



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:41 AM UTC

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

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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

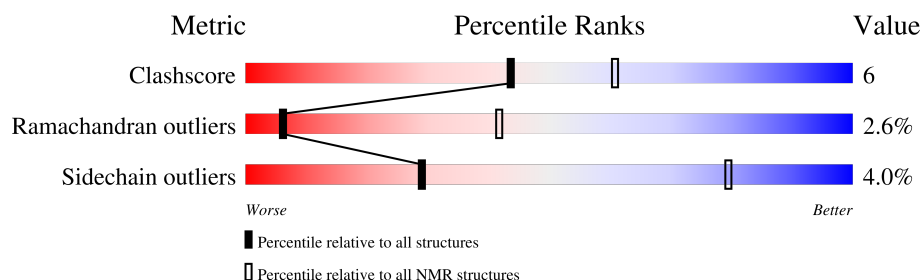
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 25%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	250	

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

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

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:75, A:82-A:244 (237)	1.20	5

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition

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

- Molecule 1 is a protein called Matrilysin.

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

There is a discrepancy between the modelled and reference sequences:

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

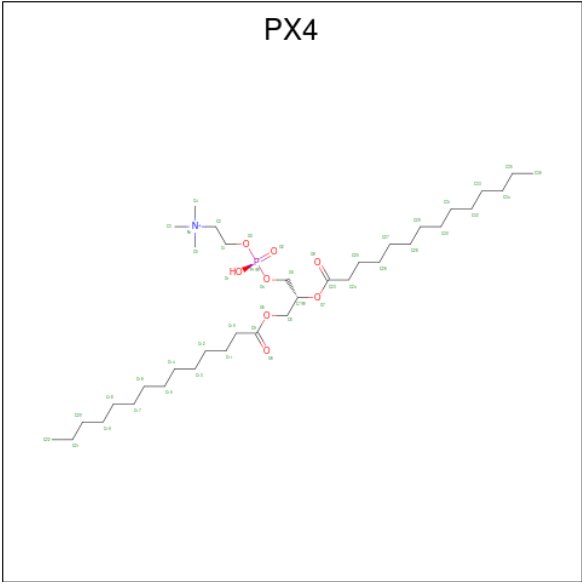
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

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

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

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



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

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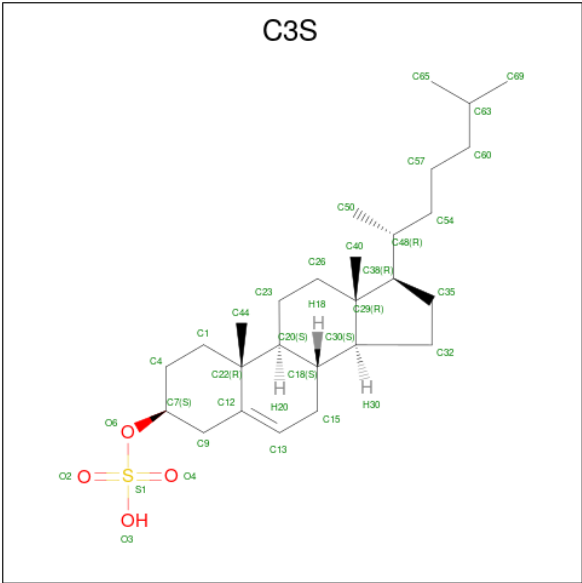
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Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

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



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

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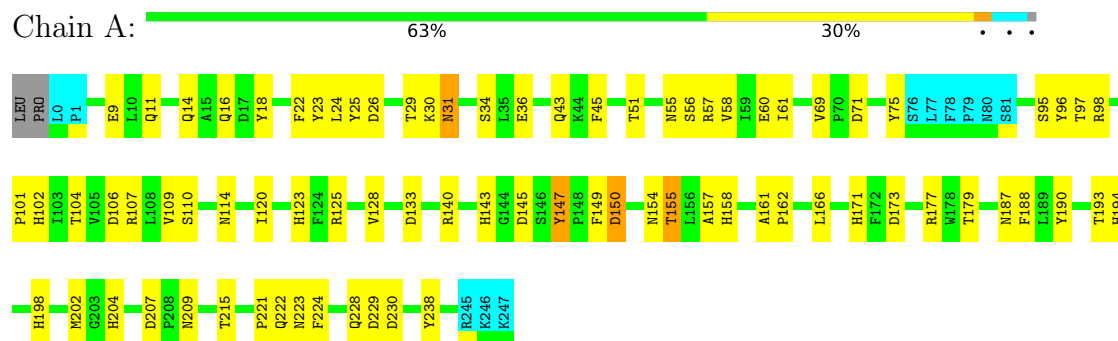
Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Matrilysin

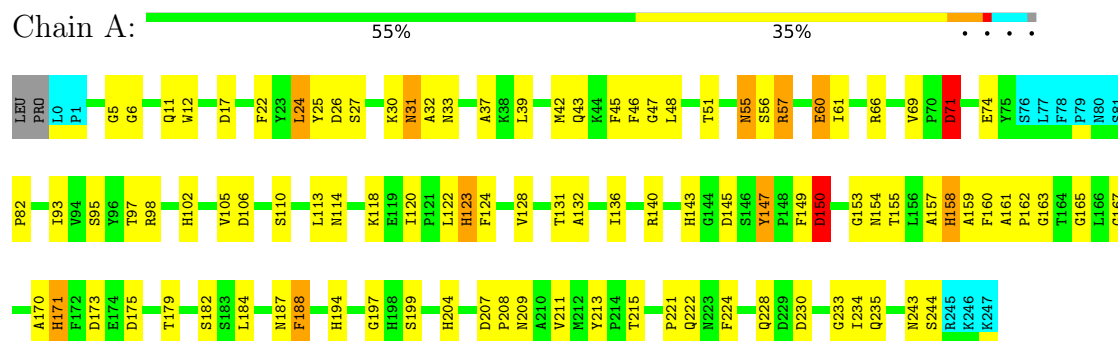


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Matrilysin



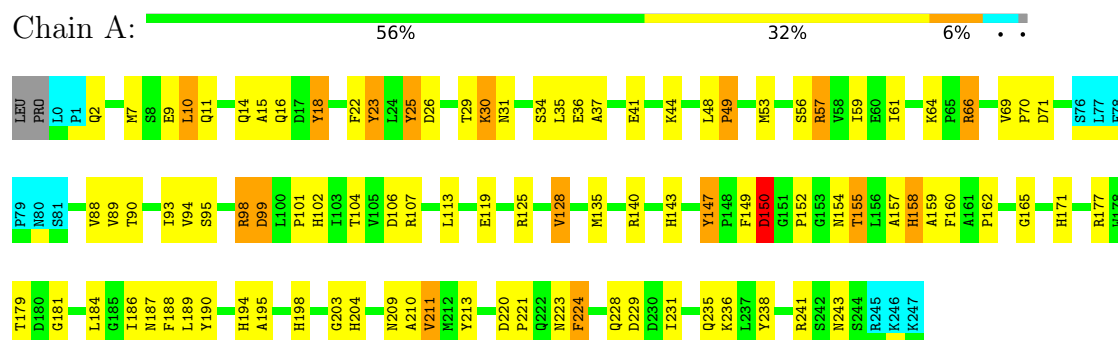
4.2.2 Score per residue for model 2

• Molecule 1: Matrilysin



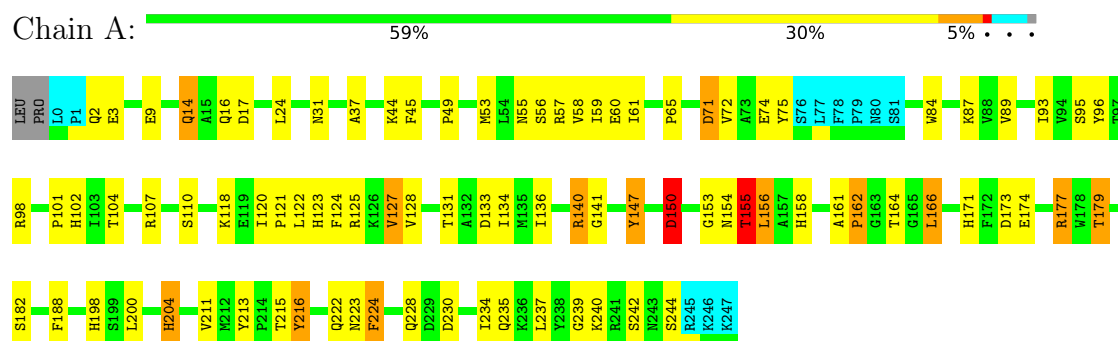
4.2.3 Score per residue for model 3

• Molecule 1: Matrilysin



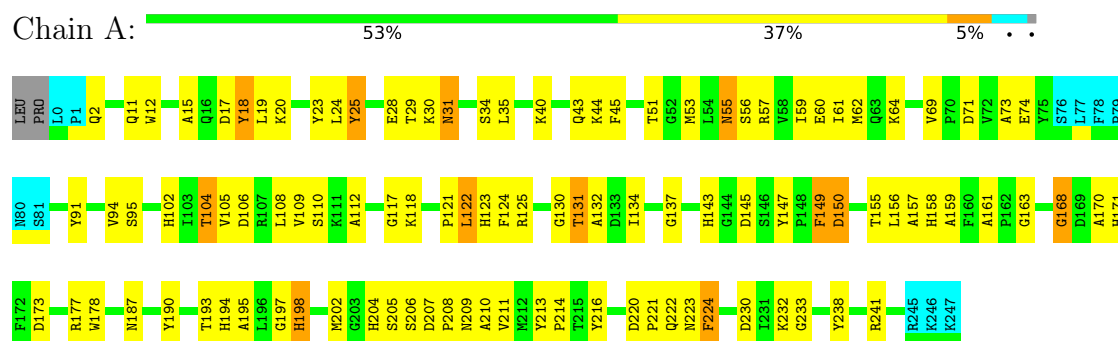
4.2.4 Score per residue for model 4

• Molecule 1: Matrilysin



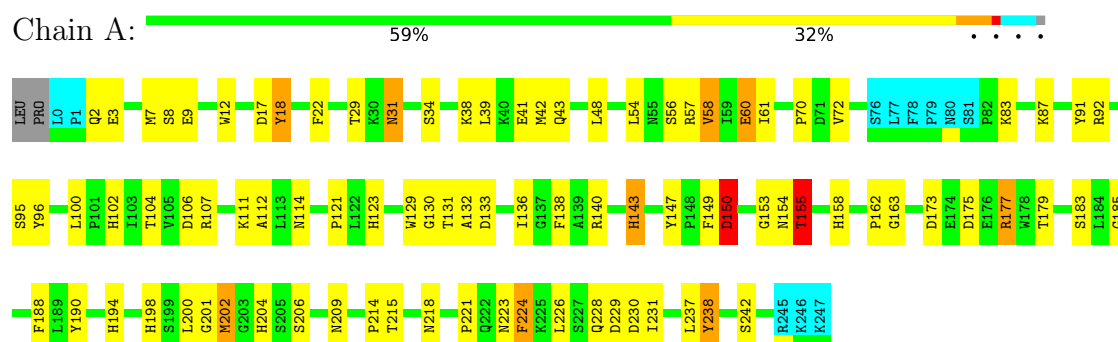
4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Matrilysin



