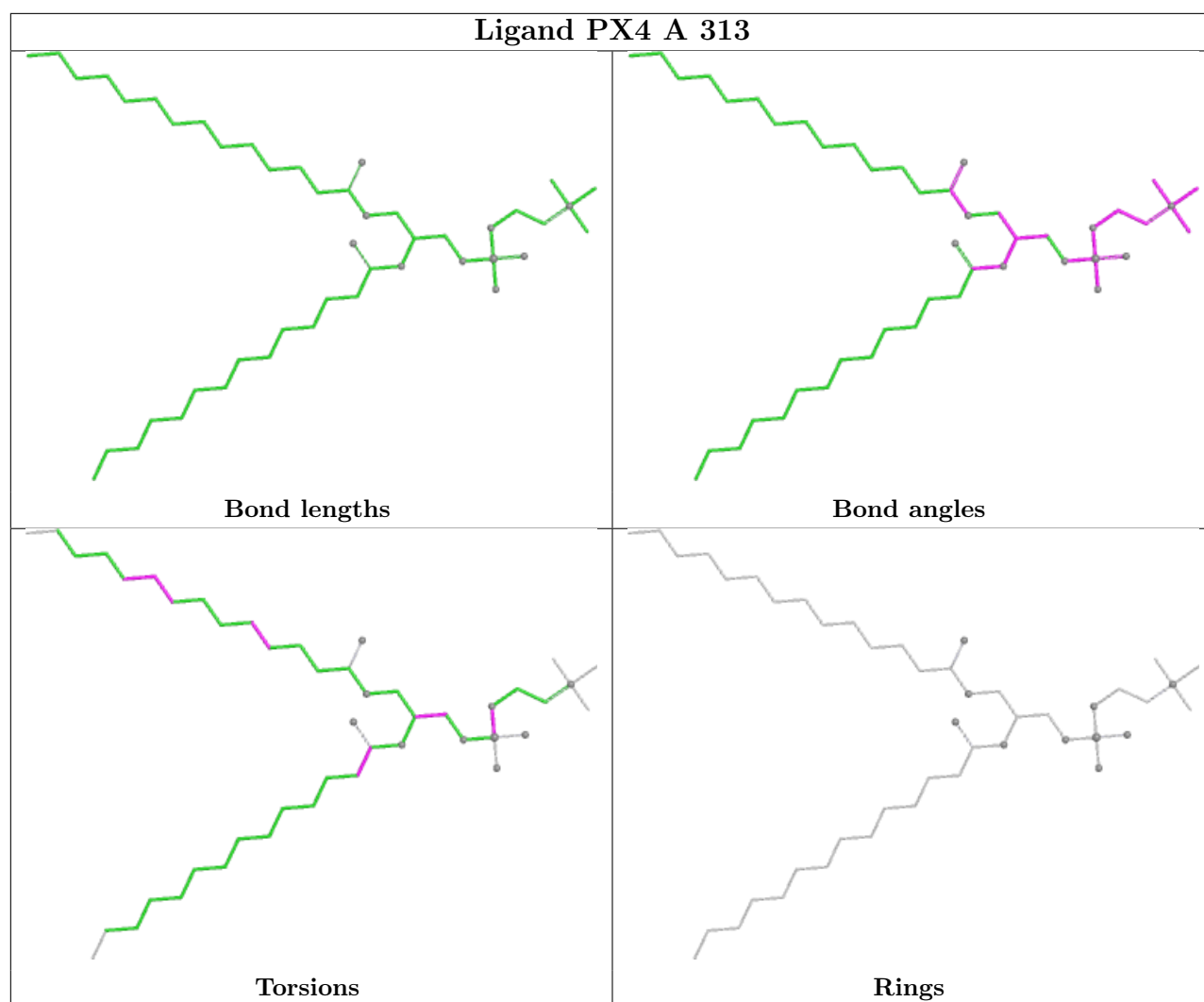


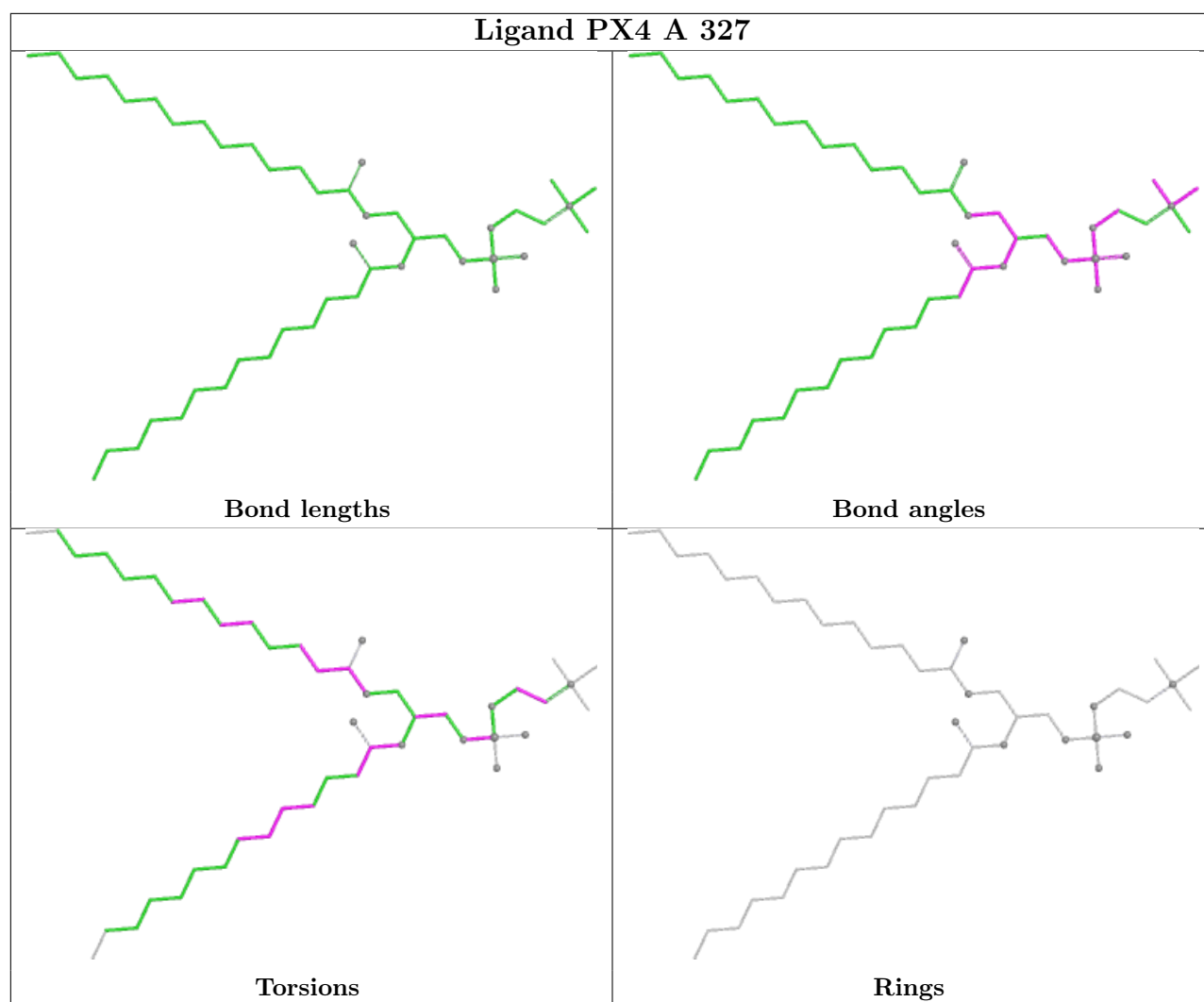


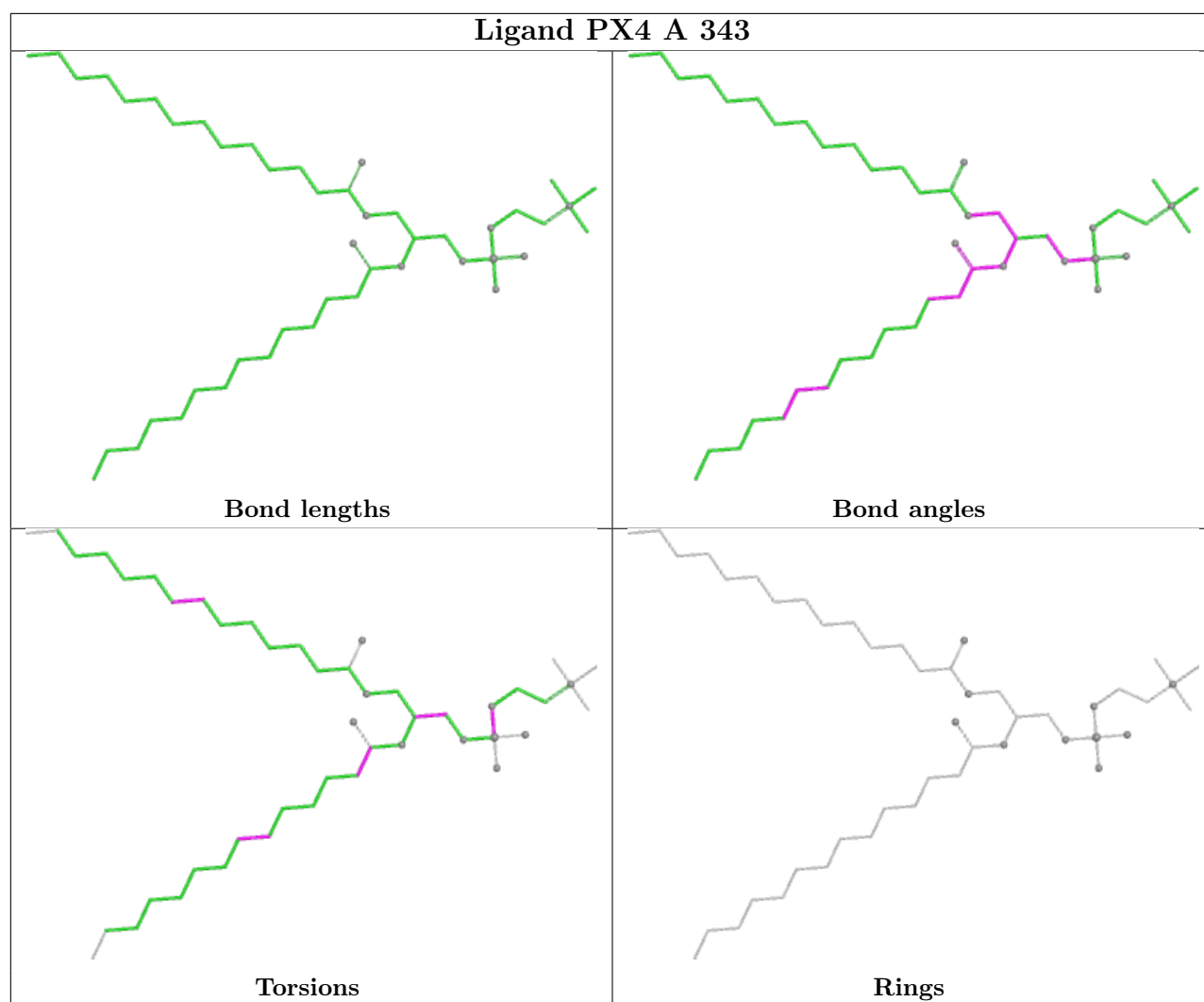




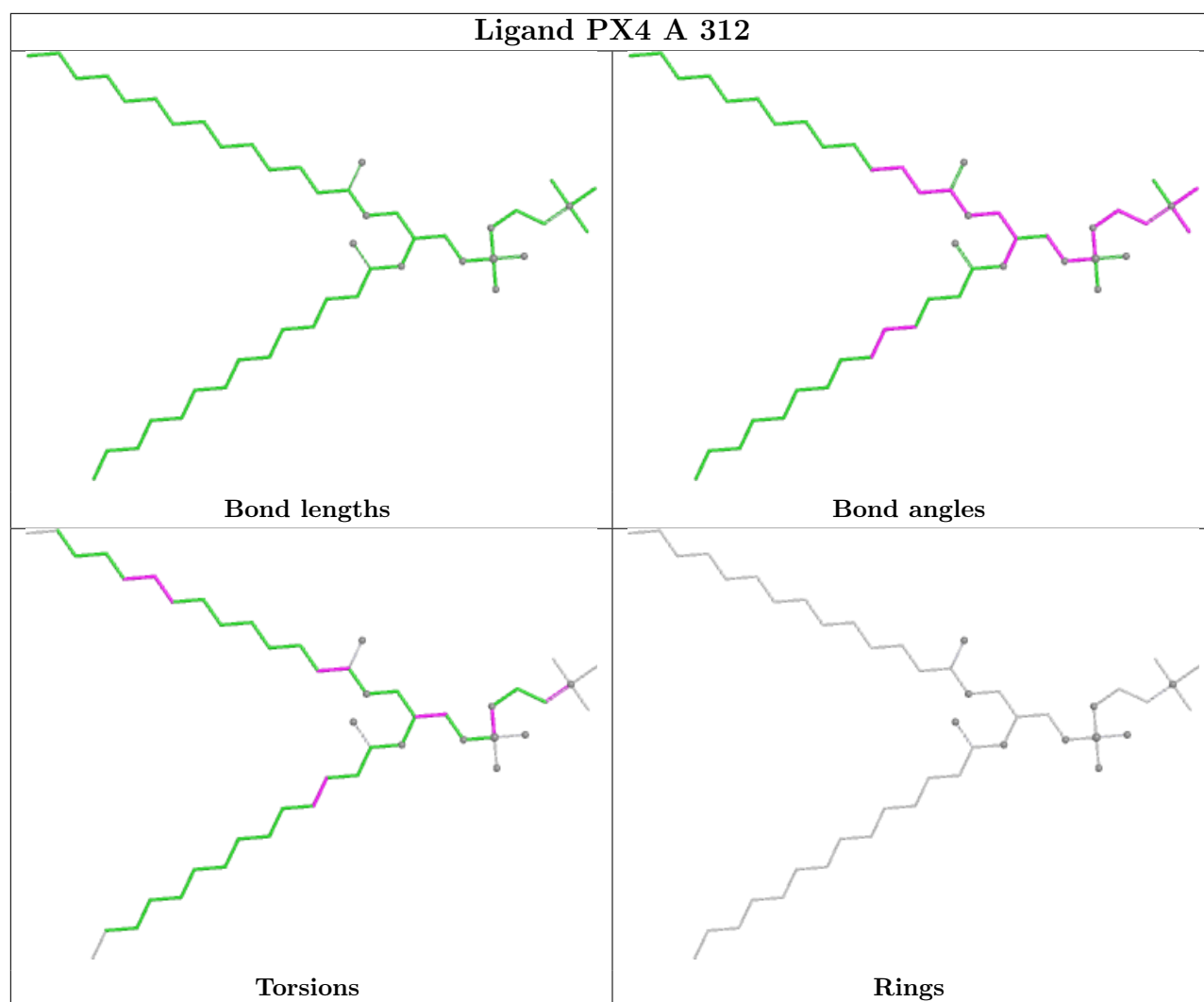


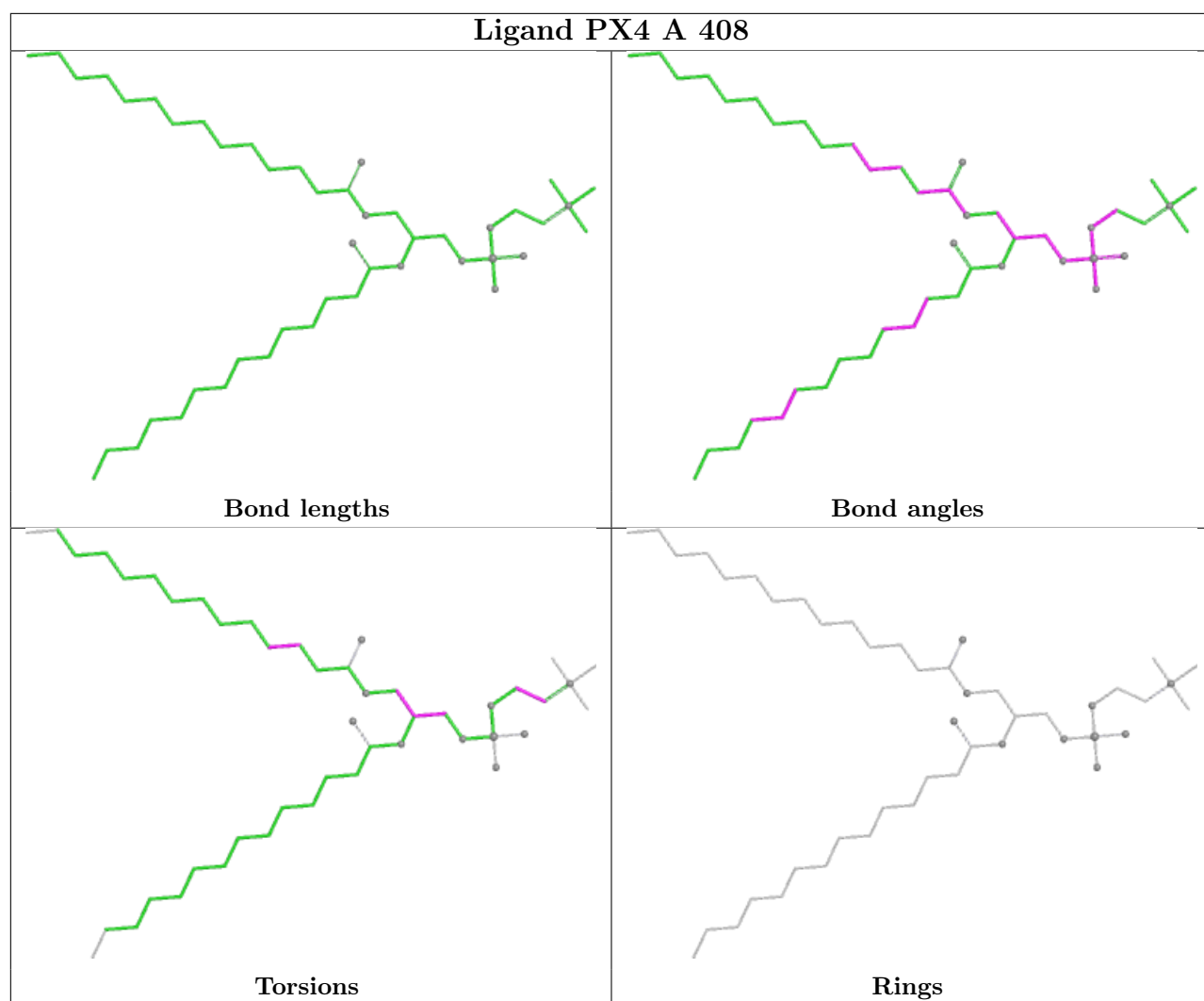


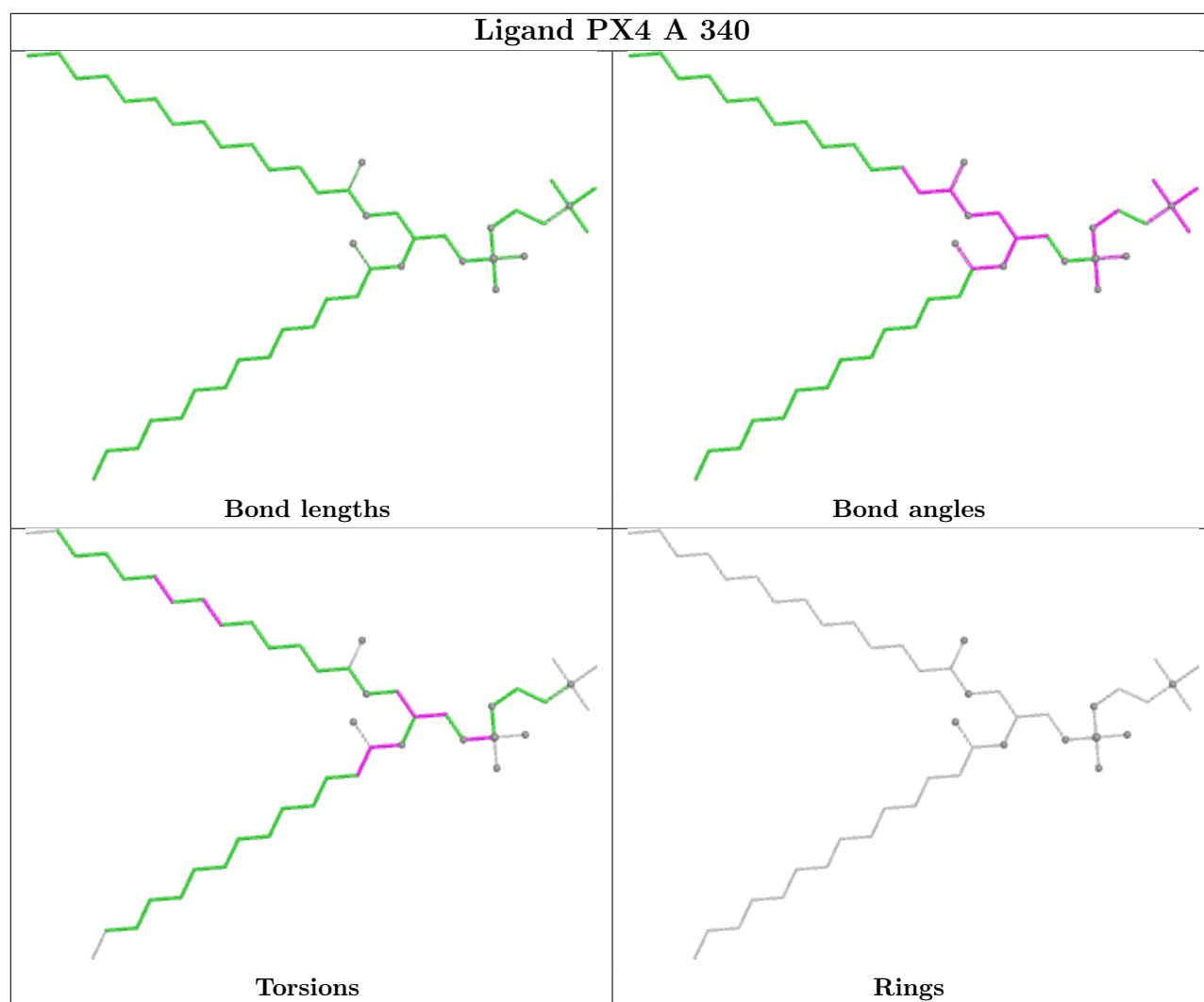