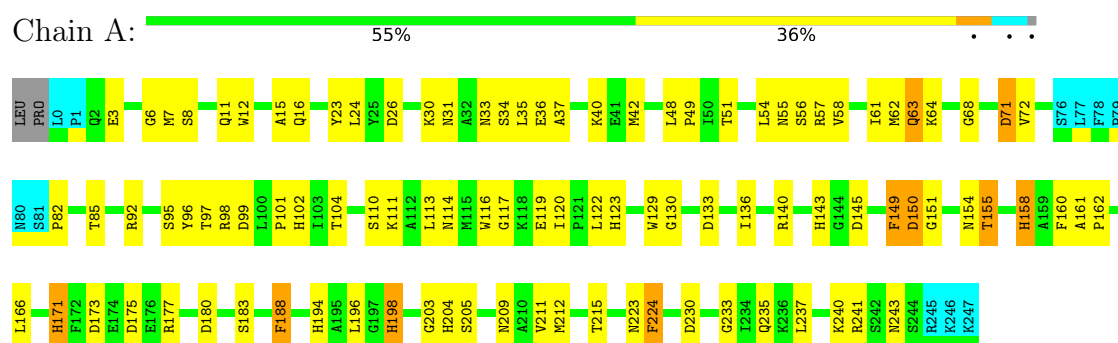
4.2.6 Score per residue for model 6

• Molecule 1: Matrilysin



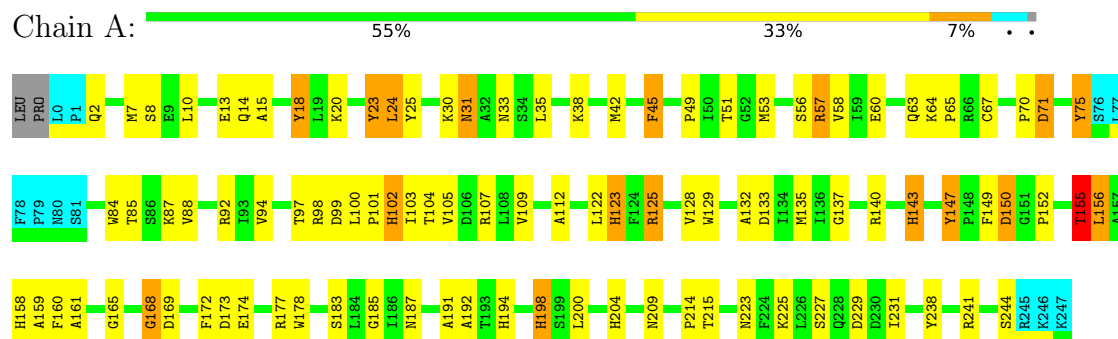
4.2.7 Score per residue for model 7

• Molecule 1: Matrilysin



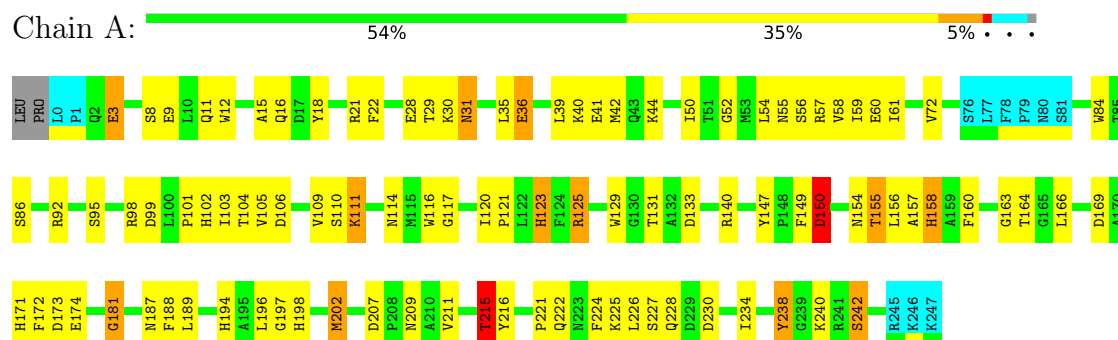
4.2.8 Score per residue for model 8

- Molecule 1: Matrilysin



4.2.9 Score per residue for model 9

- Molecule 1: Matrilysin



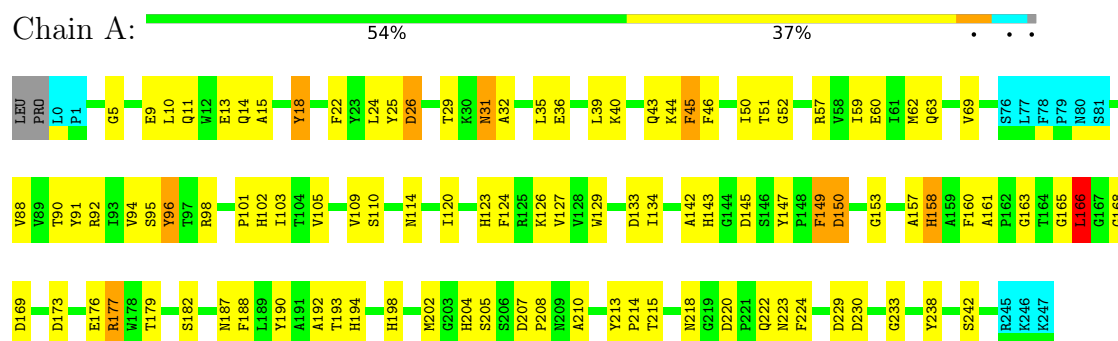
4.2.10 Score per residue for model 10

- Molecule 1: Matrilysin



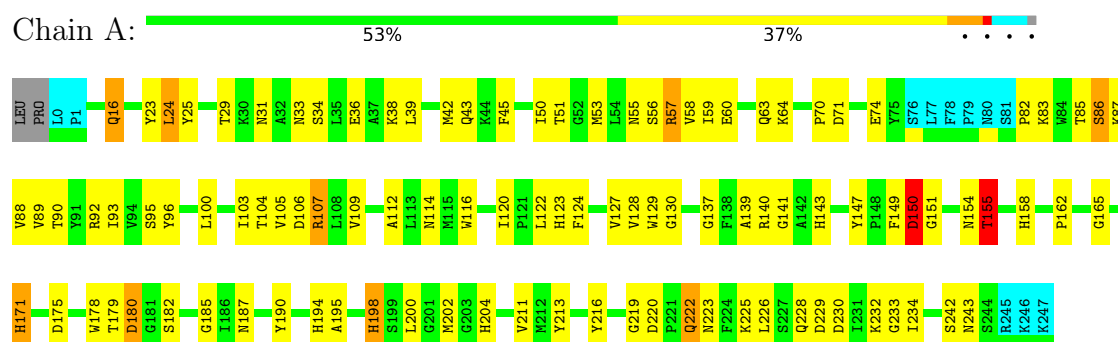
4.2.11 Score per residue for model 11

• Molecule 1: Matrilysin



4.2.12 Score per residue for model 12

• Molecule 1: Matrilysin



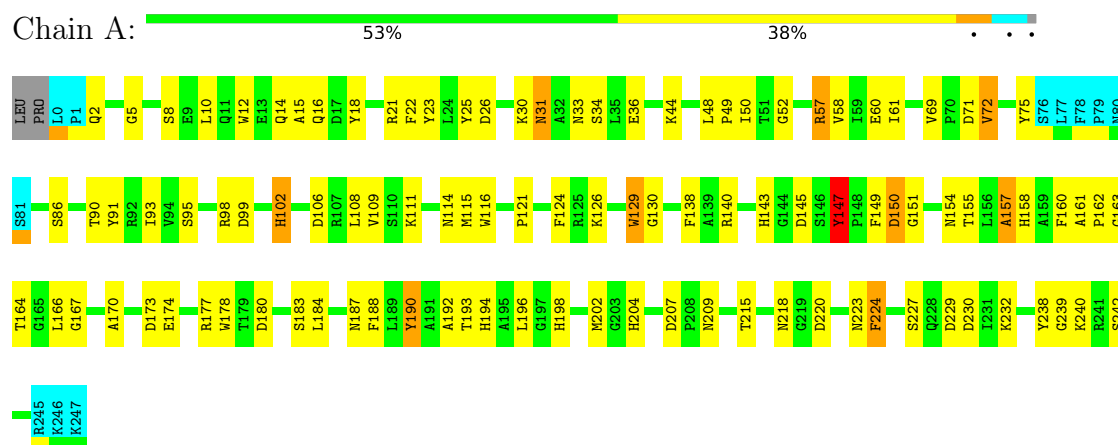
4.2.13 Score per residue for model 13

• Molecule 1: Matrilysin



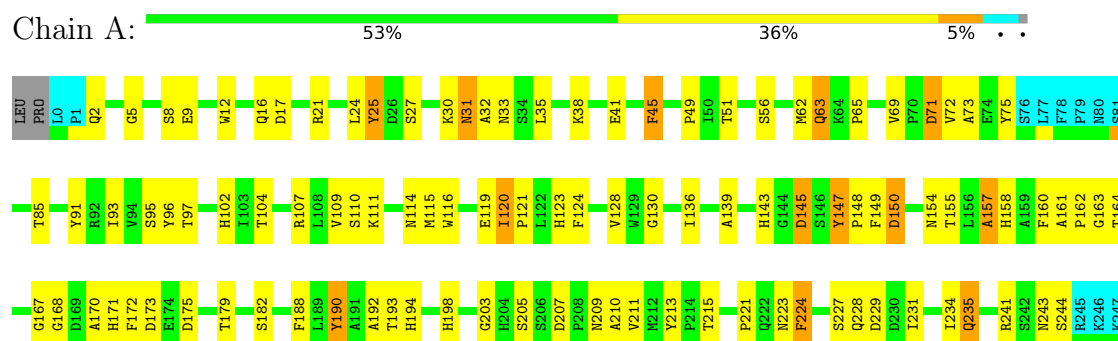
4.2.14 Score per residue for model 14

• Molecule 1: Matrilysin



4.2.15 Score per residue for model 15

• Molecule 1: Matrilysin



4.2.16 Score per residue for model 16

• Molecule 1: Matrilysin

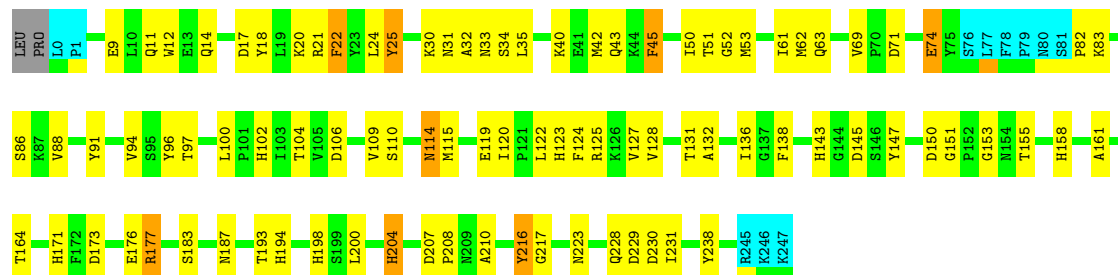




4.2.17 Score per residue for model 17

- Molecule 1: Matrilysin

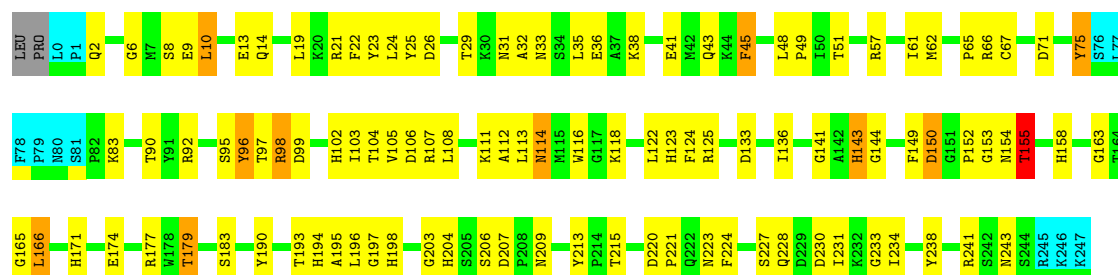
Chain A: 58% 33%



4.2.18 Score per residue for model 18

- Molecule 1: Matrilysin

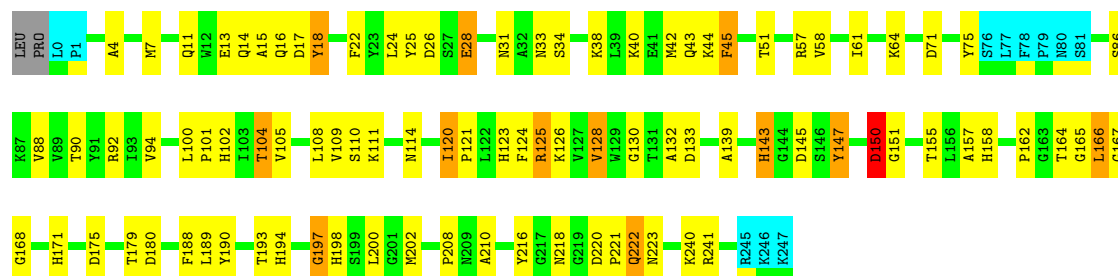
Chain A: 52% 38%



4.2.19 Score per residue for model 19

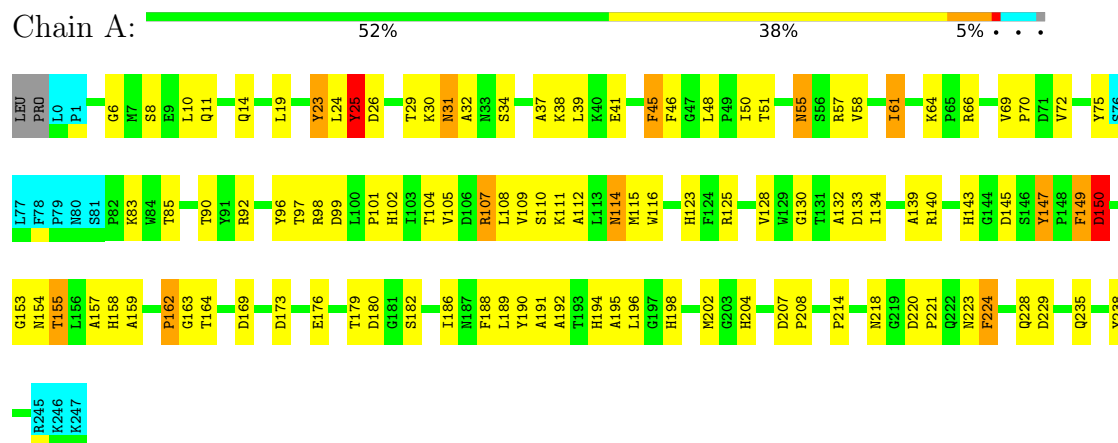
- Molecule 1: Matrilysin

Chain A: 58% 32% 5%



4.2.20 Score per residue for model 20

● Molecule 1: Matrilysin



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
HADDOCK	structure solution	2.1
GROMOS	refinement	4.5.7

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	797
Number of shifts mapped to atoms	797
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality i

6.1 Standard geometry i

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

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

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	7.2±2.1
All	All	0	144

There are no bond-length outliers.