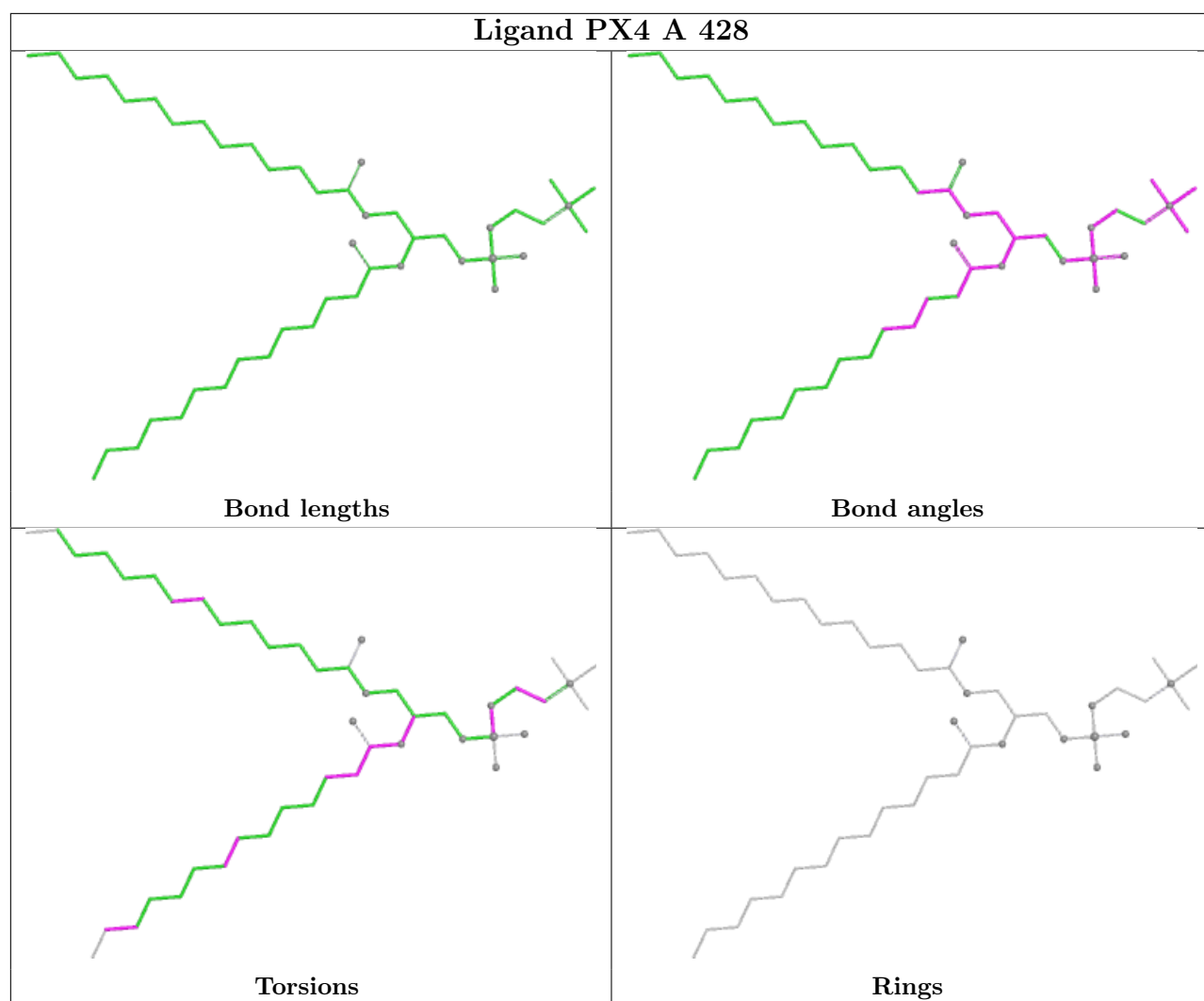


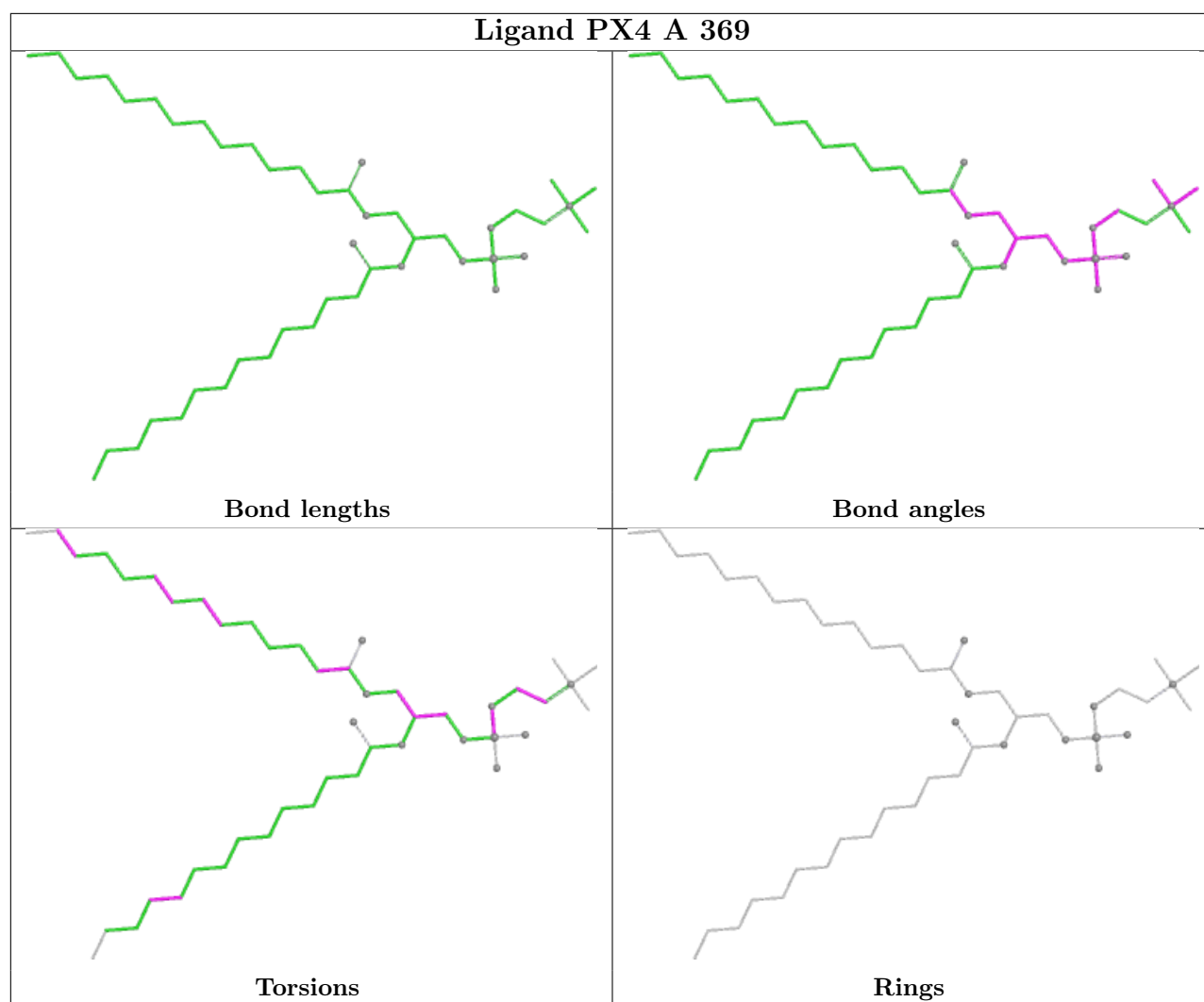


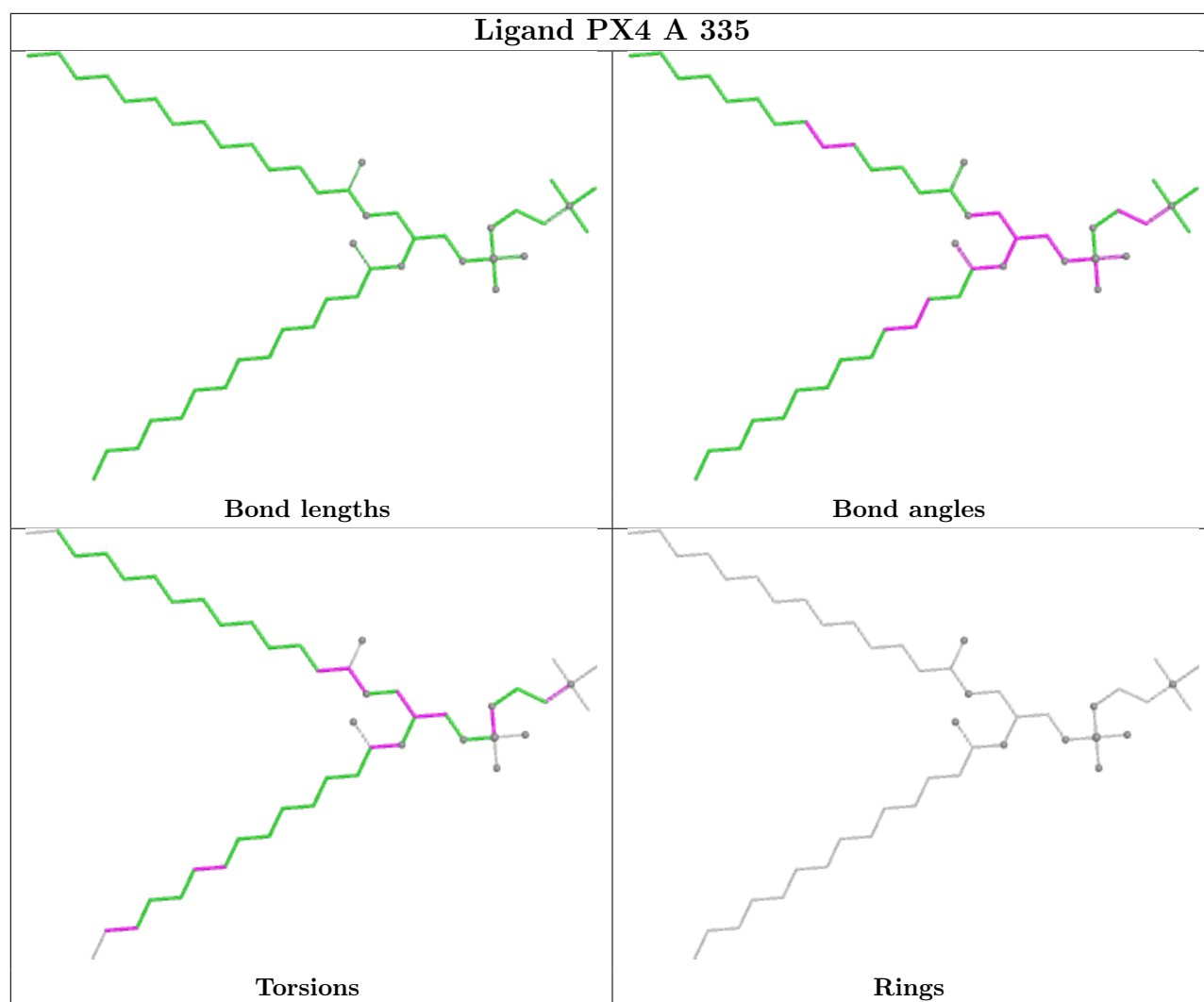


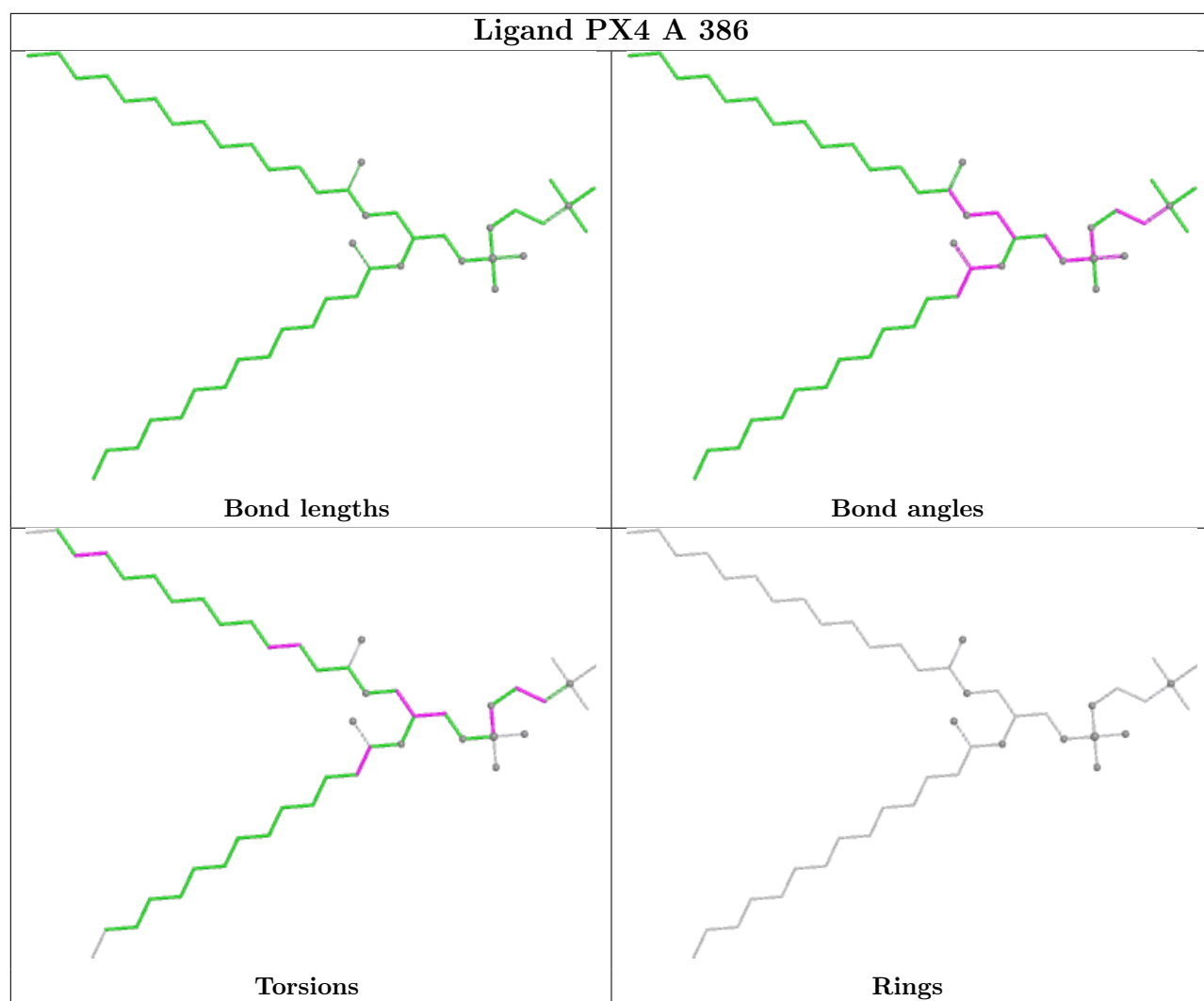


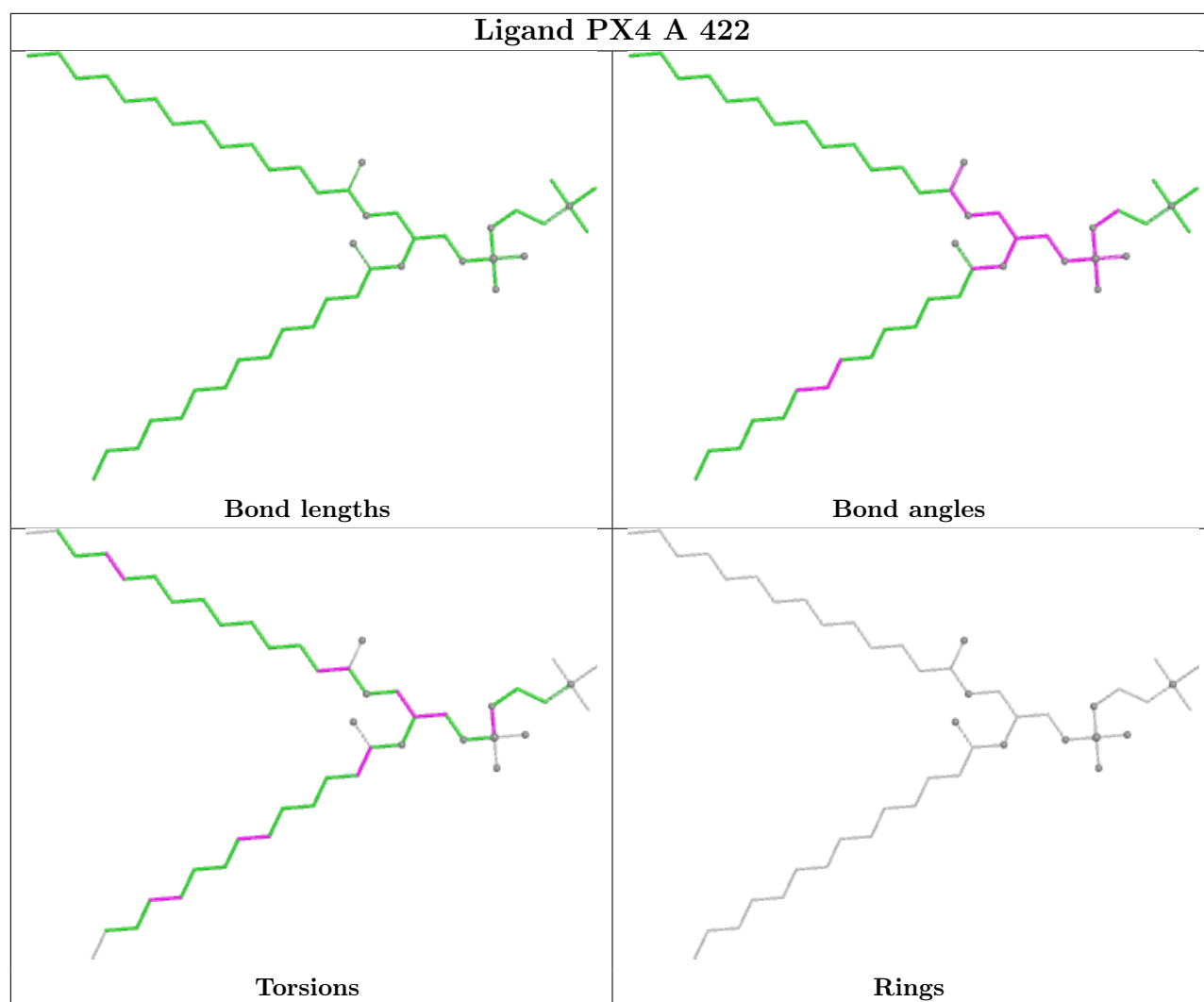


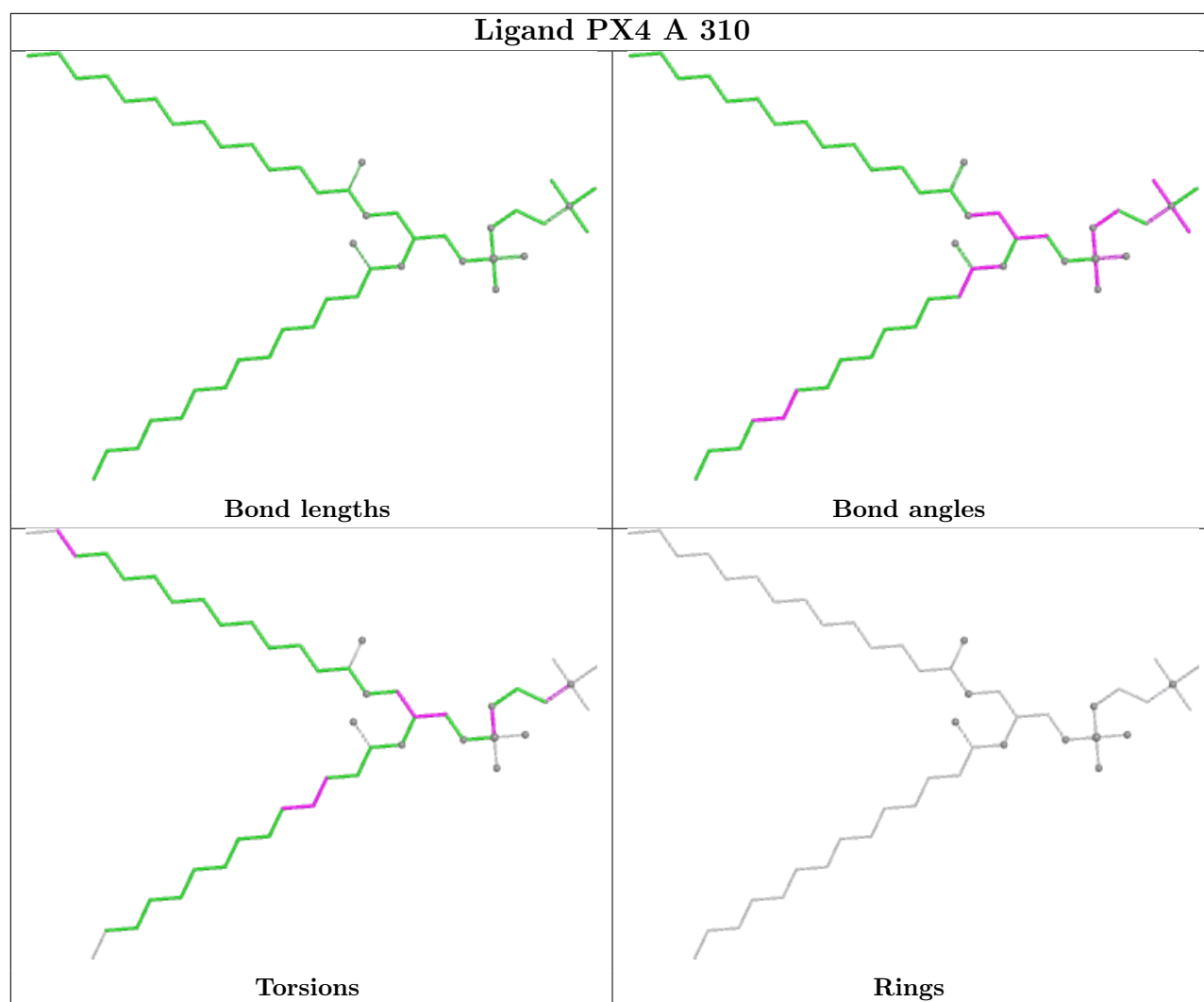