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	149	PHE	CA-CB-CG	14.12	127.92	113.80	7	13
1	A	45	PHE	CA-CB-CG	13.65	127.45	113.80	2	14
1	A	218	ASN	CA-C-N	12.62	131.33	121.61	14	4
1	A	218	ASN	C-N-CA	12.62	131.33	121.61	14	4
1	A	102	HIS	CA-CB-CG	12.54	126.34	113.80	7	5
1	A	99	ASP	CA-CB-CG	12.35	124.95	112.60	18	8
1	A	106	ASP	CA-CB-CG	12.08	124.68	112.60	17	4
1	A	224	PHE	CA-CB-CG	11.86	125.66	113.80	3	7
1	A	229	ASP	CA-C-N	11.85	136.56	120.44	15	4
1	A	229	ASP	C-N-CA	11.85	136.56	120.44	15	4
1	A	42	MET	N-CA-C	11.59	125.36	111.33	9	5
1	A	218	ASN	CA-CB-CG	11.57	124.17	112.60	6	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	VAL	N-CA-C	-11.34	98.88	108.63	5	1
1	A	111	LYS	CA-C-N	11.22	135.89	120.63	18	5
1	A	111	LYS	C-N-CA	11.22	135.89	120.63	18	5
1	A	40	LYS	CA-C-N	11.17	135.24	120.28	17	5
1	A	40	LYS	C-N-CA	11.17	135.24	120.28	17	5
1	A	204	HIS	ND1-CE1-NE2	11.07	119.47	108.40	8	9
1	A	114	ASN	CA-CB-CG	11.02	123.62	112.60	18	5
1	A	173	ASP	CA-CB-CG	10.92	123.52	112.60	7	11
1	A	123	HIS	CA-CB-CG	10.91	124.71	113.80	13	8
1	A	206	SER	CA-C-N	10.68	134.98	120.67	16	4
1	A	206	SER	C-N-CA	10.68	134.98	120.67	16	4
1	A	147	TYR	CA-C-N	10.54	130.50	119.85	10	4
1	A	147	TYR	C-N-CA	10.54	130.50	119.85	10	4
1	A	57	ARG	CA-C-N	10.46	135.28	120.53	9	12
1	A	57	ARG	C-N-CA	10.46	135.28	120.53	9	12
1	A	204	HIS	CE1-NE2-CD2	-10.35	98.65	109.00	3	9
1	A	104	THR	CA-C-N	10.33	133.92	120.60	7	8
1	A	104	THR	C-N-CA	10.33	133.92	120.60	7	8
1	A	235	GLN	OE1-CD-NE2	-10.31	112.29	122.60	20	3
1	A	198	HIS	CE1-NE2-CD2	-10.22	98.78	109.00	9	14
1	A	26	ASP	CA-C-N	10.21	133.96	120.28	11	2
1	A	26	ASP	C-N-CA	10.21	133.96	120.28	11	2
1	A	198	HIS	CA-C-N	10.16	133.90	120.28	13	1
1	A	198	HIS	C-N-CA	10.16	133.90	120.28	13	1
1	A	162	PRO	CA-C-N	10.08	131.73	121.35	4	7
1	A	162	PRO	C-N-CA	10.08	131.73	121.35	4	7
1	A	61	ILE	CA-C-N	10.05	134.11	120.54	3	11
1	A	61	ILE	C-N-CA	10.05	134.11	120.54	3	11
1	A	194	HIS	CE1-NE2-CD2	-10.02	98.98	109.00	9	12
1	A	83	LYS	O-C-N	-9.91	113.94	123.26	18	1
1	A	160	PHE	CA-CB-CG	9.91	123.71	113.80	1	4
1	A	209	ASN	CA-C-N	9.78	134.76	120.87	18	5
1	A	209	ASN	C-N-CA	9.78	134.76	120.87	18	5
1	A	17	ASP	CA-CB-CG	9.73	122.33	112.60	17	3
1	A	171	HIS	ND1-CE1-NE2	9.71	118.11	108.40	19	10
1	A	143	HIS	CA-CB-CG	9.68	123.48	113.80	11	9
1	A	177	ARG	NE-CZ-NH2	-9.62	110.54	119.20	5	5
1	A	48	LEU	CA-C-O	-9.59	112.13	120.19	20	4
1	A	194	HIS	ND1-CE1-NE2	9.57	117.97	108.40	12	7
1	A	194	HIS	CA-CB-CG	9.56	123.36	113.80	13	13
1	A	198	HIS	ND1-CE1-NE2	9.56	117.96	108.40	9	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	153	GLY	CA-C-O	-9.55	112.79	122.25	20	2
1	A	150	ASP	CA-CB-CG	9.48	122.08	112.60	5	10
1	A	3	GLU	CA-C-N	9.47	134.71	120.31	2	4
1	A	3	GLU	C-N-CA	9.47	134.71	120.31	2	4
1	A	34	SER	CA-C-N	9.46	133.91	120.28	5	11
1	A	34	SER	C-N-CA	9.46	133.91	120.28	5	11
1	A	155	THR	CA-CB-CG2	9.45	126.57	110.50	12	6
1	A	28	GLU	N-CA-C	-9.40	101.94	113.50	9	2
1	A	140	ARG	CD-NE-CZ	9.38	137.53	124.40	4	4
1	A	15	ALA	CA-C-N	9.36	133.59	120.29	3	3
1	A	15	ALA	C-N-CA	9.36	133.59	120.29	3	3
1	A	140	ARG	NE-CZ-NH2	-9.32	110.81	119.20	14	3
1	A	211	VAL	CA-CB-CG1	9.32	126.24	110.40	3	3
1	A	168	GLY	CA-C-O	-9.29	109.33	119.27	16	3
1	A	175	ASP	CA-C-N	9.28	134.04	120.87	19	4
1	A	175	ASP	C-N-CA	9.28	134.04	120.87	19	4
1	A	72	VAL	CB-CA-C	9.23	123.81	110.33	6	4
1	A	116	TRP	CA-C-N	9.18	130.37	119.99	7	4
1	A	116	TRP	C-N-CA	9.18	130.37	119.99	7	4
1	A	158	HIS	CA-CB-CG	9.12	122.92	113.80	5	10
1	A	221	PRO	CA-C-N	9.10	132.47	120.28	3	6
1	A	221	PRO	C-N-CA	9.10	132.47	120.28	3	6
1	A	69	VAL	CA-C-O	-9.09	112.01	119.47	20	5
1	A	136	ILE	CA-C-N	9.09	131.11	121.48	7	6
1	A	136	ILE	C-N-CA	9.09	131.11	121.48	7	6
1	A	179	THR	CA-C-N	9.08	133.35	121.90	16	2
1	A	179	THR	C-N-CA	9.08	133.35	121.90	16	2
1	A	120	ILE	N-CA-CB	-9.06	103.97	111.67	7	2
1	A	56	SER	CA-C-N	9.04	138.81	121.54	4	6
1	A	56	SER	C-N-CA	9.04	138.81	121.54	4	6
1	A	92	ARG	NE-CZ-NH2	9.02	127.31	119.20	6	7
1	A	243	ASN	CA-CB-CG	9.01	121.61	112.60	3	3
1	A	90	THR	CA-CB-OG1	8.98	123.07	109.60	12	3
1	A	107	ARG	CA-C-N	8.96	132.09	120.44	4	7
1	A	107	ARG	C-N-CA	8.96	132.09	120.44	4	7
1	A	134	ILE	N-CA-CB	-8.95	100.30	111.31	2	4
1	A	209	ASN	OD1-CG-ND2	-8.93	113.67	122.60	5	4
1	A	230	ASP	CA-C-N	8.89	133.07	120.53	2	7
1	A	230	ASP	C-N-CA	8.89	133.07	120.53	2	7
1	A	128	VAL	CA-C-N	8.87	135.52	122.39	8	2
1	A	128	VAL	C-N-CA	8.87	135.52	122.39	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	101	PRO	CA-C-N	8.84	132.49	120.38	3	9
1	A	101	PRO	C-N-CA	8.84	132.49	120.38	3	9
1	A	123	HIS	CE1-NE2-CD2	-8.82	100.18	109.00	6	11
1	A	97	THR	CA-CB-OG1	8.81	122.82	109.60	15	3
1	A	197	GLY	CA-C-N	8.80	132.08	120.28	9	4
1	A	197	GLY	C-N-CA	8.80	132.08	120.28	9	4
1	A	202	MET	CA-C-O	-8.80	111.30	121.16	13	2
1	A	221	PRO	N-CA-CB	8.74	111.47	103.34	2	1
1	A	123	HIS	ND1-CE1-NE2	8.73	117.13	108.40	1	8
1	A	55	ASN	CA-CB-CG	8.70	121.30	112.60	13	5
1	A	124	PHE	CA-CB-CG	8.62	122.42	113.80	5	3
1	A	198	HIS	O-C-N	-8.60	113.00	122.12	9	1
1	A	229	ASP	CA-CB-CG	8.60	121.20	112.60	14	4
1	A	207	ASP	CA-C-N	8.59	128.81	119.87	17	10
1	A	207	ASP	C-N-CA	8.59	128.81	119.87	17	10
1	A	177	ARG	CD-NE-CZ	8.59	136.43	124.40	11	2
1	A	158	HIS	ND1-CE1-NE2	8.59	116.99	108.40	6	8
1	A	51	THR	CA-CB-CG2	8.59	125.10	110.50	8	3
1	A	121	PRO	CA-C-N	8.57	134.82	123.00	9	5
1	A	121	PRO	C-N-CA	8.57	134.82	123.00	9	5
1	A	158	HIS	CE1-NE2-CD2	-8.56	100.44	109.00	3	16
1	A	57	ARG	NE-CZ-NH2	-8.55	111.51	119.20	1	1
1	A	125	ARG	NE-CZ-NH2	-8.55	111.51	119.20	2	3
1	A	35	LEU	CA-C-N	8.55	132.09	120.38	18	10
1	A	35	LEU	C-N-CA	8.55	132.09	120.38	18	10
1	A	21	ARG	NE-CZ-NH1	-8.51	112.99	121.50	9	2
1	A	172	PHE	CA-CB-CG	8.51	122.31	113.80	16	3
1	A	143	HIS	CE1-NE2-CD2	-8.49	100.50	109.00	11	9
1	A	98	ARG	CA-C-N	8.48	133.21	120.31	9	5
1	A	98	ARG	C-N-CA	8.48	133.21	120.31	9	5
1	A	6	GLY	CA-C-N	8.48	137.74	121.54	13	4
1	A	6	GLY	C-N-CA	8.48	137.74	121.54	13	4
1	A	157	ALA	CA-C-N	8.48	136.85	121.85	9	5
1	A	157	ALA	C-N-CA	8.48	136.85	121.85	9	5
1	A	57	ARG	N-CA-C	8.45	123.25	113.19	7	2
1	A	175	ASP	CA-CB-CG	8.45	121.05	112.60	12	5
1	A	225	LYS	CA-C-N	8.44	133.49	121.42	12	2
1	A	225	LYS	C-N-CA	8.44	133.49	121.42	12	2
1	A	42	MET	CA-C-O	8.44	129.50	120.55	17	1
1	A	93	ILE	N-CA-CB	8.44	119.92	110.72	4	2
1	A	60	GLU	O-C-N	8.41	131.17	122.09	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	194	HIS	CG-CD2-NE2	8.41	115.61	107.20	9	8
1	A	187	ASN	CA-CB-CG	8.39	120.99	112.60	17	2
1	A	140	ARG	NH1-CZ-NH2	8.39	130.21	119.30	14	1
1	A	154	ASN	CA-CB-CG	8.38	120.98	112.60	13	4
1	A	71	ASP	CA-CB-CG	8.38	120.98	112.60	18	2
1	A	223	ASN	CA-CB-CG	8.37	120.97	112.60	2	5
1	A	101	PRO	N-CA-CB	8.36	111.11	103.33	9	1
1	A	215	THR	CA-C-N	8.34	132.55	120.71	18	7
1	A	215	THR	C-N-CA	8.34	132.55	120.71	18	7
1	A	88	VAL	CA-C-N	8.29	135.78	122.68	3	6
1	A	88	VAL	C-N-CA	8.29	135.78	122.68	3	6
1	A	112	ALA	N-CA-C	-8.26	101.33	111.40	6	2
1	A	55	ASN	OD1-CG-ND2	-8.25	114.35	122.60	9	5
1	A	173	ASP	CA-C-N	8.23	131.66	120.38	8	6
1	A	173	ASP	C-N-CA	8.23	131.66	120.38	8	6
1	A	104	THR	CA-CB-OG1	8.18	121.86	109.60	15	9
1	A	166	LEU	CA-C-N	8.17	128.10	120.34	4	3
1	A	166	LEU	C-N-CA	8.17	128.10	120.34	4	3
1	A	114	ASN	OD1-CG-ND2	-8.15	114.45	122.60	1	7
1	A	51	THR	CB-CA-C	8.13	123.69	111.17	7	12
1	A	117	GLY	CA-C-N	8.12	133.70	120.63	7	4
1	A	117	GLY	C-N-CA	8.12	133.70	120.63	7	4
1	A	107	ARG	CA-C-O	-8.11	111.96	120.55	20	2
1	A	116	TRP	CA-C-O	-8.10	110.23	119.79	2	1
1	A	102	HIS	ND1-CE1-NE2	8.08	116.48	108.40	5	8
1	A	163	GLY	O-C-N	8.07	130.76	123.42	1	4
1	A	29	THR	CA-C-N	8.06	134.34	123.05	6	4
1	A	29	THR	C-N-CA	8.06	134.34	123.05	6	4
1	A	204	HIS	CA-CB-CG	8.06	121.86	113.80	18	5
1	A	196	LEU	CA-C-O	-8.03	111.33	120.24	16	3
1	A	103	ILE	N-CA-C	8.02	121.07	111.05	12	2
1	A	231	ILE	O-C-N	8.00	129.73	121.89	2	4
1	A	151	GLY	CA-C-N	8.00	128.30	119.90	14	2
1	A	151	GLY	C-N-CA	8.00	128.30	119.90	14	2
1	A	220	ASP	CA-C-N	8.00	128.29	119.90	19	5
1	A	220	ASP	C-N-CA	8.00	128.29	119.90	19	5
1	A	133	ASP	CA-CB-CG	7.99	120.59	112.60	11	4
1	A	105	VAL	CA-C-N	7.98	131.31	120.54	9	7
1	A	105	VAL	C-N-CA	7.98	131.31	120.54	9	7
1	A	41	GLU	CA-C-N	7.98	131.31	120.38	6	6
1	A	41	GLU	C-N-CA	7.98	131.31	120.38	6	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	210	ALA	N-CA-C	7.98	121.80	110.23	19	3
1	A	58	VAL	CA-C-O	-7.97	112.76	121.05	9	2
1	A	65	PRO	N-CA-CB	7.97	111.62	103.25	10	3
1	A	35	LEU	N-CA-C	7.96	122.43	112.87	8	1
1	A	29	THR	CA-CB-OG1	-7.96	97.66	109.60	6	1
1	A	138	PHE	CA-CB-CG	-7.96	105.84	113.80	10	3
1	A	95	SER	O-C-N	-7.96	114.57	123.48	4	4
1	A	140	ARG	NE-CZ-NH1	7.93	129.44	121.50	1	3
1	A	53	MET	CB-CA-C	7.93	125.47	109.38	10	1
1	A	149	PHE	CA-C-N	7.92	136.67	121.54	7	6
1	A	149	PHE	C-N-CA	7.92	136.67	121.54	7	6
1	A	11	GLN	CA-C-O	-7.90	112.04	120.42	9	2
1	A	180	ASP	CA-CB-CG	7.90	120.50	112.60	16	2
1	A	32	ALA	CA-C-N	7.90	131.18	120.44	17	5
1	A	32	ALA	C-N-CA	7.90	131.18	120.44	17	5
1	A	70	PRO	N-CA-CB	7.89	111.53	103.25	20	3
1	A	109	VAL	CA-C-N	7.89	130.69	120.44	12	8
1	A	109	VAL	C-N-CA	7.89	130.69	120.44	12	8
1	A	8	SER	CA-C-N	7.87	132.63	120.82	18	7
1	A	8	SER	C-N-CA	7.87	132.63	120.82	18	7
1	A	145	ASP	CA-CB-CG	7.87	120.47	112.60	15	6
1	A	152	PRO	N-CA-CB	7.87	109.89	103.36	8	2
1	A	105	VAL	CB-CA-C	7.85	124.17	111.29	19	1
1	A	31	ASN	CA-C-N	7.81	131.08	120.54	13	8
1	A	31	ASN	C-N-CA	7.81	131.08	120.54	13	8
1	A	95	SER	CA-C-O	-7.79	113.12	121.38	15	3
1	A	82	PRO	N-CA-CB	7.77	108.40	102.73	1	1
1	A	48	LEU	CA-C-N	7.76	127.40	119.56	1	5
1	A	48	LEU	C-N-CA	7.76	127.40	119.56	1	5
1	A	188	PHE	O-C-N	-7.75	113.15	122.22	4	2
1	A	25	TYR	N-CA-CB	7.74	123.57	110.49	17	1
1	A	45	PHE	N-CA-C	7.73	120.59	111.71	13	2
1	A	3	GLU	CA-C-O	7.70	128.71	120.55	13	1
1	A	214	PRO	N-CA-CB	7.70	110.62	103.46	5	2
1	A	171	HIS	CA-CB-CG	7.69	121.49	113.80	4	4
1	A	33	ASN	CA-CB-CG	7.69	120.29	112.60	7	4
1	A	188	PHE	N-CA-C	7.68	119.73	111.36	11	2
1	A	207	ASP	N-CA-CB	-7.67	99.32	110.14	9	3
1	A	110	SER	CA-C-N	7.67	131.18	120.29	11	6
1	A	110	SER	C-N-CA	7.67	131.18	120.29	11	6
1	A	38	LYS	CA-C-N	7.65	131.30	120.28	20	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	LYS	C-N-CA	7.65	131.30	120.28	20	5
1	A	155	THR	OG1-CB-CG2	-7.65	93.99	109.30	5	3
1	A	51	THR	CA-CB-OG1	7.65	121.07	109.60	17	3
1	A	16	GLN	CA-C-N	7.64	133.64	120.58	4	8
1	A	16	GLN	C-N-CA	7.64	133.64	120.58	4	8
1	A	104	THR	O-C-N	-7.63	113.79	122.03	7	1
1	A	164	THR	N-CA-C	7.62	121.67	112.38	17	2
1	A	34	SER	N-CA-C	-7.61	102.56	112.68	16	2
1	A	29	THR	CA-CB-CG2	7.61	123.44	110.50	3	6
1	A	229	ASP	CA-C-O	7.61	128.76	119.79	11	2
1	A	215	THR	CB-CA-C	7.60	121.70	111.14	11	1
1	A	229	ASP	O-C-N	7.59	130.17	122.12	12	1
1	A	221	PRO	CA-C-O	-7.59	113.30	121.27	1	2
1	A	171	HIS	CE1-NE2-CD2	-7.59	101.41	109.00	16	5
1	A	209	ASN	CA-CB-CG	7.58	120.18	112.60	7	2
1	A	30	LYS	CA-C-N	7.57	136.01	121.54	8	10
1	A	30	LYS	C-N-CA	7.57	136.01	121.54	8	10
1	A	118	LYS	CA-C-O	7.57	128.68	120.20	2	2
1	A	233	GLY	CA-C-N	7.57	130.09	120.56	11	5
1	A	233	GLY	C-N-CA	7.57	130.09	120.56	11	5
1	A	211	VAL	O-C-N	-7.55	114.51	121.91	1	1
1	A	18	TYR	CA-C-N	7.53	130.23	120.44	17	4
1	A	18	TYR	C-N-CA	7.53	130.23	120.44	17	4
1	A	198	HIS	CG-CD2-NE2	7.53	114.73	107.20	18	5
1	A	98	ARG	CA-CB-CG	-7.51	99.08	114.10	11	1
1	A	14	GLN	CA-C-N	7.50	130.34	120.28	17	8
1	A	14	GLN	C-N-CA	7.50	130.34	120.28	17	8
1	A	113	LEU	CA-C-N	7.50	130.67	120.54	7	2
1	A	113	LEU	C-N-CA	7.50	130.67	120.54	7	2
1	A	100	LEU	CA-C-N	7.48	127.46	119.76	12	3
1	A	100	LEU	C-N-CA	7.48	127.46	119.76	12	3
1	A	214	PRO	N-CA-C	7.48	123.37	113.57	20	1
1	A	113	LEU	CA-C-O	-7.47	112.63	120.55	7	1
1	A	102	HIS	CA-C-N	7.45	130.20	120.60	18	3
1	A	102	HIS	C-N-CA	7.45	130.20	120.60	18	3
1	A	133	ASP	CA-C-N	7.44	133.52	123.10	4	6
1	A	133	ASP	C-N-CA	7.44	133.52	123.10	4	6
1	A	186	ILE	CB-CA-C	7.44	121.40	111.21	3	1
1	A	227	SER	CA-C-N	7.43	130.24	120.28	2	6
1	A	227	SER	C-N-CA	7.43	130.24	120.28	2	6
1	A	183	SER	N-CA-C	7.42	121.91	112.86	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	17	ASP	N-CA-C	7.42	119.37	111.28	13	1
1	A	22	PHE	CA-CB-CG	7.41	121.21	113.80	3	5
1	A	201	GLY	CA-C-N	7.41	133.06	122.09	16	2
1	A	201	GLY	C-N-CA	7.41	133.06	122.09	16	2
1	A	36	GLU	CA-C-N	7.41	130.07	120.44	13	5
1	A	36	GLU	C-N-CA	7.41	130.07	120.44	13	5
1	A	230	ASP	CA-CB-CG	7.40	120.00	112.60	18	7
1	A	94	VAL	N-CA-C	7.40	120.36	112.96	11	3
1	A	123	HIS	CG-CD2-NE2	7.39	114.59	107.20	9	7
1	A	31	ASN	CA-CB-CG	7.39	119.99	112.60	6	2
1	A	10	LEU	CA-C-N	7.38	133.05	120.72	18	2
1	A	10	LEU	C-N-CA	7.38	133.05	120.72	18	2
1	A	71	ASP	CA-C-N	7.38	133.46	122.98	15	6
1	A	71	ASP	C-N-CA	7.38	133.46	122.98	15	6
1	A	145	ASP	N-CA-C	-7.37	99.30	110.14	20	1
1	A	232	LYS	N-CA-C	7.37	121.37	112.38	10	3
1	A	46	PHE	CA-CB-CG	7.36	121.16	113.80	11	3
1	A	160	PHE	CA-C-N	7.36	131.87	120.68	7	4
1	A	160	PHE	C-N-CA	7.36	131.87	120.68	7	4
1	A	206	SER	CA-C-O	7.36	127.94	119.18	18	1
1	A	180	ASP	CB-CA-C	7.36	125.06	110.42	2	2
1	A	143	HIS	CG-CD2-NE2	7.35	114.55	107.20	11	1
1	A	21	ARG	N-CA-C	7.34	118.93	111.07	18	3
1	A	203	GLY	CA-C-N	7.34	133.58	121.39	3	3
1	A	203	GLY	C-N-CA	7.34	133.58	121.39	3	3
1	A	12	TRP	CA-C-N	7.33	130.41	120.44	5	5
1	A	12	TRP	C-N-CA	7.33	130.41	120.44	5	5
1	A	154	ASN	CA-C-N	7.33	135.53	121.54	7	5
1	A	154	ASN	C-N-CA	7.33	135.53	121.54	7	5
1	A	88	VAL	O-C-N	-7.33	114.92	123.05	10	2
1	A	131	THR	CA-CB-OG1	7.30	120.55	109.60	5	3
1	A	83	LYS	CA-C-N	7.30	133.50	121.39	20	1
1	A	83	LYS	C-N-CA	7.30	133.50	121.39	20	1
1	A	12	TRP	CE2-CD2-CE3	-7.29	111.51	118.80	6	1
1	A	228	GLN	OE1-CD-NE2	-7.28	115.32	122.60	10	2
1	A	60	GLU	CA-C-O	-7.26	113.22	120.70	11	1
1	A	8	SER	N-CA-CB	-7.26	99.88	110.70	14	2
1	A	82	PRO	CB-CA-C	7.25	118.00	111.40	7	1
1	A	96	TYR	CA-C-N	7.25	131.17	120.87	18	4
1	A	96	TYR	C-N-CA	7.25	131.17	120.87	18	4
1	A	205	SER	CA-C-N	7.25	131.34	120.31	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	205	SER	C-N-CA	7.25	131.34	120.31	16	3
1	A	192	ALA	N-CA-C	-7.25	102.77	111.69	14	2
1	A	92	ARG	NE-CZ-NH1	7.25	128.75	121.50	20	3
1	A	192	ALA	CA-C-N	7.25	130.33	120.54	20	2
1	A	192	ALA	C-N-CA	7.25	130.33	120.54	20	2
1	A	120	ILE	CA-C-N	7.25	128.90	119.84	1	3
1	A	120	ILE	C-N-CA	7.25	128.90	119.84	1	3
1	A	132	ALA	CA-C-N	7.24	130.47	120.63	19	5
1	A	132	ALA	C-N-CA	7.24	130.47	120.63	19	5
1	A	228	GLN	CA-C-O	-7.23	112.89	120.55	18	5
1	A	71	ASP	OD1-CG-OD2	-7.23	105.55	122.90	7	15
1	A	31	ASN	OD1-CG-ND2	-7.23	115.37	122.60	16	2
1	A	122	LEU	CA-C-N	7.23	132.97	123.00	8	2
1	A	122	LEU	C-N-CA	7.23	132.97	123.00	8	2
1	A	207	ASP	N-CA-C	-7.21	98.08	109.04	10	1
1	A	11	GLN	OE1-CD-NE2	-7.21	115.39	122.60	10	3
1	A	137	GLY	O-C-N	-7.20	116.87	123.57	12	1
1	A	17	ASP	CA-C-N	7.20	129.80	120.44	5	6
1	A	17	ASP	C-N-CA	7.20	129.80	120.44	5	6
1	A	66	ARG	CD-NE-CZ	7.19	134.47	124.40	2	1
1	A	172	PHE	CA-C-N	7.19	132.14	121.72	9	4
1	A	172	PHE	C-N-CA	7.19	132.14	121.72	9	4
1	A	88	VAL	CA-C-O	7.19	127.86	120.39	16	2
1	A	52	GLY	CA-C-N	7.18	134.18	121.75	9	3
1	A	52	GLY	C-N-CA	7.18	134.18	121.75	9	3
1	A	36	GLU	CA-C-O	-7.16	112.97	120.55	9	3
1	A	145	ASP	N-CA-CB	7.16	122.21	110.69	15	1
1	A	171	HIS	CB-CG-CD2	-7.15	121.90	131.20	19	3
1	A	2	GLN	CA-C-N	7.15	129.87	120.28	4	3
1	A	2	GLN	C-N-CA	7.15	129.87	120.28	4	3
1	A	222	GLN	OE1-CD-NE2	-7.15	115.45	122.60	1	2
1	A	21	ARG	NE-CZ-NH2	7.15	125.63	119.20	9	2
1	A	243	ASN	OD1-CG-ND2	-7.15	115.45	122.60	1	2
1	A	64	LYS	CA-C-N	7.14	128.77	119.84	5	2
1	A	64	LYS	C-N-CA	7.14	128.77	119.84	5	2
1	A	130	GLY	CA-C-N	7.14	131.53	120.75	5	3
1	A	130	GLY	C-N-CA	7.14	131.53	120.75	5	3
1	A	232	LYS	CA-C-N	7.13	127.84	120.00	5	1
1	A	232	LYS	C-N-CA	7.13	127.84	120.00	5	1
1	A	88	VAL	N-CA-C	-7.13	97.83	108.46	12	1
1	A	193	THR	CA-CB-CG2	7.12	122.61	110.50	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	120	ILE	O-C-N	7.12	129.22	121.10	12	1
1	A	97	THR	CA-CB-CG2	7.12	122.59	110.50	8	2
1	A	210	ALA	CA-C-N	7.11	131.71	120.47	17	3
1	A	210	ALA	C-N-CA	7.11	131.71	120.47	17	3
1	A	9	GLU	CA-C-N	7.11	130.14	120.54	16	4
1	A	9	GLU	C-N-CA	7.11	130.14	120.54	16	4
1	A	201	GLY	CA-C-O	7.10	125.45	118.77	6	1
1	A	182	SER	N-CA-C	-7.10	104.42	113.23	11	1
1	A	59	ILE	CA-C-N	7.09	130.11	120.54	9	4
1	A	59	ILE	C-N-CA	7.09	130.11	120.54	9	4
1	A	221	PRO	CB-CA-C	-7.09	104.95	111.40	20	1
1	A	163	GLY	CA-C-O	-7.09	114.46	121.76	1	4
1	A	143	HIS	ND1-CE1-NE2	7.08	115.48	108.40	1	4
1	A	202	MET	N-CA-C	7.07	119.45	110.33	20	1
1	A	85	THR	CA-CB-OG1	7.07	120.20	109.60	15	1
1	A	204	HIS	ND1-CG-CD2	7.06	113.16	106.10	6	1
1	A	30	LYS	CA-C-O	-7.06	112.80	120.92	15	2
1	A	106	ASP	CA-C-N	7.06	130.04	120.44	18	6
1	A	106	ASP	C-N-CA	7.06	130.04	120.44	18	6
1	A	121	PRO	N-CA-CB	7.06	111.00	103.52	4	2
1	A	202	MET	CA-C-N	7.06	127.75	121.82	6	6
1	A	202	MET	C-N-CA	7.06	127.75	121.82	6	6
1	A	149	PHE	N-CA-C	7.06	121.59	113.19	16	2
1	A	42	MET	CA-C-N	7.06	129.74	120.28	7	4
1	A	42	MET	C-N-CA	7.06	129.74	120.28	7	4
1	A	150	ASP	N-CA-CB	7.05	122.41	110.49	20	2
1	A	49	PRO	CA-C-N	7.05	132.99	122.91	18	7
1	A	49	PRO	C-N-CA	7.05	132.99	122.91	18	7
1	A	34	SER	CA-C-O	7.03	128.05	119.97	2	2
1	A	223	ASN	CA-C-N	7.02	134.96	121.54	4	9
1	A	223	ASN	C-N-CA	7.02	134.96	121.54	4	9
1	A	69	VAL	CA-CB-CG1	7.02	122.34	110.40	3	3
1	A	157	ALA	CA-C-O	-7.02	113.77	121.28	15	2
1	A	26	ASP	CB-CA-C	7.01	121.92	109.65	3	3
1	A	44	LYS	O-C-N	-7.01	114.85	122.07	14	1
1	A	45	PHE	CA-C-O	-7.01	111.07	119.27	5	1
1	A	161	ALA	CA-C-N	7.00	128.59	119.84	5	9
1	A	161	ALA	C-N-CA	7.00	128.59	119.84	5	9
1	A	100	LEU	CB-CA-C	6.99	119.37	108.88	19	1
1	A	234	ILE	CA-C-N	6.99	129.98	120.54	9	2
1	A	234	ILE	C-N-CA	6.99	129.98	120.54	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	165	GLY	CA-C-N	6.98	130.57	120.38	12	9
1	A	165	GLY	C-N-CA	6.98	130.57	120.38	12	9
1	A	187	ASN	OD1-CG-ND2	-6.97	115.63	122.60	5	4
1	A	107	ARG	N-CA-C	6.96	118.87	111.28	12	2
1	A	231	ILE	CB-CA-C	6.96	120.88	111.97	8	2
1	A	204	HIS	N-CA-C	6.95	125.60	110.80	5	1
1	A	223	ASN	OD1-CG-ND2	-6.94	115.66	122.60	17	2
1	A	171	HIS	ND1-CG-CD2	6.93	113.03	106.10	18	2
1	A	209	ASN	N-CA-C	6.93	121.00	112.54	10	2
1	A	89	VAL	CB-CA-C	6.93	121.78	110.69	12	2
1	A	66	ARG	CA-C-N	6.93	132.49	122.44	3	1
1	A	66	ARG	C-N-CA	6.93	132.49	122.44	3	1
1	A	227	SER	N-CA-CB	-6.92	99.90	110.49	2	3
1	A	200	LEU	N-CA-C	6.92	121.81	113.23	12	5
1	A	21	ARG	CD-NE-CZ	6.92	134.09	124.40	16	1
1	A	189	LEU	O-C-N	6.92	129.28	122.09	3	1
1	A	108	LEU	CA-C-O	-6.91	113.47	121.07	18	2
1	A	125	ARG	NE-CZ-NH1	6.91	128.41	121.50	2	2
1	A	73	ALA	N-CA-CB	-6.91	100.69	111.05	15	1
1	A	9	GLU	O-C-N	-6.91	114.80	122.12	2	1
1	A	52	GLY	CA-C-O	-6.90	111.31	118.97	14	1
1	A	188	PHE	CA-C-N	6.89	129.85	120.54	14	7
1	A	188	PHE	C-N-CA	6.89	129.85	120.54	14	7
1	A	104	THR	CA-CB-CG2	6.89	122.21	110.50	20	2
1	A	235	GLN	CA-C-O	-6.88	110.42	119.10	13	1
1	A	190	TYR	CA-C-N	6.88	130.77	120.31	18	4
1	A	190	TYR	C-N-CA	6.88	130.77	120.31	18	4
1	A	44	LYS	CA-C-O	-6.88	113.13	120.42	19	3
1	A	103	ILE	CA-CB-CG1	6.88	122.09	110.40	9	1
1	A	241	ARG	NE-CZ-NH1	-6.87	114.63	121.50	19	2
1	A	112	ALA	CA-C-N	6.86	129.47	120.28	20	2
1	A	112	ALA	C-N-CA	6.86	129.47	120.28	20	2
1	A	193	THR	O-C-N	-6.85	114.20	122.22	17	1
1	A	16	GLN	CG-CD-NE2	6.84	126.66	116.40	15	3
1	A	84	TRP	CA-C-N	6.84	133.14	122.26	4	1
1	A	84	TRP	C-N-CA	6.84	133.14	122.26	4	1
1	A	46	PHE	N-CA-C	-6.84	104.83	113.72	20	1
1	A	24	LEU	CA-C-N	6.83	134.59	121.54	15	9
1	A	24	LEU	C-N-CA	6.83	134.59	121.54	15	9
1	A	22	PHE	CA-C-O	6.82	127.81	120.24	2	1
1	A	194	HIS	CB-CG-CD2	6.82	140.07	131.20	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	187	ASN	CA-C-O	-6.82	113.15	120.92	9	3
1	A	175	ASP	N-CA-C	-6.82	105.00	113.38	15	2
1	A	86	SER	N-CA-CB	-6.81	99.56	110.46	9	4
1	A	56	SER	CB-CA-C	6.80	123.96	110.42	7	1
1	A	170	ALA	CA-C-N	6.80	132.59	123.00	1	6
1	A	170	ALA	C-N-CA	6.80	132.59	123.00	1	6
1	A	228	GLN	N-CA-C	6.80	121.03	112.87	17	3
1	A	74	GLU	CB-CA-C	6.80	120.55	110.62	12	3
1	A	113	LEU	N-CA-C	6.80	119.53	111.71	18	3
1	A	215	THR	CA-CB-OG1	6.80	119.80	109.60	4	1
1	A	185	GLY	O-C-N	-6.80	117.97	123.14	12	2
1	A	66	ARG	NE-CZ-NH2	-6.79	113.09	119.20	3	2
1	A	59	ILE	CA-CB-CG2	6.79	122.04	110.50	13	2
1	A	228	GLN	CA-C-N	6.79	129.92	120.29	20	4
1	A	228	GLN	C-N-CA	6.79	129.92	120.29	20	4
1	A	221	PRO	O-C-N	-6.78	115.50	123.10	19	1
1	A	15	ALA	N-CA-C	6.78	119.53	111.33	5	2
1	A	186	ILE	N-CA-CB	-6.78	103.14	110.53	20	1
1	A	28	GLU	O-C-N	-6.76	113.37	122.43	10	1
1	A	164	THR	CA-CB-CG2	6.76	122.00	110.50	19	1
1	A	27	SER	CA-C-O	6.76	127.69	119.38	1	1
1	A	23	TYR	CA-C-N	6.76	134.45	121.54	8	6
1	A	23	TYR	C-N-CA	6.76	134.45	121.54	8	6
1	A	129	TRP	CZ3-CH2-CZ2	-6.76	112.71	121.50	11	1
1	A	26	ASP	CA-CB-CG	6.76	119.36	112.60	16	3
1	A	102	HIS	CE1-NE2-CD2	-6.75	102.25	109.00	7	4
1	A	223	ASN	CB-CA-C	6.75	118.26	109.28	13	1
1	A	136	ILE	CA-CB-CG1	6.75	121.87	110.40	15	1
1	A	58	VAL	CB-CA-C	6.74	122.34	111.29	6	2
1	A	244	SER	CA-C-N	-6.74	112.12	122.09	15	1
1	A	244	SER	C-N-CA	-6.74	112.12	122.09	15	1
1	A	225	LYS	O-C-N	-6.74	116.19	123.26	9	1
1	A	36	GLU	N-CA-CB	-6.74	99.93	110.30	2	1
1	A	60	GLU	N-CA-C	6.73	119.48	111.33	12	4
1	A	223	ASN	CA-C-O	-6.72	111.94	119.81	7	1
1	A	17	ASP	O-C-N	-6.72	115.00	122.12	2	1
1	A	65	PRO	N-CD-CG	6.72	113.28	103.20	8	2
1	A	111	LYS	CA-C-O	-6.71	113.43	120.55	20	2
1	A	222	GLN	CA-C-O	-6.71	113.31	120.42	16	1
1	A	214	PRO	CA-C-N	6.71	133.59	122.66	8	2
1	A	214	PRO	C-N-CA	6.71	133.59	122.66	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	197	GLY	CA-C-O	-6.70	112.93	120.30	18	1
1	A	15	ALA	O-C-N	6.69	129.24	122.08	8	2
1	A	200	LEU	CA-C-O	-6.69	111.77	119.60	8	2
1	A	43	GLN	OE1-CD-NE2	-6.69	115.91	122.60	17	2
1	A	98	ARG	CD-NE-CZ	6.69	133.77	124.40	14	1
1	A	136	ILE	N-CA-C	-6.69	98.22	107.99	1	1
1	A	155	THR	N-CA-CB	6.69	121.79	110.49	10	1
1	A	242	SER	CA-C-N	6.68	133.31	122.29	4	5
1	A	242	SER	C-N-CA	6.68	133.31	122.29	4	5
1	A	43	GLN	N-CA-CB	6.68	120.05	110.16	17	1
1	A	37	ALA	N-CA-C	6.66	118.34	111.14	16	2
1	A	20	LYS	N-CA-C	6.66	119.37	111.71	8	1
1	A	102	HIS	ND1-CG-CD2	6.65	112.75	106.10	20	4
1	A	198	HIS	CA-CB-CG	-6.65	107.15	113.80	11	2