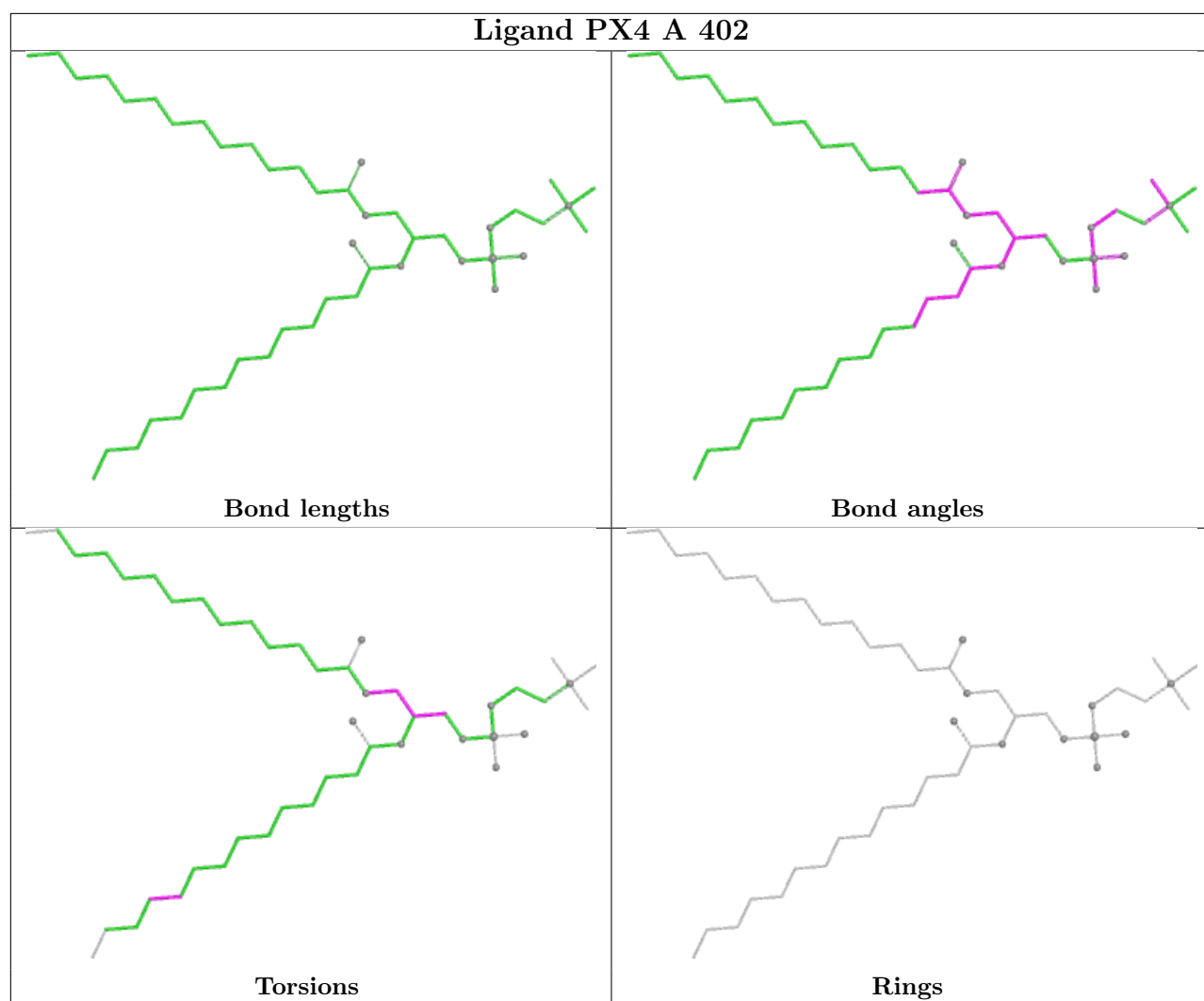


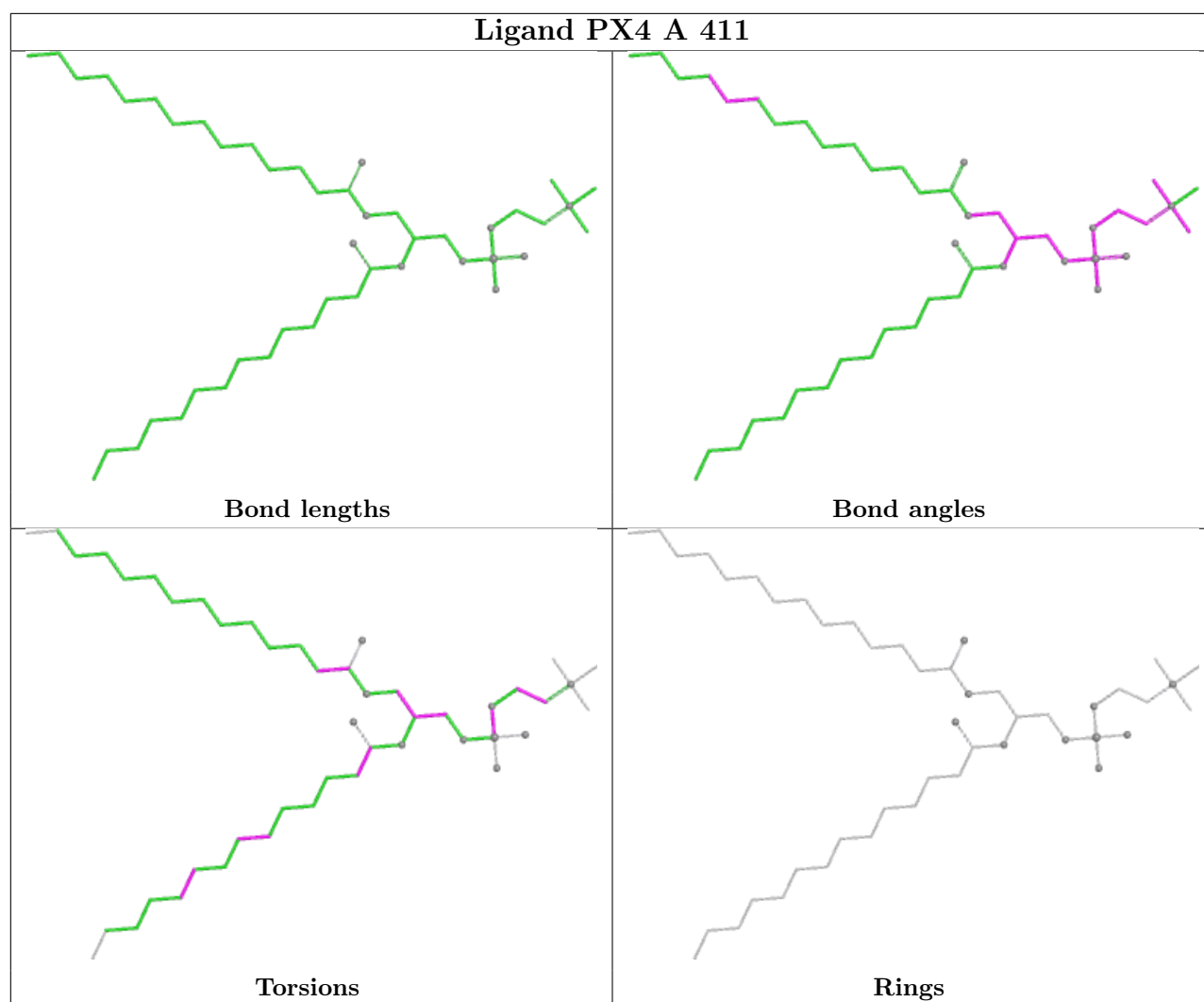


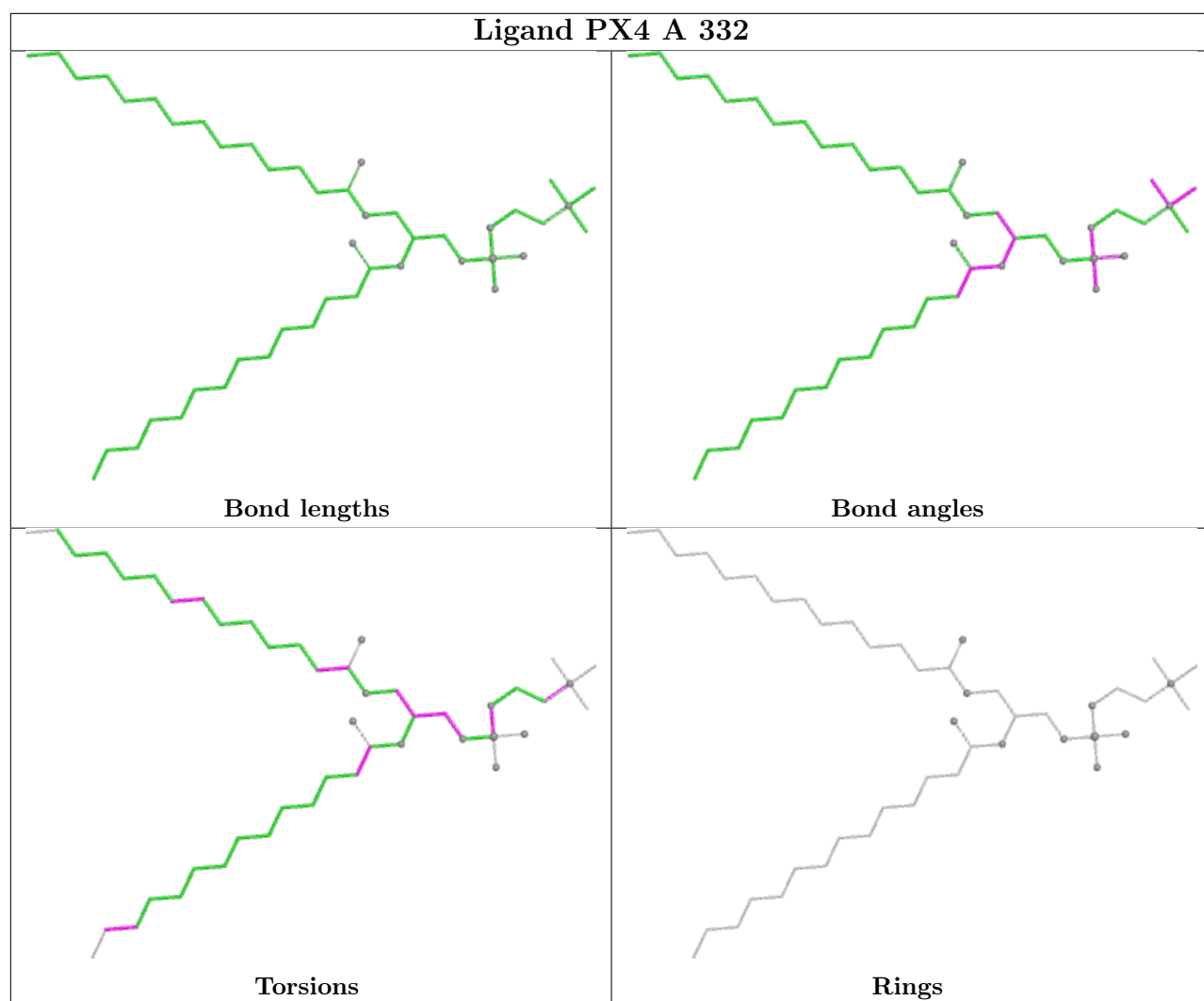


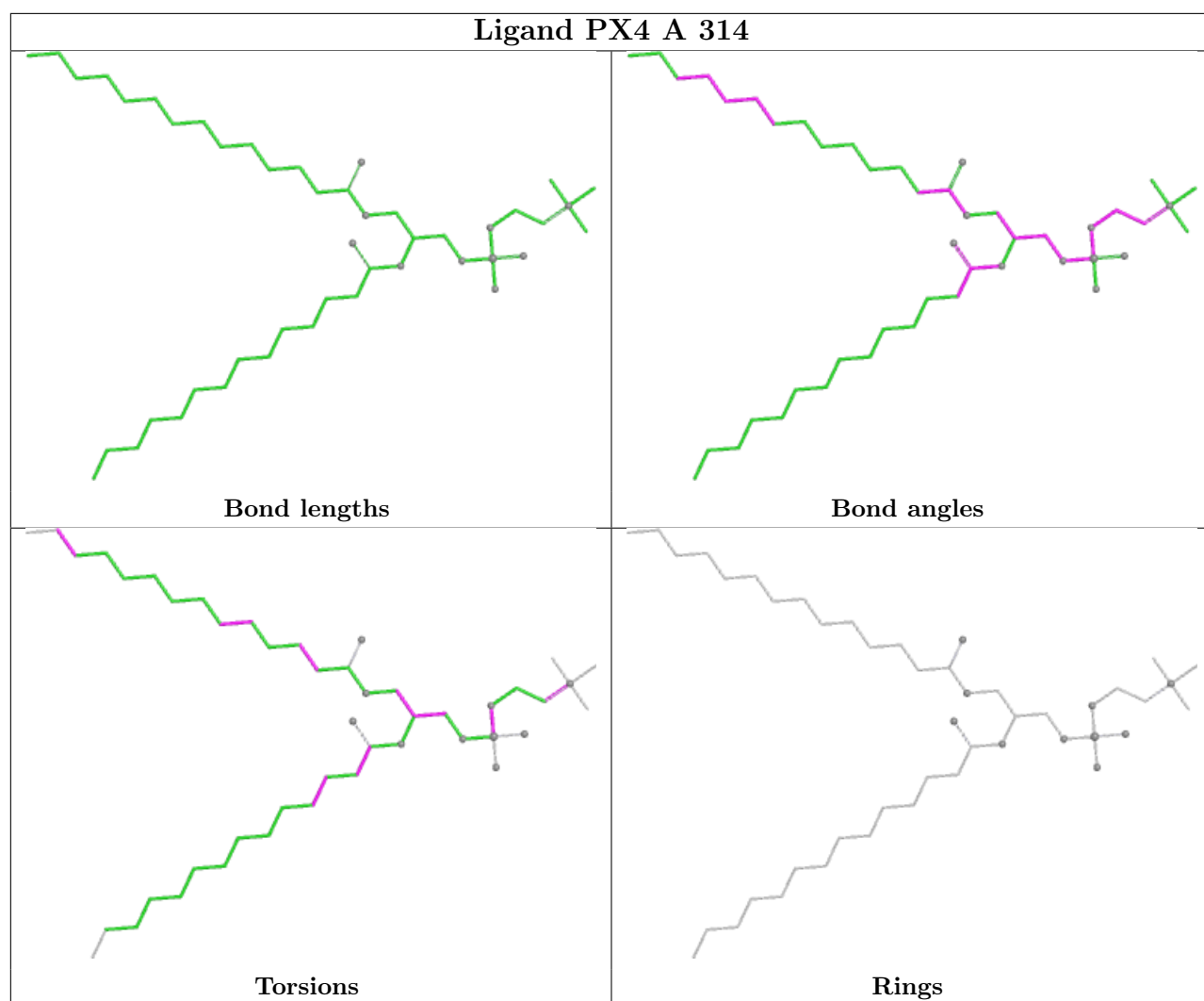


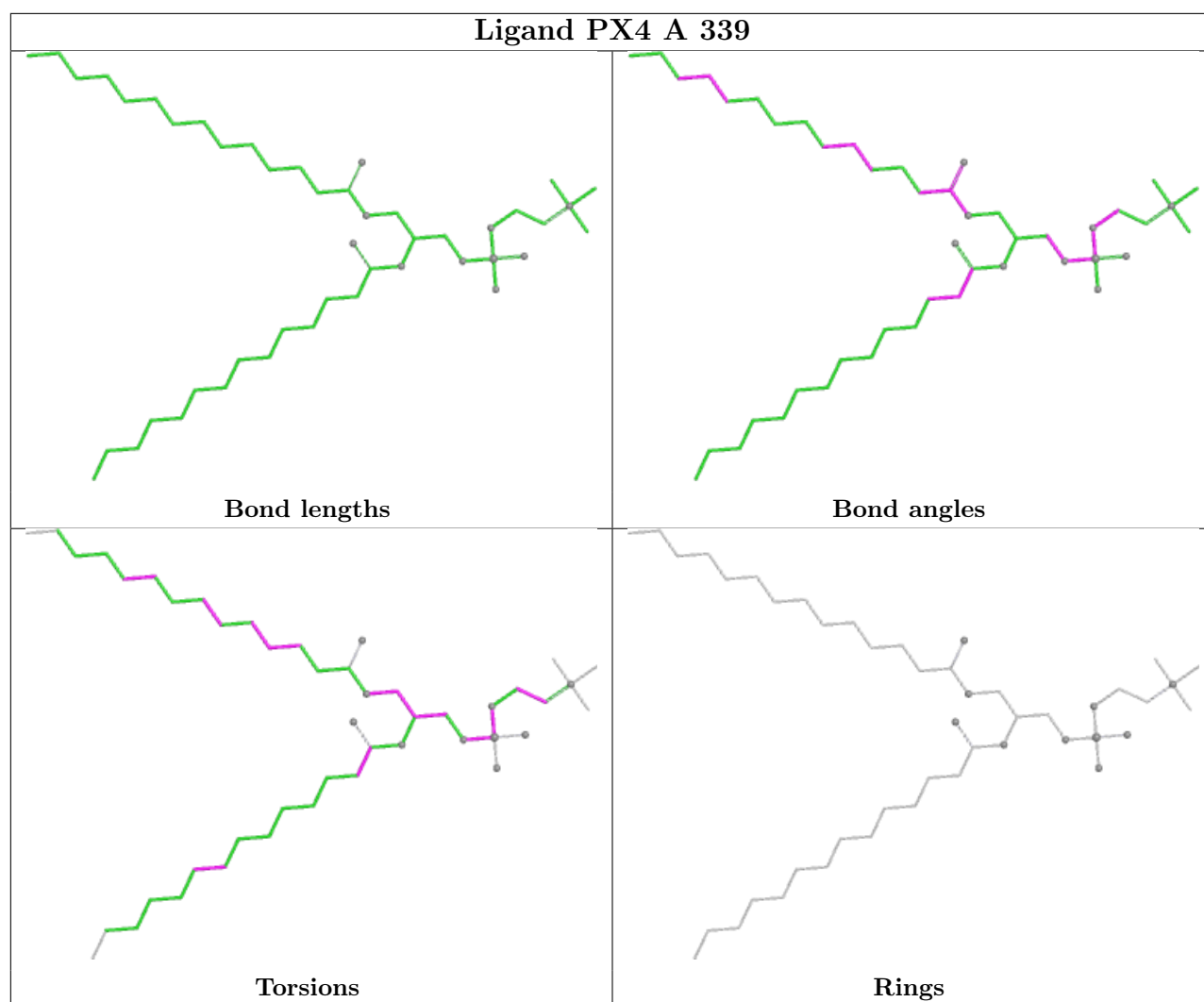


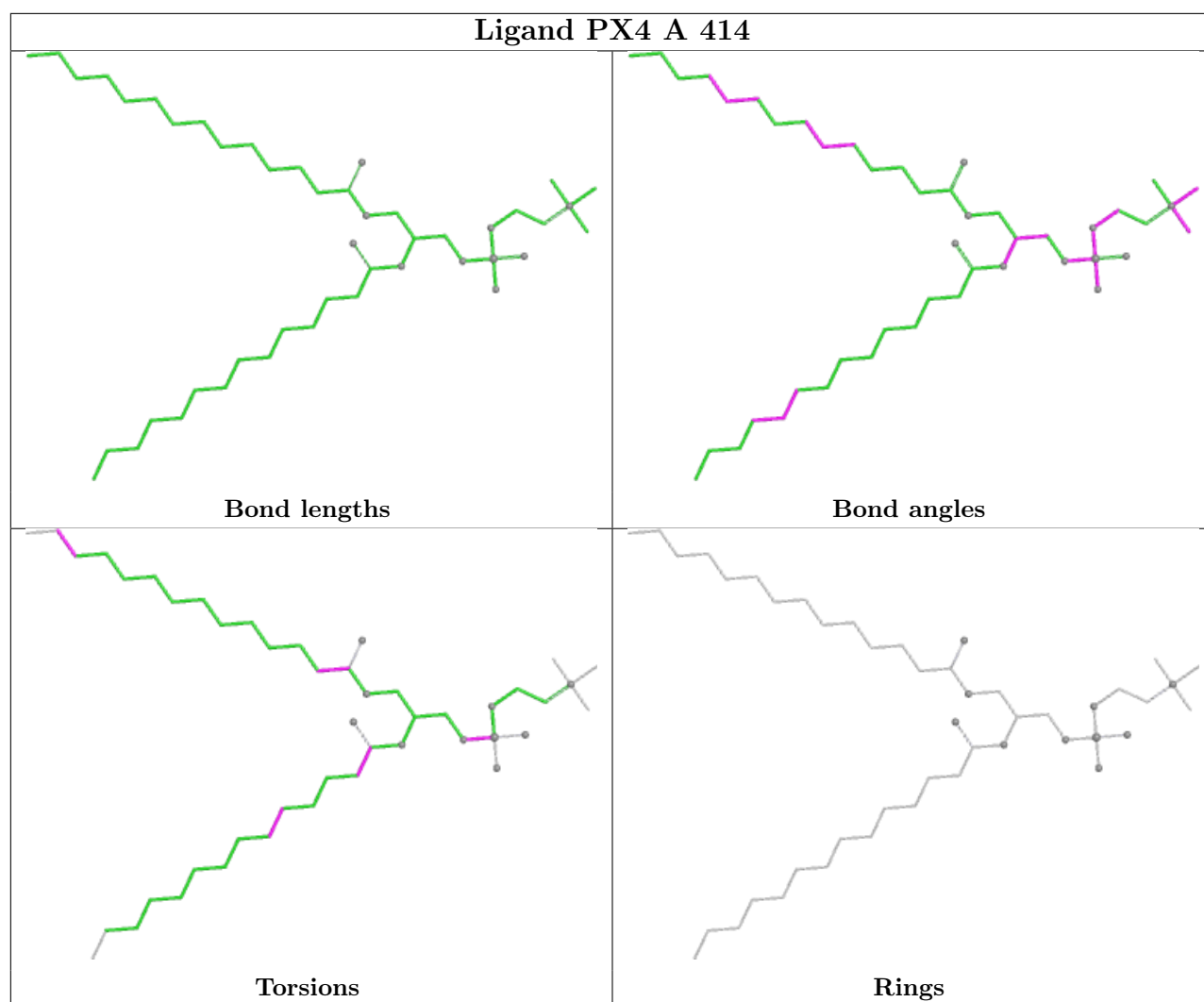