1	A	154	ASN	N-CA-C	6.65	120.12	110.42	15	2
1	A	145	ASP	OD1-CG-OD2	-6.64	106.96	122.90	17	2
1	A	98	ARG	NE-CZ-NH2	6.64	125.17	119.20	1	1
1	A	12	TRP	CA-CB-CG	6.62	126.19	113.60	1	1
1	A	220	ASP	CA-CB-CG	6.62	119.22	112.60	13	3
1	A	94	VAL	N-CA-CB	-6.62	103.22	112.35	8	1
1	A	199	SER	CA-C-O	-6.62	112.62	120.10	1	1
1	A	118	LYS	N-CA-C	6.61	120.80	112.87	4	4
1	A	143	HIS	CA-C-N	6.61	131.94	122.63	13	2
1	A	143	HIS	C-N-CA	6.61	131.94	122.63	13	2
1	A	182	SER	N-CA-CB	-6.59	100.14	110.30	20	2
1	A	164	THR	CA-C-N	6.59	134.33	121.41	19	2
1	A	164	THR	C-N-CA	6.59	134.33	121.41	19	2
1	A	161	ALA	CA-C-O	-6.59	113.52	120.70	7	2
1	A	231	ILE	CA-C-O	6.58	127.79	120.95	3	1
1	A	157	ALA	N-CA-C	6.57	117.15	107.88	3	4
1	A	12	TRP	CA-C-O	-6.57	111.29	119.38	15	1
1	A	69	VAL	CA-C-N	6.56	126.52	120.03	14	4
1	A	69	VAL	C-N-CA	6.56	126.52	120.03	14	4
1	A	95	SER	CB-CA-C	6.56	122.16	110.16	14	5
1	A	86	SER	CB-CA-C	6.55	120.60	109.53	16	2
1	A	102	HIS	N-CA-C	6.55	124.75	110.80	5	2
1	A	193	THR	CA-C-N	6.55	129.06	120.28	16	2
1	A	193	THR	C-N-CA	6.55	129.06	120.28	16	2
1	A	20	LYS	CA-C-N	6.54	129.70	120.28	8	3
1	A	20	LYS	C-N-CA	6.54	129.70	120.28	8	3
1	A	48	LEU	O-C-N	6.54	128.03	121.30	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	194	HIS	CA-C-N	6.52	129.55	120.29	14	5
1	A	194	HIS	C-N-CA	6.52	129.55	120.29	14	5
1	A	204	HIS	CB-CG-CD2	-6.51	122.73	131.20	6	1
1	A	204	HIS	CA-C-O	-6.51	114.13	121.81	12	1
1	A	189	LEU	CA-C-N	6.51	129.65	120.28	19	1
1	A	189	LEU	C-N-CA	6.51	129.65	120.28	19	1
1	A	64	LYS	CA-C-O	-6.51	113.94	120.64	8	4
1	A	224	PHE	CA-C-N	6.51	133.01	121.75	16	4
1	A	224	PHE	C-N-CA	6.51	133.01	121.75	16	4
1	A	147	TYR	N-CA-CB	6.51	121.95	110.37	4	2
1	A	196	LEU	CA-C-N	6.51	127.03	119.94	9	3
1	A	196	LEU	C-N-CA	6.51	127.03	119.94	9	3
1	A	59	ILE	CA-C-O	-6.50	113.24	120.46	5	2
1	A	171	HIS	CB-CA-C	6.50	121.60	109.71	15	2
1	A	60	GLU	CA-C-N	6.49	131.61	121.35	9	2
1	A	60	GLU	C-N-CA	6.49	131.61	121.35	9	2
1	A	121	PRO	N-CA-C	6.49	121.99	114.20	13	1
1	A	82	PRO	CA-C-N	6.48	133.92	121.54	17	2
1	A	82	PRO	C-N-CA	6.48	133.92	121.54	17	2
1	A	210	ALA	CA-C-O	-6.47	114.07	121.19	19	1
1	A	153	GLY	CA-C-N	6.46	133.88	121.54	16	6
1	A	153	GLY	C-N-CA	6.46	133.88	121.54	16	6
1	A	209	ASN	CA-C-O	-6.46	112.11	119.41	16	2
1	A	122	LEU	O-C-N	6.45	130.75	123.27	7	1
1	A	120	ILE	N-CA-C	6.45	115.00	107.84	2	1
1	A	239	GLY	O-C-N	-6.45	114.32	122.70	14	1
1	A	59	ILE	CA-CB-CG1	6.43	121.34	110.40	12	1
1	A	106	ASP	CA-C-O	6.43	127.78	120.90	13	1
1	A	63	GLN	OE1-CD-NE2	-6.42	116.18	122.60	11	5
1	A	87	LYS	N-CA-C	-6.42	105.60	113.50	6	1
1	A	163	GLY	CA-C-N	6.42	131.55	121.99	15	2
1	A	163	GLY	C-N-CA	6.42	131.55	121.99	15	2
1	A	14	GLN	OE1-CD-NE2	-6.41	116.19	122.60	8	2
1	A	110	SER	O-C-N	6.41	128.67	122.07	20	1
1	A	37	ALA	CA-C-N	6.39	129.37	120.29	3	4
1	A	37	ALA	C-N-CA	6.39	129.37	120.29	3	4
1	A	168	GLY	N-CA-C	-6.38	105.70	114.64	8	3
1	A	127	VAL	CA-CB-CG2	6.38	121.25	110.40	17	4
1	A	43	GLN	O-C-N	6.38	128.64	122.07	2	1
1	A	4	ALA	N-CA-C	6.37	120.31	112.54	19	2
1	A	53	MET	O-C-N	6.36	130.75	123.31	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	190	TYR	O-C-N	-6.36	114.44	122.27	14	1
1	A	155	THR	CA-C-N	6.36	132.23	122.24	5	2
1	A	155	THR	C-N-CA	6.36	132.23	122.24	5	2
1	A	85	THR	CA-C-N	6.36	132.15	122.93	8	2
1	A	85	THR	C-N-CA	6.36	132.15	122.93	8	2
1	A	132	ALA	N-CA-CB	-6.36	101.17	111.22	1	3
1	A	71	ASP	CA-C-O	6.35	126.13	119.14	14	1
1	A	93	ILE	CA-C-N	6.35	131.62	121.34	3	1
1	A	93	ILE	C-N-CA	6.35	131.62	121.34	3	1
1	A	56	SER	O-C-N	-6.32	114.87	122.65	9	2
1	A	11	GLN	CA-C-N	6.32	128.75	120.28	9	3
1	A	11	GLN	C-N-CA	6.32	128.75	120.28	9	3
1	A	89	VAL	CA-C-N	6.32	132.09	122.93	3	1
1	A	89	VAL	C-N-CA	6.32	132.09	122.93	3	1
1	A	122	LEU	CA-C-O	-6.32	115.38	122.01	5	1
1	A	159	ALA	CA-C-N	6.31	132.47	122.62	1	2
1	A	159	ALA	C-N-CA	6.31	132.47	122.62	1	2
1	A	135	MET	CA-C-N	6.31	130.98	122.90	2	2
1	A	135	MET	C-N-CA	6.31	130.98	122.90	2	2
1	A	36	GLU	CB-CG-CD	6.31	123.32	112.60	9	2
1	A	98	ARG	CA-C-O	6.30	127.13	119.31	20	1
1	A	198	HIS	N-CA-C	6.30	118.95	111.33	19	1
1	A	236	LYS	CA-C-N	6.30	132.16	121.14	3	2
1	A	236	LYS	C-N-CA	6.30	132.16	121.14	3	2
1	A	73	ALA	CA-C-N	6.30	131.57	122.44	16	1
1	A	73	ALA	C-N-CA	6.30	131.57	122.44	16	1
1	A	85	THR	N-CA-C	-6.29	106.14	113.88	20	1
1	A	67	CYS	CB-CA-C	-6.29	99.87	110.19	8	1
1	A	35	LEU	CA-C-O	-6.29	112.73	119.97	17	1
1	A	41	GLU	O-C-N	-6.29	113.84	122.46	15	1
1	A	220	ASP	N-CA-C	-6.28	102.15	109.93	18	1
1	A	50	ILE	O-C-N	-6.27	115.74	122.45	13	1
1	A	70	PRO	CA-C-N	6.27	131.30	120.58	6	4
1	A	70	PRO	C-N-CA	6.27	131.30	120.58	6	4
1	A	141	GLY	CA-C-N	6.26	132.37	122.60	12	3
1	A	141	GLY	C-N-CA	6.26	132.37	122.60	12	3
1	A	56	SER	N-CA-CB	-6.26	97.98	109.18	2	2
1	A	25	TYR	CA-C-N	6.25	131.58	122.77	20	1
1	A	25	TYR	C-N-CA	6.25	131.58	122.77	20	1
1	A	31	ASN	N-CA-CB	6.24	121.04	110.49	11	1
1	A	175	ASP	CA-C-O	-6.24	111.12	119.11	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	GLY	CA-C-N	6.24	133.63	121.41	11	3
1	A	5	GLY	C-N-CA	6.24	133.63	121.41	11	3
1	A	101	PRO	CA-C-O	-6.24	113.83	121.31	11	1
1	A	24	LEU	CB-CA-C	6.22	122.81	110.42	12	3
1	A	11	GLN	CB-CG-CD	6.22	123.18	112.60	1	1
1	A	151	GLY	CA-C-O	-6.22	112.62	121.52	19	4
1	A	104	THR	N-CA-C	-6.22	103.81	111.40	19	2
1	A	169	ASP	CA-C-N	6.22	132.88	122.87	9	1
1	A	169	ASP	C-N-CA	6.22	132.88	122.87	9	1
1	A	189	LEU	N-CA-C	6.22	118.57	111.11	3	3
1	A	229	ASP	N-CA-C	-6.22	104.76	112.90	17	2
1	A	114	ASN	CA-C-N	6.21	128.60	120.28	20	3
1	A	114	ASN	C-N-CA	6.21	128.60	120.28	20	3
1	A	84	TRP	CE2-CD2-CE3	-6.21	112.59	118.80	2	2
1	A	53	MET	CA-C-O	-6.21	114.62	121.33	3	4
1	A	156	LEU	CA-C-O	-6.21	112.07	119.15	2	1
1	A	244	SER	CB-CA-C	6.20	121.02	110.85	1	2
1	A	241	ARG	CA-C-N	6.20	132.47	121.75	19	2
1	A	241	ARG	C-N-CA	6.20	132.47	121.75	19	2
1	A	88	VAL	CA-CB-CG2	6.19	120.93	110.40	19	1
1	A	211	VAL	CA-C-N	6.19	131.78	122.87	9	2
1	A	211	VAL	C-N-CA	6.19	131.78	122.87	9	2
1	A	238	TYR	CA-C-N	6.19	133.54	121.41	9	2
1	A	238	TYR	C-N-CA	6.19	133.54	121.41	9	2
1	A	208	PRO	N-CA-CB	6.18	109.39	103.52	5	6
1	A	47	GLY	CA-C-O	6.17	126.06	119.03	1	1
1	A	93	ILE	CA-CB-CG2	6.16	120.97	110.50	1	1
1	A	68	GLY	CA-C-N	6.16	129.73	121.23	7	1
1	A	68	GLY	C-N-CA	6.16	129.73	121.23	7	1
1	A	72	VAL	CA-C-O	-6.16	114.85	121.19	9	2
1	A	57	ARG	O-C-N	-6.16	114.40	122.59	9	1
1	A	202	MET	O-C-N	6.16	130.40	122.89	13	2
1	A	48	LEU	N-CA-C	6.16	117.46	109.64	13	2
1	A	39	LEU	CA-C-N	6.16	129.14	120.28	6	3
1	A	39	LEU	C-N-CA	6.16	129.14	120.28	6	3
1	A	66	ARG	NE-CZ-NH1	6.15	127.65	121.50	2	1
1	A	115	MET	CA-C-O	-6.15	112.49	120.00	2	1
1	A	40	LYS	O-C-N	-6.15	115.14	122.15	11	1
1	A	193	THR	N-CA-C	6.15	118.49	111.11	19	4
1	A	90	THR	CA-C-N	6.14	132.65	122.33	19	1
1	A	90	THR	C-N-CA	6.14	132.65	122.33	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	129	TRP	CA-C-N	6.14	133.44	121.41	12	3
1	A	129	TRP	C-N-CA	6.14	133.44	121.41	12	3
1	A	191	ALA	N-CA-C	-6.13	104.67	111.36	20	2
1	A	18	TYR	CA-C-O	-6.13	114.38	120.82	5	1
1	A	111	LYS	N-CA-CB	-6.13	101.11	110.12	9	1
1	A	21	ARG	CA-C-N	6.13	128.41	120.44	13	1
1	A	21	ARG	C-N-CA	6.13	128.41	120.44	13	1
1	A	176	GLU	N-CA-CB	-6.13	100.97	110.29	17	1
1	A	90	THR	O-C-N	-6.13	115.44	123.16	19	1
1	A	2	GLN	CB-CA-C	6.13	121.08	111.77	6	1
1	A	32	ALA	N-CA-C	6.12	118.75	111.71	1	3
1	A	94	VAL	CA-C-N	6.12	135.59	121.87	10	1
1	A	94	VAL	C-N-CA	6.12	135.59	121.87	10	1
1	A	71	ASP	N-CA-C	-6.12	106.35	113.88	18	1
1	A	102	HIS	CG-CD2-NE2	-6.11	101.09	107.20	20	3
1	A	102	HIS	O-C-N	6.11	130.72	122.59	14	1
1	A	213	TYR	CA-C-N	6.11	125.81	119.64	4	1
1	A	213	TYR	C-N-CA	6.11	125.81	119.64	4	1
1	A	126	LYS	CA-C-N	6.09	131.41	122.94	14	1
1	A	126	LYS	C-N-CA	6.09	131.41	122.94	14	1
1	A	90	THR	CA-C-O	-6.09	114.25	120.71	3	1
1	A	138	PHE	N-CA-C	-6.09	98.98	108.90	2	1
1	A	120	ILE	CA-CB-CG1	6.08	120.74	110.40	1	3
1	A	129	TRP	CB-CA-C	6.08	119.50	110.62	11	2
1	A	215	THR	N-CA-CB	-6.08	102.10	110.42	15	2
1	A	214	PRO	O-C-N	6.07	130.47	122.27	10	1
1	A	145	ASP	CB-CA-C	-6.06	99.96	110.45	11	2
1	A	140	ARG	N-CA-C	-6.06	101.55	110.52	7	1
1	A	177	ARG	NH1-CZ-NH2	6.05	127.17	119.30	7	2
1	A	72	VAL	CA-C-N	6.05	131.43	121.39	20	2
1	A	72	VAL	C-N-CA	6.05	131.43	121.39	20	2
1	A	128	VAL	CB-CA-C	6.05	119.53	111.85	3	4
1	A	43	GLN	N-CA-C	6.05	118.66	111.71	13	3
1	A	200	LEU	N-CA-CB	-6.04	100.55	110.40	16	2
1	A	23	TYR	N-CA-CB	-6.04	101.01	110.44	2	1
1	A	101	PRO	O-C-N	-6.04	115.63	123.00	2	1
1	A	57	ARG	N-CA-CB	-6.04	101.16	110.46	19	1
1	A	112	ALA	O-C-N	6.04	128.55	122.03	18	2
1	A	33	ASN	OD1-CG-ND2	-6.03	116.57	122.60	14	2
1	A	179	THR	CA-C-O	6.03	127.75	121.36	2	2
1	A	74	GLU	CA-C-N	6.03	132.24	122.29	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	GLU	C-N-CA	6.03	132.24	122.29	13	3
1	A	200	LEU	CA-C-N	6.02	130.84	122.29	19	2
1	A	200	LEU	C-N-CA	6.02	130.84	122.29	19	2
1	A	156	LEU	CB-CA-C	6.02	119.14	109.02	5	2
1	A	169	ASP	CA-CB-CG	6.02	118.62	112.60	8	2
1	A	43	GLN	CA-C-N	6.02	129.46	120.31	12	5
1	A	43	GLN	C-N-CA	6.02	129.46	120.31	12	5
1	A	168	GLY	O-C-N	-6.01	116.40	122.65	11	1
1	A	193	THR	OG1-CB-CG2	-6.01	97.28	109.30	11	1
1	A	106	ASP	O-C-N	6.01	128.28	122.03	1	1
1	A	57	ARG	CD-NE-CZ	6.01	132.81	124.40	13	4
1	A	70	PRO	N-CD-CG	6.01	112.21	103.20	8	2
1	A	138	PHE	CA-C-N	6.01	132.07	121.80	2	2
1	A	138	PHE	C-N-CA	6.01	132.07	121.80	2	2
1	A	195	ALA	N-CA-CB	-6.01	101.24	110.13	12	2
1	A	75	TYR	N-CA-C	6.00	118.24	108.76	18	2
1	A	18	TYR	N-CA-CB	-5.99	101.31	110.12	6	1
1	A	115	MET	CA-C-N	5.99	128.80	120.29	17	1
1	A	115	MET	C-N-CA	5.99	128.80	120.29	17	1
1	A	187	ASN	CA-C-N	5.99	128.22	120.44	8	2
1	A	187	ASN	C-N-CA	5.99	128.22	120.44	8	2
1	A	54	LEU	CB-CA-C	5.99	119.54	109.48	9	1
1	A	13	GLU	CA-C-N	5.99	128.62	120.54	8	2
1	A	13	GLU	C-N-CA	5.99	128.62	120.54	8	2
1	A	154	ASN	OD1-CG-ND2	-5.98	116.62	122.60	18	1
1	A	16	GLN	OE1-CD-NE2	-5.98	116.62	122.60	15	3
1	A	200	LEU	O-C-N	5.98	130.85	122.36	8	1
1	A	14	GLN	CA-C-O	-5.98	114.54	120.82	11	3
1	A	164	THR	CA-CB-OG1	5.98	118.57	109.60	20	3
1	A	145	ASP	CA-C-N	5.98	130.94	122.09	20	2
1	A	145	ASP	C-N-CA	5.98	130.94	122.09	20	2
1	A	139	ALA	N-CA-C	5.98	118.16	109.07	15	3
1	A	94	VAL	CB-CA-C	5.98	117.04	111.30	16	1
1	A	112	ALA	CA-C-O	5.98	127.08	120.63	8	2
1	A	226	LEU	CA-C-O	-5.97	115.22	121.55	6	1
1	A	148	PRO	N-CD-CG	5.97	112.16	103.20	15	1
1	A	173	ASP	CA-C-O	5.97	127.50	120.58	13	1
1	A	211	VAL	CB-CA-C	5.96	119.61	111.97	10	1
1	A	183	SER	CA-C-N	5.96	133.18	122.38	17	1
1	A	183	SER	C-N-CA	5.96	133.18	122.38	17	1
1	A	116	TRP	NE1-CE2-CD2	-5.96	99.65	107.40	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	234	ILE	N-CA-C	5.96	116.70	110.62	15	3
1	A	137	GLY	CA-C-N	5.96	131.21	122.39	8	2
1	A	137	GLY	C-N-CA	5.96	131.21	122.39	8	2
1	A	14	GLN	N-CA-C	5.95	118.53	111.33	14	1
1	A	58	VAL	N-CA-C	5.95	116.60	110.36	10	6
1	A	164	THR	OG1-CB-CG2	-5.95	97.41	109.30	17	1
1	A	94	VAL	O-C-N	5.94	128.40	122.04	11	2
1	A	233	GLY	N-CA-C	-5.94	106.97	114.16	1	1
1	A	125	ARG	N-CA-C	5.94	119.22	109.72	20	1
1	A	10	LEU	N-CA-C	5.94	119.78	112.54	20	2