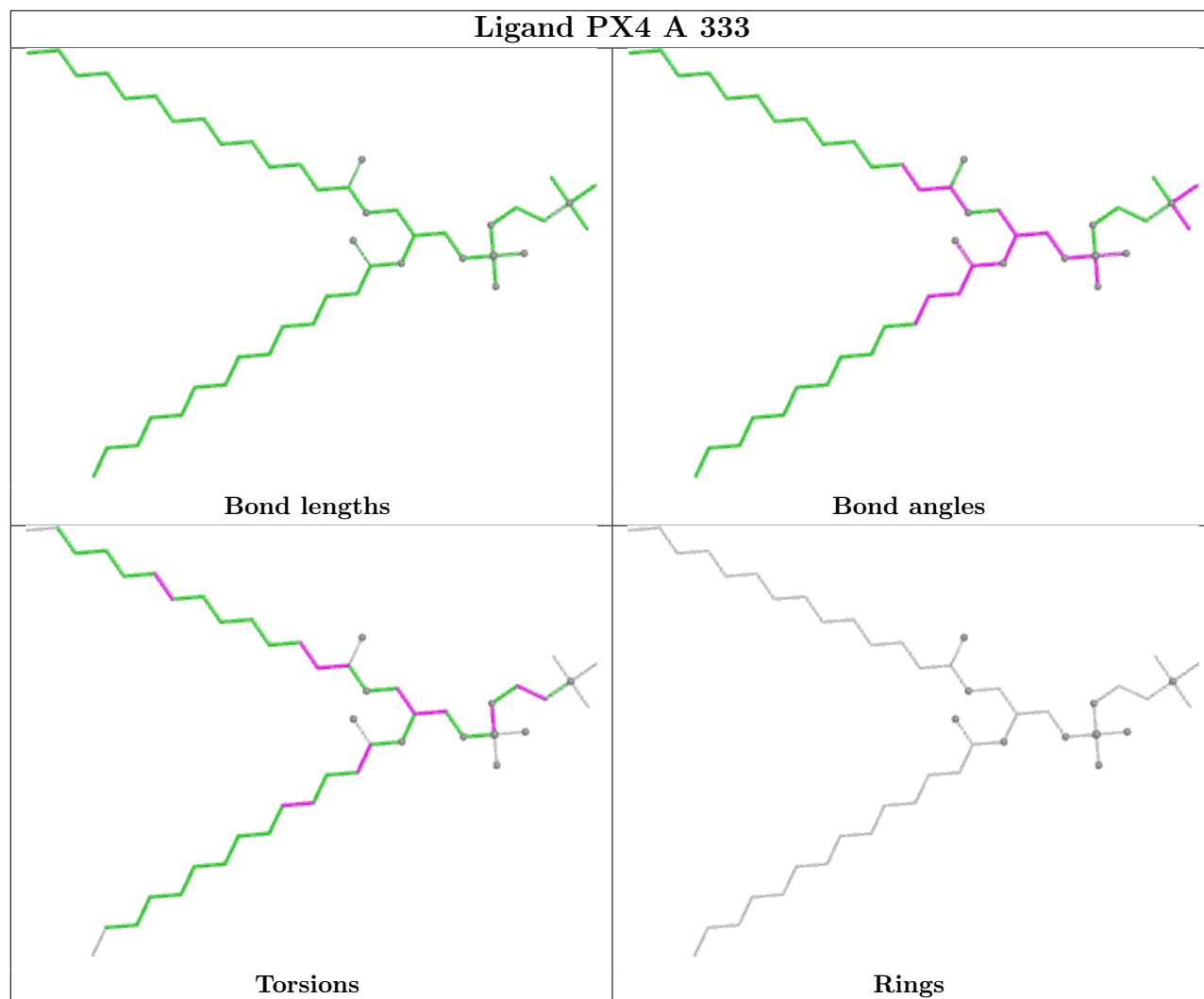


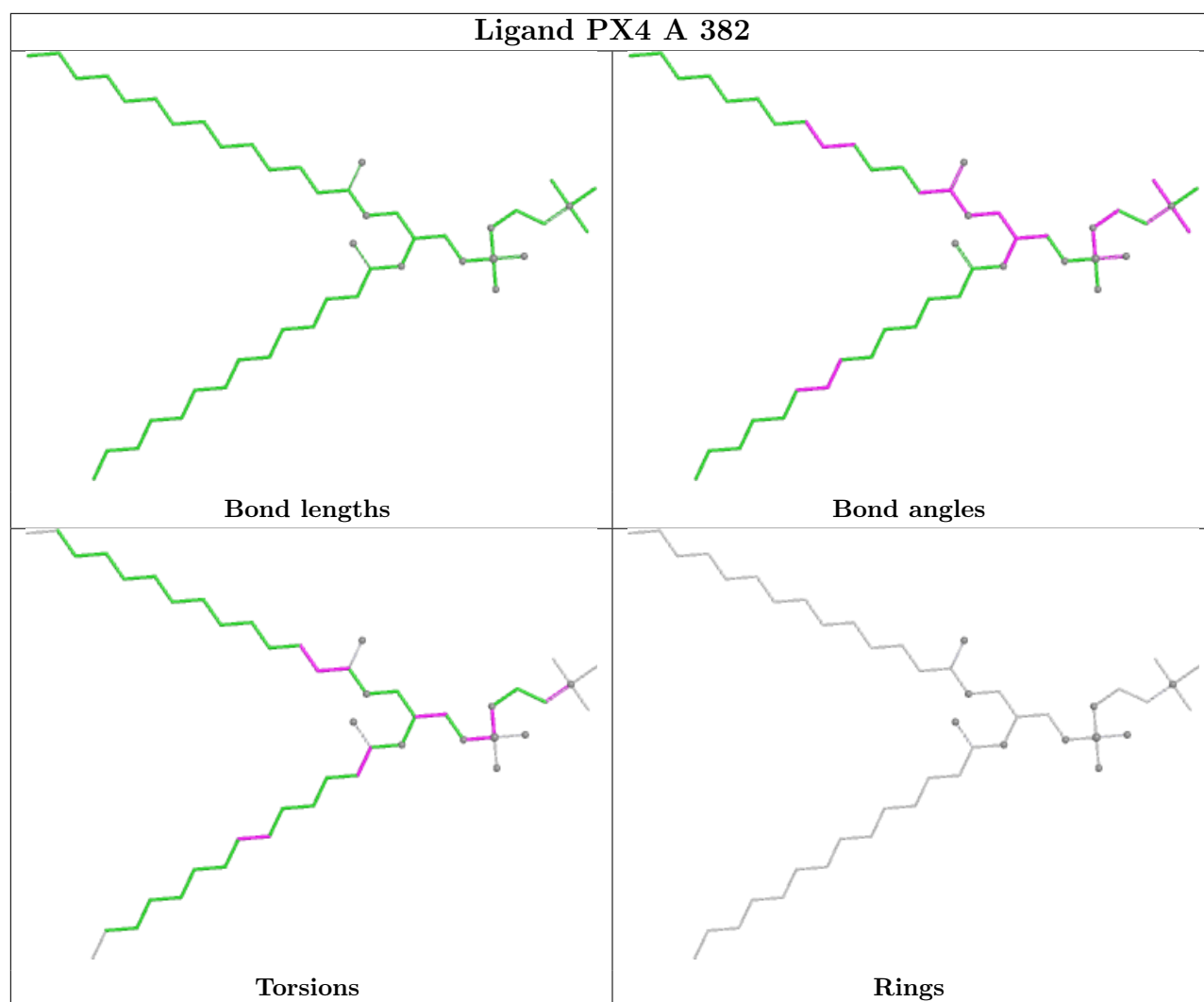


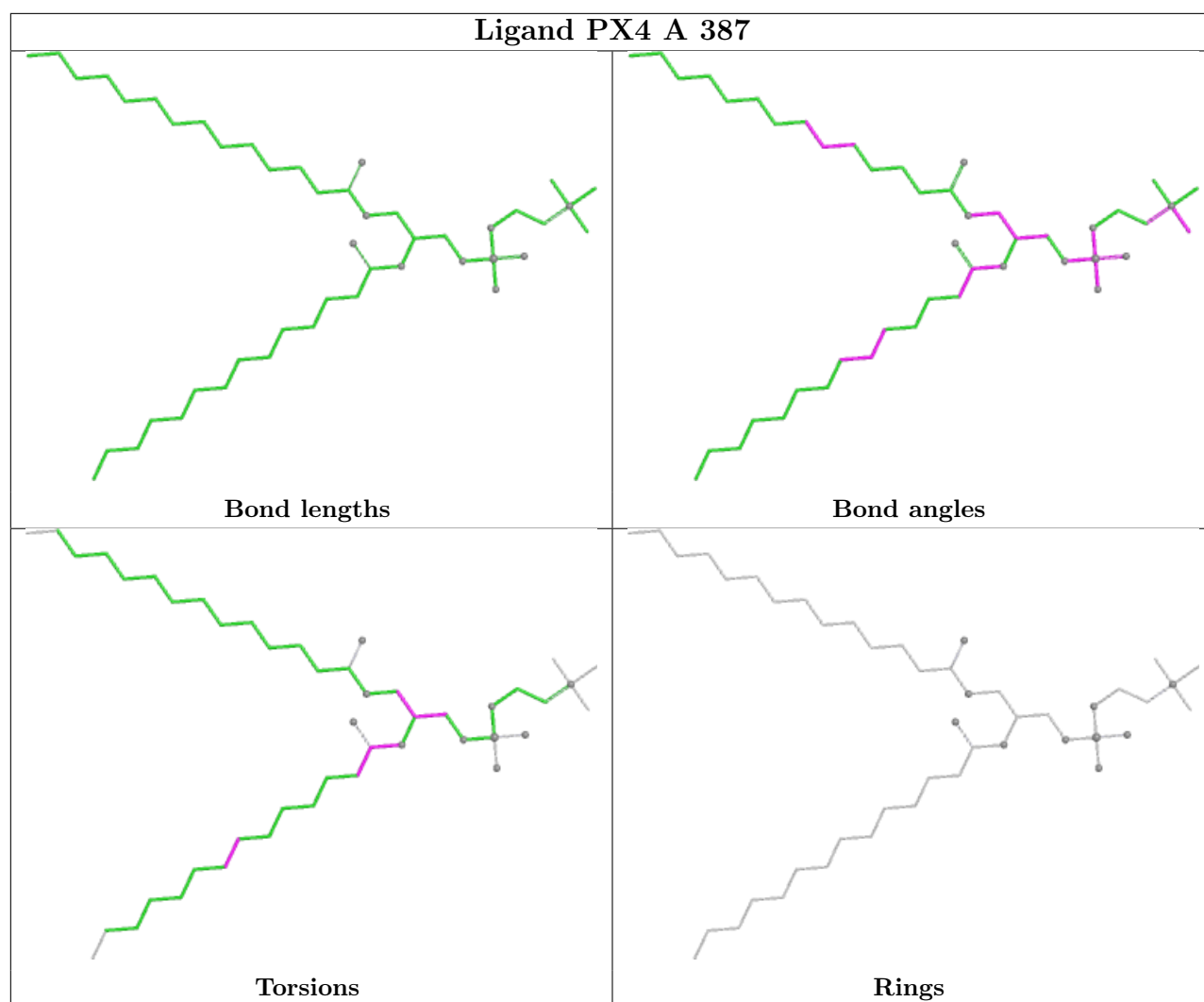


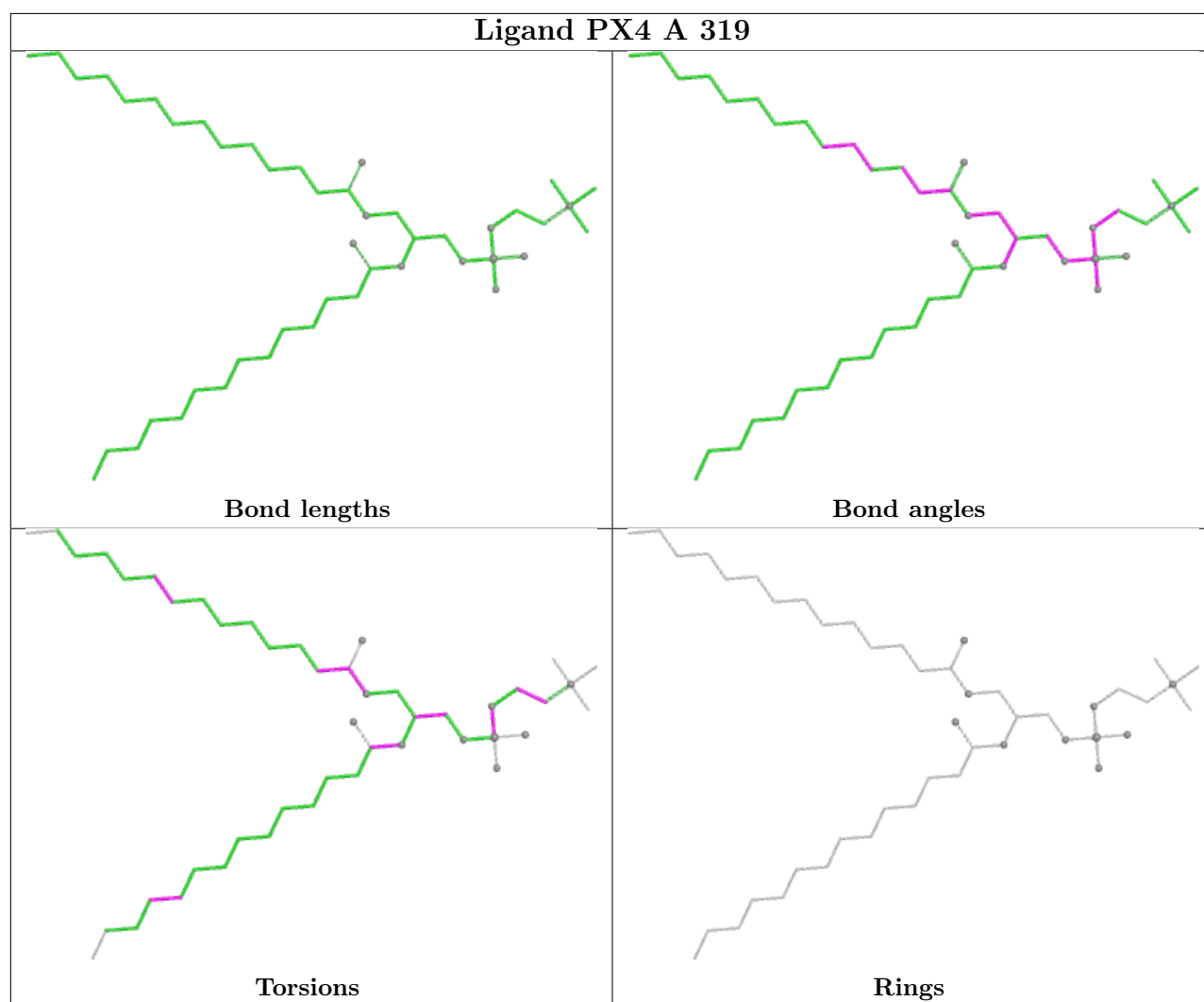


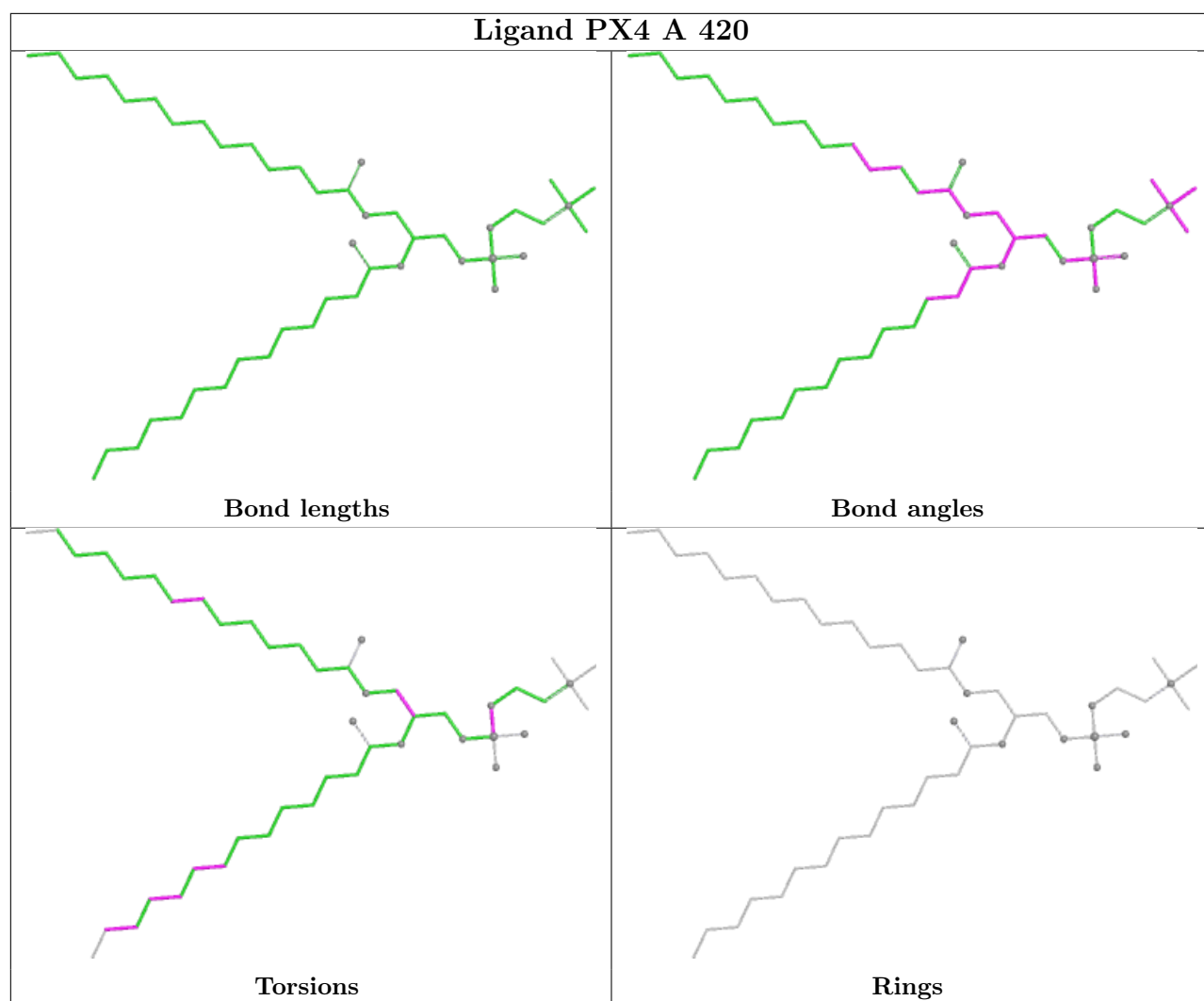


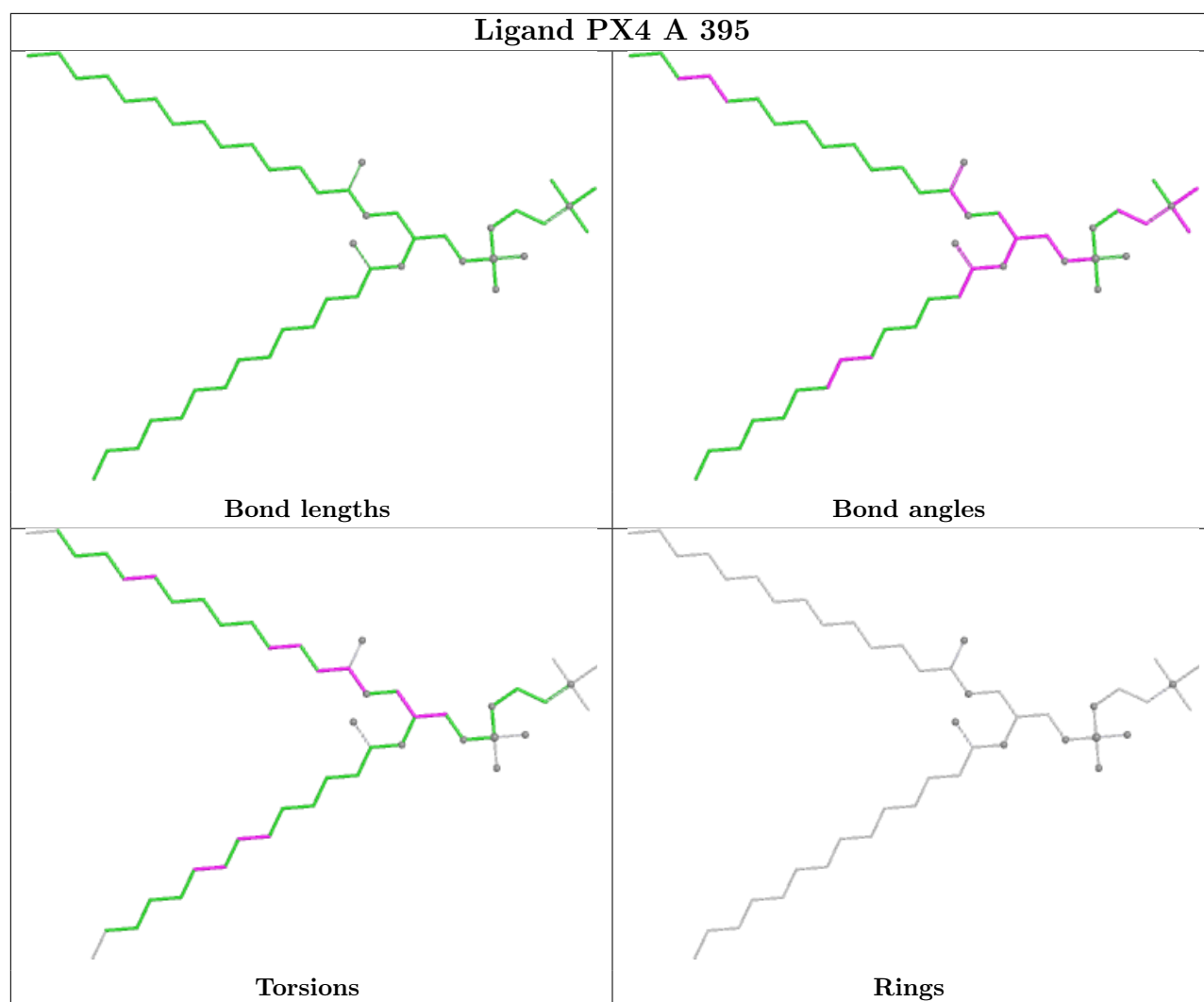