1	A	218	ASN	OD1-CG-ND2	-5.94	116.66	122.60	11	2
1	A	205	SER	CA-CB-OG	5.93	122.97	111.10	5	1
1	A	24	LEU	CA-C-O	5.93	128.99	120.51	8	1
1	A	178	TRP	CA-C-O	-5.93	113.92	120.38	12	1
1	A	64	LYS	N-CA-CB	-5.93	102.86	110.03	20	3
1	A	74	GLU	N-CA-C	-5.93	100.05	109.59	4	1
1	A	95	SER	CA-C-N	5.92	131.84	122.36	6	4
1	A	95	SER	C-N-CA	5.92	131.84	122.36	6	4
1	A	29	THR	OG1-CB-CG2	-5.92	97.47	109.30	9	2
1	A	241	ARG	CD-NE-CZ	5.91	132.68	124.40	18	1
1	A	170	ALA	CA-C-O	-5.91	114.19	121.11	1	1
1	A	207	ASP	CA-C-O	-5.91	113.64	119.49	13	2
1	A	121	PRO	CB-CA-C	5.90	120.62	112.89	6	1
1	A	117	GLY	N-CA-C	5.90	121.30	114.16	9	1
1	A	36	GLU	O-C-N	5.90	129.12	122.22	16	1
1	A	108	LEU	CA-C-N	5.90	129.97	120.30	5	2
1	A	108	LEU	C-N-CA	5.90	129.97	120.30	5	2
1	A	57	ARG	CA-C-O	-5.90	112.08	120.51	8	1
1	A	3	GLU	O-C-N	-5.90	114.38	122.46	9	1
1	A	84	TRP	NE1-CE2-CD2	-5.88	99.76	107.40	4	1
1	A	92	ARG	CA-C-N	5.88	129.05	122.59	6	2
1	A	92	ARG	C-N-CA	5.88	129.05	122.59	6	2
1	A	62	MET	CA-C-N	5.87	130.66	120.68	7	2
1	A	62	MET	C-N-CA	5.87	130.66	120.68	7	2
1	A	98	ARG	CB-CA-C	5.87	120.82	110.37	8	1
1	A	167	GLY	CA-C-N	5.86	132.66	122.05	1	4
1	A	167	GLY	C-N-CA	5.86	132.66	122.05	1	4
1	A	12	TRP	CZ3-CH2-CZ2	-5.86	113.88	121.50	1	1
1	A	15	ALA	CA-C-O	5.86	127.17	120.90	11	2
1	A	12	TRP	CE3-CZ3-CH2	5.86	128.72	121.10	1	1
1	A	152	PRO	N-CD-CG	5.85	111.98	103.20	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	MET	N-CA-CB	-5.85	101.21	110.28	5	1
1	A	89	VAL	O-C-N	-5.85	116.68	122.76	2	1
1	A	58	VAL	CA-C-N	5.84	129.84	121.02	7	3
1	A	58	VAL	C-N-CA	5.84	129.84	121.02	7	3
1	A	177	ARG	CA-C-N	5.84	131.98	122.81	6	1
1	A	177	ARG	C-N-CA	5.84	131.98	122.81	6	1
1	A	221	PRO	N-CA-C	5.83	120.40	110.95	1	1
1	A	125	ARG	CA-C-O	-5.83	114.53	120.71	4	1
1	A	215	THR	CA-CB-CG2	5.83	120.42	110.50	11	1
1	A	210	ALA	N-CA-CB	-5.83	101.03	109.83	19	1
1	A	19	LEU	CA-C-N	5.83	128.36	120.38	18	2
1	A	19	LEU	C-N-CA	5.83	128.36	120.38	18	2
1	A	129	TRP	CB-CG-CD2	5.82	134.95	126.80	6	1
1	A	109	VAL	N-CA-CB	5.82	121.30	110.77	5	2
1	A	102	HIS	CA-C-O	-5.81	112.20	120.51	11	1
1	A	241	ARG	N-CA-CB	-5.80	100.76	110.22	8	1
1	A	52	GLY	O-C-N	5.80	129.12	122.33	14	2
1	A	158	HIS	CG-CD2-NE2	5.80	113.00	107.20	9	6
1	A	108	LEU	O-C-N	-5.80	114.56	122.33	5	1
1	A	92	ARG	O-C-N	-5.80	116.87	123.48	11	1
1	A	65	PRO	CB-CA-C	5.80	116.68	111.40	15	2
1	A	182	SER	CA-C-N	5.80	132.62	121.54	12	3
1	A	182	SER	C-N-CA	5.80	132.62	121.54	12	3
1	A	105	VAL	CA-CB-CG1	5.80	120.26	110.40	18	2
1	A	90	THR	CA-CB-CG2	5.80	120.35	110.50	11	1
1	A	174	GLU	N-CA-C	5.79	118.34	111.33	8	3
1	A	111	LYS	CG-CD-CE	5.79	124.62	111.30	20	2
1	A	55	ASN	O-C-N	-5.78	114.90	122.59	1	1
1	A	50	ILE	N-CA-CB	-5.78	104.17	111.46	14	3
1	A	2	GLN	OE1-CD-NE2	-5.78	116.82	122.60	4	2
1	A	63	GLN	CB-CG-CD	5.78	122.43	112.60	15	2
1	A	44	LYS	CA-C-N	5.78	128.02	120.28	9	4
1	A	44	LYS	C-N-CA	5.78	128.02	120.28	9	4
1	A	161	ALA	N-CA-C	5.78	118.05	110.08	7	1
1	A	220	ASP	CB-CA-C	-5.76	100.38	109.42	20	1
1	A	93	ILE	CA-CB-CG1	5.76	120.19	110.40	15	2
1	A	234	ILE	CA-CB-CG1	5.76	120.18	110.40	18	1
1	A	28	GLU	CA-C-N	5.76	130.47	120.68	19	1
1	A	28	GLU	C-N-CA	5.76	130.47	120.68	19	1
1	A	211	VAL	N-CA-CB	-5.75	101.74	111.23	15	2
1	A	194	HIS	ND1-CG-CD2	-5.75	100.35	106.10	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	GLU	CB-CG-CD	5.75	122.37	112.60	19	1
1	A	62	MET	CA-CB-CG	5.75	125.60	114.10	7	2
1	A	213	TYR	CA-CB-CG	5.74	124.24	113.90	5	1
1	A	69	VAL	O-C-N	5.74	127.38	121.07	15	1
1	A	110	SER	N-CA-CB	-5.74	101.67	110.16	7	2
1	A	7	MET	CA-C-N	5.74	129.94	120.94	8	2
1	A	7	MET	C-N-CA	5.74	129.94	120.94	8	2
1	A	58	VAL	O-C-N	-5.74	116.27	121.89	8	1
1	A	109	VAL	CA-C-O	-5.73	114.28	120.47	17	1
1	A	154	ASN	CA-C-O	5.73	126.26	120.88	13	3
1	A	159	ALA	CA-C-O	-5.72	115.15	121.33	5	1
1	A	4	ALA	N-CA-CB	-5.72	100.90	110.39	19	1
1	A	225	LYS	CA-C-O	5.72	127.44	121.38	9	1
1	A	50	ILE	CA-CB-CG2	5.72	120.22	110.50	12	1
1	A	176	GLU	CA-C-O	-5.71	115.33	121.56	20	1
1	A	56	SER	N-CA-C	5.71	115.95	108.07	8	1
1	A	103	ILE	CA-C-O	-5.71	114.80	120.85	8	1
1	A	158	HIS	CA-C-N	5.71	131.63	121.75	20	1
1	A	158	HIS	C-N-CA	5.71	131.63	121.75	20	1
1	A	159	ALA	O-C-N	-5.71	116.75	123.25	20	1
1	A	222	GLN	N-CA-CB	-5.70	101.73	110.16	2	2
1	A	128	VAL	CA-CB-CG2	5.70	120.09	110.40	10	4
1	A	166	LEU	O-C-N	-5.70	115.01	122.59	19	1
1	A	60	GLU	CB-CG-CD	5.69	122.28	112.60	1	1
1	A	11	GLN	N-CA-C	-5.69	105.06	112.23	5	1
1	A	116	TRP	CE2-CD2-CE3	-5.69	113.11	118.80	14	2
1	A	123	HIS	CB-CG-CD2	5.69	138.59	131.20	6	2
1	A	243	ASN	CA-C-N	5.69	128.47	120.28	7	1
1	A	243	ASN	C-N-CA	5.69	128.47	120.28	7	1
1	A	171	HIS	CG-ND1-CE1	-5.69	99.63	109.30	18	2
1	A	182	SER	CA-C-O	-5.68	113.08	119.79	4	1
1	A	91	TYR	CA-C-N	5.68	131.90	121.85	14	2
1	A	91	TYR	C-N-CA	5.68	131.90	121.85	14	2
1	A	222	GLN	N-CA-C	-5.68	105.17	111.36	9	4
1	A	209	ASN	CB-CG-ND2	5.67	124.91	116.40	8	1
1	A	120	ILE	CA-C-O	-5.67	112.35	119.95	1	1
1	A	178	TRP	NE1-CE2-CD2	-5.67	100.03	107.40	5	1
1	A	103	ILE	CA-CB-CG2	5.66	120.13	110.50	8	2
1	A	158	HIS	CB-CA-C	5.66	122.00	109.94	1	1
1	A	89	VAL	CA-CB-CG1	5.66	120.02	110.40	4	1
1	A	238	TYR	CB-CA-C	5.66	119.05	109.55	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	GLN	CA-C-O	-5.65	114.43	120.42	10	1
1	A	43	GLN	CB-CG-CD	5.65	122.21	112.60	6	2
1	A	109	VAL	N-CA-C	5.65	117.06	110.62	14	3
1	A	125	ARG	NH1-CZ-NH2	-5.65	111.95	119.30	18	2
1	A	2	GLN	N-CA-C	-5.65	102.54	110.50	15	1
1	A	18	TYR	N-CA-C	5.64	117.88	111.11	19	1
1	A	44	LYS	N-CA-C	5.64	117.43	111.28	13	2
1	A	22	PHE	N-CA-C	5.64	117.50	111.36	19	2
1	A	103	ILE	CA-C-N	5.63	128.29	120.29	2	1
1	A	103	ILE	C-N-CA	5.63	128.29	120.29	2	1
1	A	213	TYR	CA-C-O	-5.63	113.99	119.51	3	1
1	A	228	GLN	O-C-N	5.63	128.09	122.12	18	2
1	A	230	ASP	N-CA-C	-5.63	104.54	111.40	5	1
1	A	46	PHE	CB-CG-CD2	-5.62	111.14	120.70	10	1
1	A	237	LEU	CA-C-N	5.62	131.60	122.67	7	2
1	A	237	LEU	C-N-CA	5.62	131.60	122.67	7	2
1	A	131	THR	O-C-N	5.62	129.31	122.96	9	1
1	A	219	GLY	CA-C-N	5.62	129.42	121.61	12	1
1	A	219	GLY	C-N-CA	5.62	129.42	121.61	12	1
1	A	93	ILE	N-CA-C	-5.62	99.14	107.51	3	3
1	A	235	GLN	N-CA-C	-5.61	106.44	113.28	3	2
1	A	69	VAL	N-CA-CB	5.61	116.39	110.17	11	2
1	A	231	ILE	CA-CB-CG2	5.61	120.03	110.50	3	1
1	A	167	GLY	O-C-N	-5.60	118.72	123.59	2	1
1	A	108	LEU	N-CA-C	-5.60	104.56	111.40	14	1
1	A	187	ASN	CB-CA-C	5.60	118.66	110.26	1	1
1	A	14	GLN	CG-CD-NE2	5.60	124.80	116.40	8	1
1	A	218	ASN	CA-C-O	-5.60	115.14	120.90	13	2
1	A	192	ALA	CA-C-O	-5.60	113.78	120.10	15	2
1	A	14	GLN	O-C-N	-5.59	115.68	122.22	18	1
1	A	152	PRO	CB-CA-C	-5.59	104.57	111.11	8	1
1	A	92	ARG	CD-NE-CZ	5.59	132.23	124.40	9	2
1	A	9	GLU	N-CA-C	5.59	118.14	111.71	11	2
1	A	153	GLY	N-CA-C	-5.59	105.15	111.85	4	1
1	A	2	GLN	N-CA-CB	-5.58	101.54	110.63	10	1
1	A	84	TRP	CD2-CE3-CZ3	5.58	125.85	118.60	10	1
1	A	41	GLU	CA-C-O	5.58	125.80	119.27	15	1
1	A	87	LYS	CA-C-N	5.58	130.90	122.98	4	2
1	A	87	LYS	C-N-CA	5.58	130.90	122.98	4	2
1	A	185	GLY	CA-C-N	5.58	129.35	121.66	8	1
1	A	185	GLY	C-N-CA	5.58	129.35	121.66	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	171	HIS	N-CA-C	-5.57	99.20	108.34	16	1
1	A	228	GLN	CG-CD-NE2	5.57	124.76	116.40	20	2
1	A	181	GLY	CA-C-N	5.57	131.56	121.92	3	2
1	A	181	GLY	C-N-CA	5.57	131.56	121.92	3	2
1	A	193	THR	CA-CB-OG1	5.57	117.95	109.60	2	2
1	A	223	ASN	O-C-N	5.57	128.94	122.09	7	1
1	A	228	GLN	CB-CG-CD	5.57	122.07	112.60	12	1
1	A	110	SER	CA-CB-OG	5.57	122.24	111.10	2	1
1	A	62	MET	O-C-N	5.57	127.80	122.07	17	3
1	A	204	HIS	CG-CD2-NE2	5.56	112.76	107.20	12	4
1	A	121	PRO	N-CD-CG	5.56	111.55	103.20	14	1
1	A	127	VAL	CB-CA-C	5.56	119.07	110.50	10	1
1	A	61	ILE	CA-C-O	-5.55	112.86	119.58	4	1
1	A	226	LEU	O-C-N	-5.55	116.46	123.01	12	1
1	A	192	ALA	CB-CA-C	-5.55	100.55	110.70	14	1
1	A	90	THR	CB-CA-C	5.55	120.33	109.35	18	1
1	A	144	GLY	CA-C-N	5.55	132.28	121.63	18	1
1	A	144	GLY	C-N-CA	5.55	132.28	121.63	18	1
1	A	121	PRO	O-C-N	-5.54	115.16	122.64	15	1
1	A	208	PRO	N-CD-CG	5.54	111.51	103.20	20	2
1	A	96	TYR	CB-CA-C	5.54	121.86	109.56	13	1
1	A	159	ALA	N-CA-CB	5.54	120.80	110.99	3	1
1	A	89	VAL	CA-CB-CG2	5.54	119.82	110.40	13	1
1	A	39	LEU	O-C-N	-5.54	115.74	122.22	20	2
1	A	91	TYR	CB-CA-C	5.54	120.62	109.38	11	1
1	A	125	ARG	N-CA-CB	-5.54	101.22	110.80	10	2
1	A	160	PHE	CB-CG-CD2	5.53	130.10	120.70	9	1
1	A	50	ILE	CA-C-N	5.53	131.17	122.21	9	2
1	A	50	ILE	C-N-CA	5.53	131.17	122.21	9	2
1	A	18	TYR	O-C-N	5.53	127.76	122.07	5	2
1	A	168	GLY	CA-C-N	5.53	130.56	121.39	5	2
1	A	168	GLY	C-N-CA	5.53	130.56	121.39	5	2
1	A	184	LEU	CD1-CG-CD2	-5.53	98.64	110.80	14	1
1	A	41	GLU	CA-CB-CG	5.53	125.15	114.10	16	1
1	A	24	LEU	O-C-N	5.52	129.94	122.59	13	2
1	A	66	ARG	CB-CA-C	5.52	116.62	109.28	18	1
1	A	200	LEU	CB-CA-C	5.52	118.82	109.55	4	2
1	A	206	SER	O-C-N	-5.52	114.58	122.41	18	1
1	A	25	TYR	CB-CA-C	5.51	121.39	110.42	5	1
1	A	65	PRO	CA-N-CD	-5.51	104.28	112.00	8	1
1	A	223	ASN	N-CA-C	-5.51	106.23	113.12	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	143	HIS	N-CA-CB	-5.51	101.18	110.49	6	3
1	A	140	ARG	O-C-N	-5.51	115.31	122.97	2	3
1	A	75	TYR	CB-CG-CD2	-5.50	112.54	120.80	19	1
1	A	11	GLN	O-C-N	5.49	128.41	122.15	9	1
1	A	149	PHE	CA-C-O	5.49	126.14	119.11	12	1
1	A	49	PRO	N-CA-C	5.49	121.21	114.35	14	1
1	A	31	ASN	CB-CG-ND2	5.49	124.63	116.40	15	1
1	A	129	TRP	N-CA-C	-5.49	99.15	108.26	8	1
1	A	109	VAL	CA-CB-CG2	5.48	119.72	110.40	17	2
1	A	133	ASP	N-CA-C	-5.48	104.71	111.40	9	2
1	A	123	HIS	N-CA-C	-5.48	100.77	109.76	12	1
1	A	84	TRP	CB-CG-CD2	5.48	134.47	126.80	9	1
1	A	44	LYS	N-CA-CB	5.48	118.01	110.07	4	1
1	A	206	SER	N-CA-C	-5.48	106.37	113.16	5	1
1	A	240	LYS	O-C-N	5.48	129.45	123.04	10	2
1	A	128	VAL	N-CA-CB	-5.48	104.82	111.94	12	1
1	A	45	PHE	N-CA-CB	5.47	118.65	110.22	11	2
1	A	195	ALA	CA-C-N	5.47	132.88	121.94	20	2
1	A	195	ALA	C-N-CA	5.47	132.88	121.94	20	2
1	A	94	VAL	CA-CB-CG2	5.47	119.70	110.40	8	3
1	A	125	ARG	CD-NE-CZ	5.47	132.05	124.40	8	4
1	A	188	PHE	CA-CB-CG	5.46	119.26	113.80	16	2
1	A	107	ARG	NE-CZ-NH1	-5.46	116.04	121.50	6	3
1	A	17	ASP	CA-C-O	5.46	126.30	120.24	19	1
1	A	64	LYS	CB-CA-C	-5.44	101.19	108.87	7	1
1	A	84	TRP	CD2-CE2-CZ2	5.44	127.84	122.40	2	1
1	A	39	LEU	N-CA-C	5.44	117.21	111.28	12	1
1	A	24	LEU	N-CA-CB	5.44	119.69	110.49	17	1
1	A	38	LYS	N-CA-C	-5.44	105.77	112.90	15	2
1	A	92	ARG	CA-C-O	5.43	126.84	120.43	11	1
1	A	94	VAL	CA-CB-CG1	5.43	119.63	110.40	3	1
1	A	194	HIS	N-CA-C	5.43	117.28	111.36	17	1
1	A	194	HIS	N-CA-CB	-5.43	101.55	110.40	12	3
1	A	7	MET	N-CA-C	5.43	116.97	109.15	6	1
1	A	162	PRO	N-CA-CB	5.42	107.63	103.30	2	3
1	A	3	GLU	N-CA-C	-5.42	106.52	113.23	9	2
1	A	44	LYS	CA-CB-CG	5.41	124.93	114.10	11	1
1	A	61	ILE	CA-CB-CG1	5.41	119.60	110.40	19	2
1	A	208	PRO	N-CA-C	5.41	120.95	113.98	5	3
1	A	118	LYS	CA-C-N	5.41	130.42	121.99	10	2
1	A	118	LYS	C-N-CA	5.41	130.42	121.99	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	226	LEU	N-CA-CB	-5.40	101.91	110.06	9	1
1	A	148	PRO	CA-C-O	-5.39	115.09	121.67	2	1
1	A	136	ILE	N-CA-CB	5.39	117.46	110.99	4	1
1	A	178	TRP	O-C-N	-5.39	117.02	123.06	14	1
1	A	240	LYS	CA-C-N	5.38	130.87	122.26	16	1
1	A	240	LYS	C-N-CA	5.38	130.87	122.26	16	1
1	A	152	PRO	CA-C-O	-5.37	114.91	121.03	3	1
1	A	243	ASN	O-C-N	-5.37	116.89	122.96	15	2
1	A	7	MET	N-CA-CB	5.37	119.56	110.49	19	1
1	A	37	ALA	O-C-N	-5.37	116.45	122.03	20	1
1	A	118	LYS	O-C-N	5.36	129.56	122.43	4	1
1	A	71	ASP	CB-CG-OD1	5.36	130.73	118.40	4	2
1	A	74	GLU	CB-CG-CD	5.36	121.71	112.60	5	1
1	A	52	GLY	N-CA-C	-5.36	107.64	115.63	11	1
1	A	53	MET	CA-C-N	5.36	130.33	122.77	12	1
1	A	53	MET	C-N-CA	5.36	130.33	122.77	12	1
1	A	176	GLU	N-CA-C	-5.36	102.55	110.48	11	1
1	A	220	ASP	O-C-N	5.36	126.52	120.68	3	1
1	A	231	ILE	N-CA-C	5.36	115.98	110.36	15	1
1	A	14	GLN	CB-CG-CD	5.35	121.69	112.60	3	1
1	A	85	THR	CA-C-O	5.35	125.53	119.27	8	1
1	A	25	TYR	CA-C-O	-5.34	114.13	120.43	3	1
1	A	63	GLN	CA-C-O	-5.34	113.49	119.79	7	1
1	A	183	SER	N-CA-CB	-5.33	104.02	112.08	6	1
1	A	21	ARG	N-CA-CB	-5.33	102.01	110.28	16	1
1	A	133	ASP	N-CA-CB	5.33	118.02	110.13	6	1
1	A	94	VAL	CA-C-O	5.33	123.77	119.29	19	1
1	A	244	SER	CA-CB-OG	5.33	121.76	111.10	13	2
1	A	179	THR	N-CA-C	5.33	116.09	108.74	13	1
1	A	98	ARG	NE-CZ-NH1	5.33	126.83	121.50	18	1
1	A	103	ILE	O-C-N	-5.32	116.62	121.94	18	1
1	A	105	VAL	O-C-N	5.32	127.13	121.91	18	1
1	A	179	THR	CB-CA-C	5.32	120.84	110.30	12	1
1	A	37	ALA	CA-C-O	-5.32	115.22	120.70	16	1
1	A	8	SER	CA-C-O	-5.32	115.32	121.49	9	1
1	A	240	LYS	N-CA-CB	-5.32	102.13	110.69	9	2
1	A	173	ASP	CB-CA-C	5.31	118.22	110.26	16	1
1	A	197	GLY	N-CA-C	-5.30	105.91	113.86	5	1
1	A	229	ASP	CB-CA-C	-5.30	101.83	110.85	20	1
1	A	61	ILE	N-CA-C	5.30	119.49	112.76	14	2
1	A	163	GLY	N-CA-C	-5.30	103.01	110.91	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	GLU	CA-C-O	-5.30	113.57	120.25	5	1
1	A	92	ARG	CB-CG-CD	5.30	123.49	111.30	11	1
1	A	39	LEU	N-CA-CB	-5.30	101.60	110.39	1	1
1	A	148	PRO	N-CA-CB	5.30	108.26	103.33	10	1
1	A	145	ASP	O-C-N	5.29	129.41	123.27	19	1
1	A	69	VAL	CB-CA-C	-5.29	106.02	110.94	2	1
1	A	66	ARG	N-CA-CB	5.29	119.43	110.49	20	1
1	A	20	LYS	O-C-N	5.29	128.77	122.27	5	1
1	A	135	MET	CA-C-O	5.29	126.13	120.32	8	1
1	A	119	GLU	CB-CA-C	5.29	119.19	109.99	17	1
1	A	9	GLU	N-CA-CB	-5.28	102.10	110.22	11	2
1	A	240	LYS	N-CA-C	5.28	117.35	108.96	19	1
1	A	199	SER	N-CA-C	-5.27	106.69	113.01	10	1
1	A	128	VAL	CA-C-O	5.27	126.42	120.42	15	1
1	A	120	ILE	CB-CA-C	5.26	115.58	109.89	19	1
1	A	97	THR	O-C-N	-5.26	117.17	123.06	17	2
1	A	164	THR	CA-C-O	-5.26	114.95	120.58	19	1
1	A	211	VAL	CA-C-O	5.25	127.35	120.78	7	1
1	A	84	TRP	CE2-CD2-CG	5.25	113.50	107.20	8	1
1	A	75	TYR	CB-CG-CD1	5.25	128.68	120.80	2	1
1	A	230	ASP	N-CA-CB	5.25	117.68	110.07	4	2
1	A	54	LEU	CA-C-O	-5.24	114.85	120.46	6	1
1	A	84	TRP	NE1-CE2-CZ2	5.24	137.96	130.10	4	1
1	A	33	ASN	CA-C-N	5.24	128.28	120.31	12	1
1	A	33	ASN	C-N-CA	5.24	128.28	120.31	12	1
1	A	218	ASN	N-CA-C	5.24	116.99	111.28	14	1
1	A	50	ILE	CB-CA-C	-5.24	104.41	110.91	20	1
1	A	8	SER	CB-CA-C	5.24	121.81	111.22	6	1
1	A	70	PRO	CB-CA-C	5.24	118.12	110.63	3	1
1	A	225	LYS	N-CA-C	5.24	117.22	108.99	13	1
1	A	154	ASN	O-C-N	5.24	128.98	123.11	18	1
1	A	188	PHE	CB-CA-C	-5.24	102.63	110.90	9	1
1	A	98	ARG	N-CA-C	5.23	118.77	112.38	16	1
1	A	28	GLU	CA-CB-CG	5.23	124.56	114.10	5	1
1	A	82	PRO	N-CD-CG	5.23	111.05	103.20	13	2
1	A	50	ILE	CA-CB-CG1	5.23	119.29	110.40	10	1
1	A	42	MET	O-C-N	-5.23	116.58	122.12	17	1
1	A	234	ILE	O-C-N	-5.22	116.45	121.83	9	1
1	A	241	ARG	NE-CZ-NH2	5.22	123.90	119.20	7	1
1	A	46	PHE	CA-C-O	5.22	125.78	119.31	11	1
1	A	97	THR	CA-C-N	5.22	130.27	121.14	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	97	THR	C-N-CA	5.22	130.27	121.14	20	1
1	A	111	LYS	N-CA-C	5.21	117.64	111.33	19	2
1	A	107	ARG	CD-NE-CZ	5.21	131.70	124.40	6	1
1	A	11	GLN	N-CA-CB	-5.21	101.74	110.39	11	1
1	A	242	SER	CA-CB-OG	5.21	121.52	111.10	14	1
1	A	86	SER	CA-C-N	5.21	127.68	120.29	12	1
1	A	86	SER	C-N-CA	5.21	127.68	120.29	12	1
1	A	91	TYR	CB-CG-CD2	-5.21	112.99	120.80	13	1
1	A	27	SER	N-CA-CB	-5.21	102.21	110.28	15	1
1	A	131	THR	CB-CA-C	5.20	118.75	109.38	17	1
1	A	13	GLU	N-CA-C	-5.20	105.05	111.40	18	1
1	A	45	PHE	CA-C-N	5.20	131.71	121.58	8	1
1	A	45	PHE	C-N-CA	5.20	131.71	121.58	8	1
1	A	216	TYR	N-CA-C	5.20	118.17	110.48	5	3
1	A	124	PHE	CA-C-O	-5.19	114.90	120.46	15	1
1	A	238	TYR	CA-C-O	-5.19	113.49	119.56	6	1
1	A	53	MET	N-CA-C	-5.19	99.99	108.76	17	1
1	A	186	ILE	O-C-N	-5.19	116.81	122.83	10	1
1	A	179	THR	OG1-CB-CG2	-5.19	98.93	109.30	20	1
1	A	174	GLU	CA-CB-CG	5.19	124.47	114.10	14	1
1	A	178	TRP	CE2-CD2-CE3	-5.18	113.62	118.80	8	1
1	A	207	ASP	O-C-N	5.18	126.46	121.28	16	1
1	A	238	TYR	N-CA-CB	-5.18	102.64	110.92	18	1
1	A	12	TRP	CG-CD2-CE3	5.17	139.07	133.90	14	1
1	A	7	MET	O-C-N	5.17	129.48	122.96	7	1
1	A	16	GLN	N-CA-C	-5.17	105.73	111.36	3	1
1	A	43	GLN	CA-CB-CG	-5.17	103.76	114.10	11	1
1	A	33	ASN	CB-CA-C	5.17	119.06	110.90	19	1
1	A	132	ALA	O-C-N	-5.16	116.48	123.19	8	1
1	A	243	ASN	N-CA-C	5.16	117.77	108.48	18	1
1	A	105	VAL	N-CA-CB	-5.16	102.84	110.58	2	1
1	A	16	GLN	CB-CA-C	5.16	119.62	110.85	3	1
1	A	87	LYS	O-C-N	-5.16	116.27	122.15	12	1
1	A	63	GLN	CA-CB-CG	5.15	124.41	114.10	8	1
1	A	134	ILE	N-CA-C	-5.15	99.74	107.37	11	1
1	A	239	GLY	N-CA-C	-5.15	100.97	113.18	4	1
1	A	92	ARG	NH1-CZ-NH2	5.15	126.00	119.30	18	1
1	A	190	TYR	CB-CG-CD1	5.14	128.51	120.80	11	1
1	A	114	ASN	CA-C-O	-5.14	115.10	120.55	17	1
1	A	43	GLN	CA-C-O	5.14	125.70	119.38	16	1
1	A	212	MET	CA-C-N	5.14	128.40	121.20	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	212	MET	C-N-CA	5.14	128.40	121.20	2	1
1	A	237	LEU	N-CA-CB	-5.14	103.10	110.65	4	1
1	A	171	HIS	CA-C-O	-5.13	114.81	120.30	1	1
1	A	213	TYR	N-CA-C	-5.13	102.18	109.62	1	1
1	A	181	GLY	O-C-N	-5.13	116.03	122.70	9	1
1	A	89	VAL	N-CA-C	5.13	117.42	108.95	3	1
1	A	161	ALA	N-CA-CB	-5.13	102.59	110.03	8	1
1	A	29	THR	O-C-N	-5.13	115.46	122.33	13	1
1	A	180	ASP	CA-C-O	-5.13	113.17	120.51	19	1
1	A	216	TYR	CA-C-O	5.13	127.86	121.81	19	1
1	A	122	LEU	N-CA-C	-5.13	101.34	109.59	16	1
1	A	185	GLY	CA-C-O	5.12	126.95	120.54	12	1
1	A	195	ALA	N-CA-C	5.12	117.60	111.71	16	2
1	A	190	TYR	CB-CG-CD2	-5.12	113.11	120.80	19	1
1	A	45	PHE	CB-CA-C	5.12	120.83	110.38	10	1
1	A	60	GLU	CB-CA-C	5.12	119.06	110.92	4	1
1	A	23	TYR	CA-C-O	-5.12	113.08	119.18	20	1
1	A	177	ARG	N-CA-CB	-5.12	102.09	110.43	16	2
1	A	73	ALA	N-CA-C	5.12	117.45	109.52	5	1
1	A	116	TRP	O-C-N	-5.12	114.76	122.28	18	1
1	A	217	GLY	N-CA-C	-5.11	106.65	112.79	17	1
1	A	184	LEU	CA-C-O	5.11	125.69	119.05	1	1
1	A	26	ASP	CA-C-O	5.11	126.54	120.66	14	1
1	A	242	SER	O-C-N	5.11	129.10	123.33	11	2
1	A	224	PHE	CB-CA-C	5.11	120.58	110.42	6	1
1	A	61	ILE	CB-CA-C	5.10	122.03	111.32	14	1
1	A	205	SER	N-CA-C	-5.10	100.98	108.99	7	1
1	A	119	GLU	CA-C-N	5.10	128.87	121.68	16	2
1	A	119	GLU	C-N-CA	5.10	128.87	121.68	16	2
1	A	158	HIS	CB-CG-CD2	5.10	137.82	131.20	9	2
1	A	131	THR	CA-C-O	-5.09	115.80	121.81	16	2
1	A	116	TRP	CA-CB-CG	5.09	123.28	113.60	15	1
1	A	91	TYR	N-CA-C	5.09	116.99	108.99	2	1
1	A	33	ASN	N-CA-C	-5.09	105.73	111.28	15	2
1	A	155	THR	CA-CB-OG1	5.09	117.23	109.60	8	2
1	A	213	TYR	CB-CA-C	5.09	118.04	109.85	11	1
1	A	113	LEU	O-C-N	-5.08	116.02	122.27	2	1
1	A	235	GLN	CA-CB-CG	5.08	124.26	114.10	7	1
1	A	58	VAL	CA-CB-CG1	5.08	119.03	110.40	16	1
1	A	166	LEU	N-CA-C	5.07	121.61	110.80	11	1
1	A	153	GLY	O-C-N	5.07	128.43	123.10	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	212	MET	N-CA-C	-5.07	104.00	111.81	7	1
1	A	85	THR	N-CA-CB	-5.07	103.24	110.80	12	1
1	A	88	VAL	CB-CA-C	-5.07	104.29	111.38	19	1
1	A	150	ASP	CA-C-O	-5.07	113.27	120.51	5	1
1	A	187	ASN	N-CA-C	5.07	117.04	109.59	16	1
1	A	193	THR	CA-C-O	-5.06	115.06	120.42	14	1
1	A	198	HIS	CA-C-O	5.06	125.19	119.27	2	1
1	A	41	GLU	N-CA-CB	-5.05	102.52	110.30	20	1
1	A	58	VAL	CA-CB-CG2	5.05	118.99	110.40	12	1
1	A	162	PRO	CB-CA-C	-5.05	104.49	111.21	10	1
1	A	142	ALA	CA-C-O	-5.05	113.31	119.32	11	1
1	A	173	ASP	CB-CG-OD2	-5.05	106.78	118.40	14	1
1	A	186	ILE	CA-CB-CG1	5.05	118.98	110.40	20	1
1	A	235	GLN	CA-C-N	5.05	127.55	120.28	1	1
1	A	235	GLN	C-N-CA	5.05	127.55	120.28	1	1
1	A	178	TRP	CA-C-N	5.04	130.13	122.11	8	1
1	A	178	TRP	C-N-CA	5.04	130.13	122.11	8	1
1	A	30	LYS	O-C-N	-5.04	117.31	123.16	17	1
1	A	180	ASP	O-C-N	-5.04	115.89	122.59	14	1
1	A	5	GLY	O-C-N	-5.04	116.15	122.70	15	1
1	A	98	ARG	NH1-CZ-NH2	-5.04	112.75	119.30	18	1
1	A	89	VAL	CA-C-O	-5.04	116.64	121.63	13	1
1	A	16	GLN	N-CA-CB	-5.03	102.71	110.16	3	1
1	A	203	GLY	CA-C-O	-5.03	116.89	121.47	15	1
1	A	179	THR	CA-CB-CG2	5.03	119.05	110.50	18	1
1	A	8	SER	CA-CB-OG	5.03	121.16	111.10	14	1
1	A	62	MET	N-CA-C	5.02	117.49	111.71	11	1
1	A	49	PRO	O-C-N	-5.02	115.40	122.38	2	1
1	A	167	GLY	CA-C-O	-5.02	116.16	121.88	19	1
1	A	107	ARG	N-CA-CB	-5.02	102.80	110.07	18	1
1	A	215	THR	N-CA-C	-5.01	107.66	112.97	8	1
1	A	215	THR	O-C-N	-5.01	116.44	122.71	14	1
1	A	231	ILE	N-CA-CB	-5.01	103.72	110.54	3	1
1	A	9	GLU	CB-CA-C	5.01	119.20	110.68	6	1
1	A	29	THR	CA-C-O	5.01	126.93	118.91	6	1
1	A	242	SER	CA-C-O	-5.01	115.70	120.56	10	1
1	A	6	GLY	O-C-N	5.01	129.21	122.70	7	1
1	A	216	TYR	CA-C-N	5.01	128.91	122.85	17	1
1	A	216	TYR	C-N-CA	5.01	128.91	122.85	17	1
1	A	237	LEU	N-CA-C	-5.00	105.92	112.23	6	1
1	A	9	GLU	CB-CG-CD	5.00	121.11	112.60	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	GLN	CG-CD-NE2	-5.00	108.89	116.40	19	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	238	TYR	Sidechain	11
1	A	18	TYR	Sidechain	8
1	A	96	TYR	Sidechain	7
1	A	190	TYR	Sidechain	7
1	A	147	TYR	Sidechain	6
1	A	149	PHE	Sidechain,Peptide	6
1	A	213	TYR	Sidechain	5
1	A	25	TYR	Sidechain	5
1	A	91	TYR	Sidechain	5
1	A	22	PHE	Sidechain	4
1	A	188	PHE	Sidechain	4
1	A	23	TYR	Sidechain	4
1	A	216	TYR	Sidechain	4
1	A	45	PHE	Sidechain	4
1	A	157	ALA	Peptide	4
1	A	71	ASP	Sidechain	3
1	A	140	ARG	Peptide,Sidechain	3
1	A	143	HIS	Sidechain,Mainchain	3
1	A	75	TYR	Sidechain	3
1	A	123	HIS	Sidechain	2
1	A	124	PHE	Sidechain	2
1	A	158	HIS	Sidechain	2
1	A	66	ARG	Sidechain	2
1	A	198	HIS	Sidechain	2
1	A	138	PHE	Sidechain	2
1	A	168	GLY	Peptide	2
1	A	150	ASP	Peptide	1
1	A	30	LYS	Peptide	1
1	A	41	GLU	Peptide	1
1	A	49	PRO	Mainchain	1
1	A	98	ARG	Sidechain	1
1	A	14	GLN	Mainchain	1
1	A	179	THR	Peptide	1
1	A	235	GLN	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	240	LYS	Mainchain	1
1	A	224	PHE	Sidechain	1
1	A	241	ARG	Sidechain	1
1	A	177	ARG	Sidechain	1
1	A	125	ARG	Sidechain	1
1	A	215	THR	Mainchain	1
1	A	46	PHE	Peptide	1
1	A	160	PHE	Sidechain	1
1	A	219	GLY	Peptide	1
1	A	169	ASP	Sidechain	1
1	A	57	ARG	Sidechain	1
1	A	95	SER	Mainchain	1
1	A	107	ARG	Sidechain	1
1	A	139	ALA	Peptide	1
1	A	36	GLU	Mainchain	1
1	A	102	HIS	Sidechain	1
1	A	129	TRP	Peptide	1
1	A	167	GLY	Mainchain	1
1	A	183	SER	Mainchain	1
1	A	133	ASP	Peptide	1
1	A	181	GLY	Peptide	1
1	A	204	HIS	Sidechain	1
1	A	28	GLU	Mainchain	1
1	A	130	GLY	Peptide	1
1	A	197	GLY	Peptide	1
1	A	61	ILE	Mainchain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1861	1796	1796	4±2
4	A	5796	0	9072	122±10
5	A	192	270	272	3±2
All	All	157060	41320	222802	2461

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H50	4:A:427:PX4:H60	0.91	1.43	1	1
4:A:328:PX4:H39	4:A:351:PX4:H23	0.90	1.41	12	1
4:A:386:PX4:H42	4:A:417:PX4:H38	0.85	1.47	3	1
4:A:308:PX4:H17	4:A:326:PX4:H55	0.84	1.49	15	1
4:A:367:PX4:H16	4:A:399:PX4:H47	0.84	1.48	17	1
4:A:353:PX4:H53	4:A:361:PX4:H21	0.84	1.47	13	1
4:A:309:PX4:H17	4:A:328:PX4:H24	0.84	1.47	20	1
4:A:372:PX4:H31	4:A:410:PX4:H66	0.84	1.50	6	1
4:A:316:PX4:H17	4:A:352:PX4:H19	0.84	1.48	17	1
4:A:381:PX4:H14	4:A:394:PX4:H47	0.82	1.49	6	1
4:A:327:PX4:H23	4:A:348:PX4:H47	0.82	1.49	18	1
4:A:326:PX4:H35	4:A:355:PX4:H31	0.82	1.50	5	1
4:A:329:PX4:H19	4:A:335:PX4:H26	0.82	1.52	11	1
4:A:359:PX4:H64	4:A:375:PX4:H43	0.82	1.52	15	1
4:A:327:PX4:H35	4:A:359:PX4:H60	0.82	1.52	10	1
4:A:313:PX4:H25	4:A:362:PX4:H26	0.81	1.52	15	1
4:A:345:PX4:H46	4:A:358:PX4:H16	0.81	1.53	13	1
4:A:319:PX4:H34	4:A:319:PX4:H67	0.81	1.49	16	1
4:A:386:PX4:H16	4:A:402:PX4:H14	0.81	1.50	16	1
4:A:412:PX4:H50	4:A:424:PX4:H48	0.81	1.51	14	1
4:A:417:PX4:H21	4:A:421:PX4:H61	0.80	1.52	20	1
4:A:392:PX4:H47	4:A:425:PX4:H16	0.80	1.53	19	1
4:A:306:PX4:H52	4:A:342:PX4:H25	0.80	1.52	9	1
4:A:382:PX4:H46	4:A:423:PX4:H32	0.79	1.53	20	1
4:A:367:PX4:H38	4:A:389:PX4:H29	0.78	1.56	14	1
4:A:373:PX4:H50	4:A:410:PX4:H19	0.78	1.54	15	1
4:A:369:PX4:H52	4:A:419:PX4:H19	0.78	1.56	6	1
4:A:308:PX4:H42	4:A:332:PX4:H38	0.78	1.55	17	1
4:A:390:PX4:H31	4:A:416:PX4:H33	0.77	1.56	11	1
4:A:328:PX4:H58	4:A:347:PX4:H53	0.77	1.55	14	1
4:A:352:PX4:H40	4:A:375:PX4:H44	0.77	1.56	18	1
4:A:398:PX4:H30	4:A:399:PX4:H34	0.77	1.54	6	1
4:A:384:PX4:H59	4:A:427:PX4:H63	0.77	1.57	13	1
4:A:374:PX4:H69	4:A:429:PX4:H63	0.76	1.54	20	1
4:A:319:PX4:H62	4:A:343:PX4:H23	0.76	1.56	1	1
4:A:365:PX4:H63	4:A:376:PX4:H23	0.75	1.57	14	1
4:A:322:PX4:H66	4:A:430:PX4:H69	0.75	1.57	17	1
4:A:366:PX4:H47	4:A:403:PX4:H16	0.75	1.59	12	2
4:A:324:PX4:H53	4:A:333:PX4:H28	0.75	1.59	13	1
4:A:360:PX4:H66	4:A:379:PX4:H39	0.75	1.57	12	1
4:A:323:PX4:H61	4:A:325:PX4:H62	0.75	1.57	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:383:PX4:H61	4:A:394:PX4:H50	0.75	1.55	2	1
4:A:397:PX4:H56	4:A:430:PX4:H27	0.75	1.56	16	1
4:A:365:PX4:H30	4:A:383:PX4:H35	0.75	1.57	19	1
4:A:429:PX4:H69	4:A:430:PX4:H31	0.74	1.59	14	1
4:A:306:PX4:H62	4:A:342:PX4:H39	0.74	1.59	11	1
4:A:329:PX4:H42	4:A:335:PX4:H59	0.74	1.57	7	1
4:A:332:PX4:H47	4:A:348:PX4:H47	0.74	1.58	13	1
4:A:391:PX