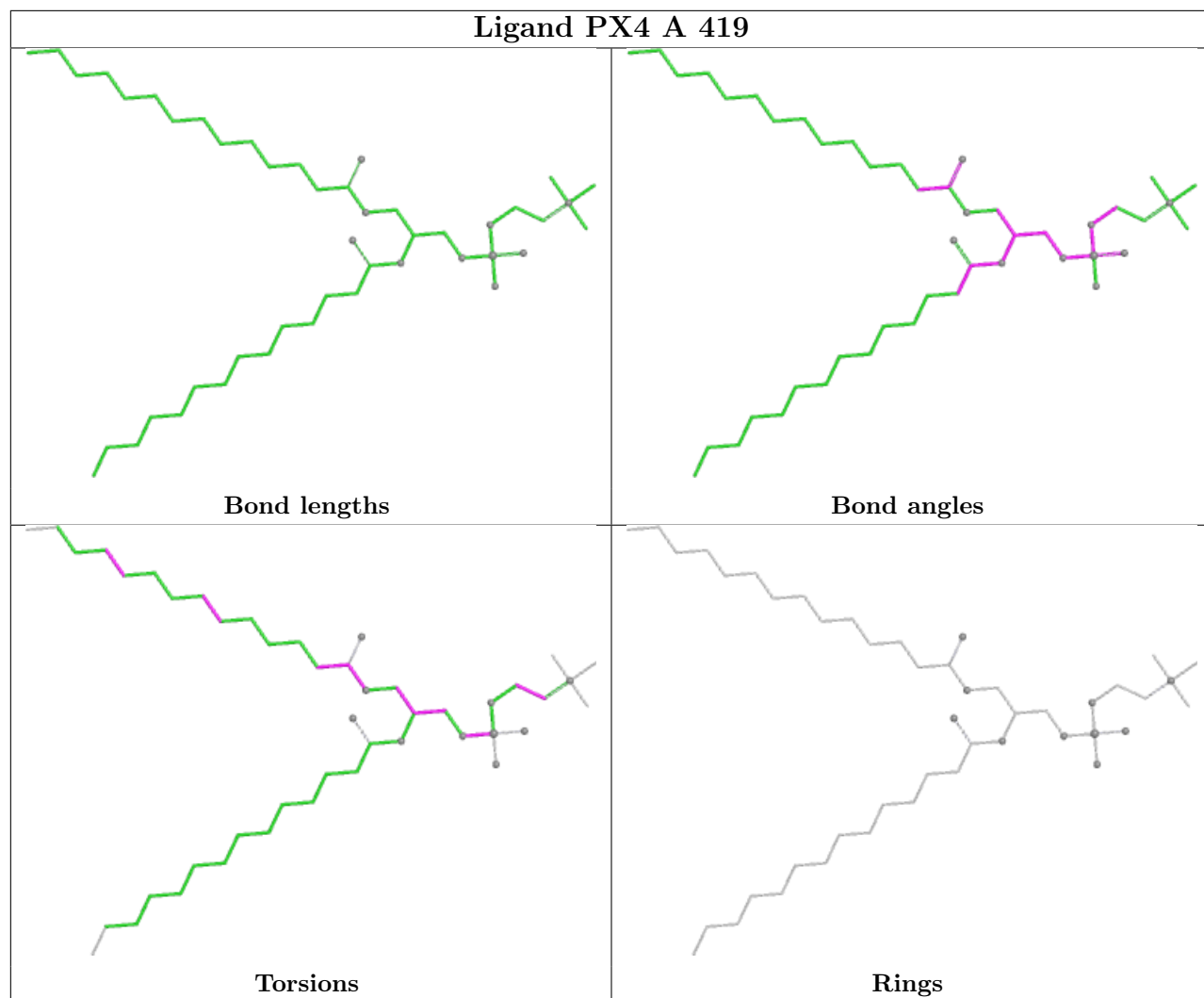


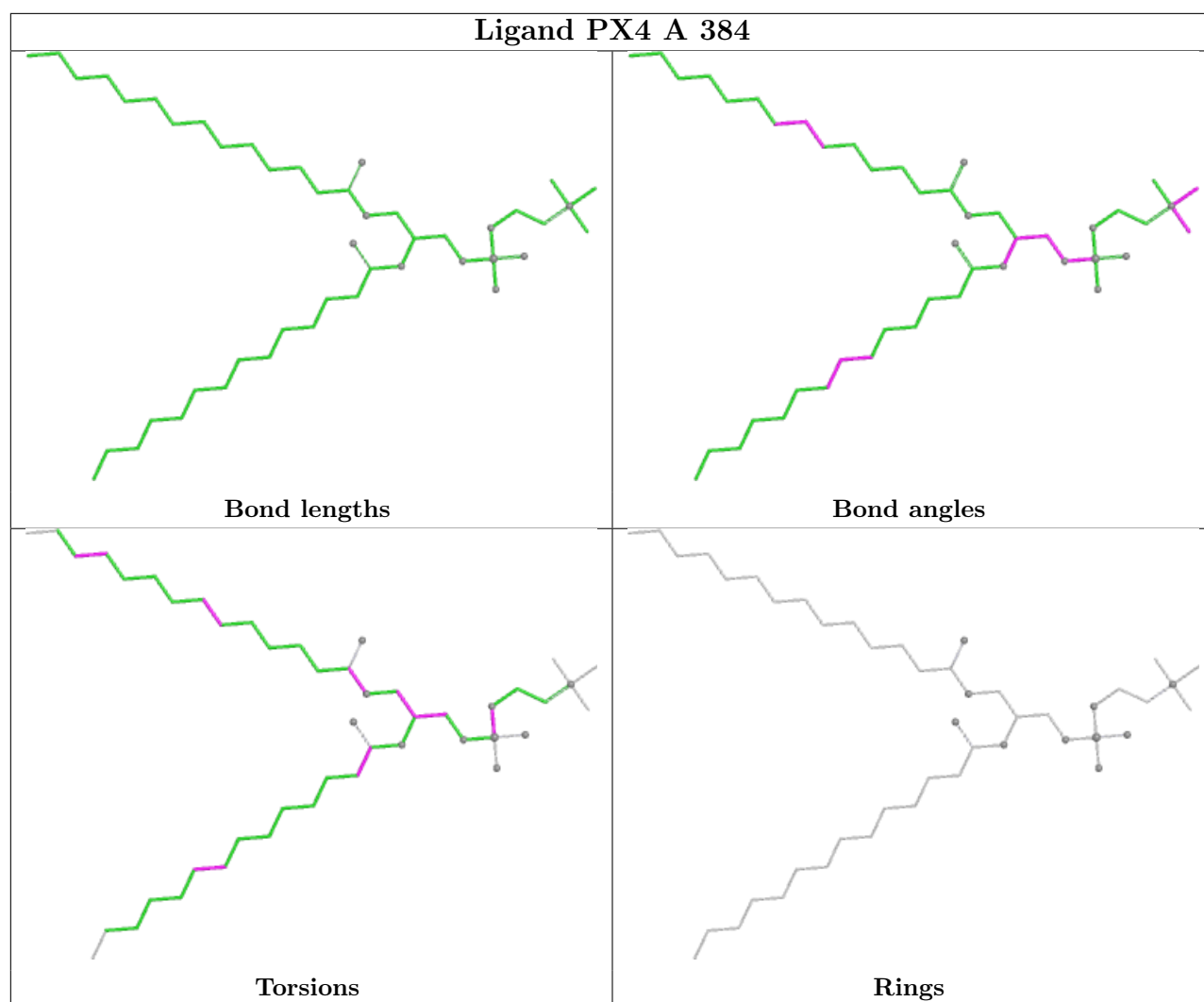












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	160	-0.25 ± 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 82%, i.e. 1756 atoms were assigned a chemical shift out of a possible 2153. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

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

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	158/272 (58%)	79/137 (58%)	76/123 (62%)	3/12 (25%)
Overall	1756/2153 (82%)	955/1169 (82%)	636/777 (82%)	165/207 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1762 atoms were assigned a chemical shift out of a possible 2177. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	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 [i](#)

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

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

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

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

Random coil index (RCI) for chain A:

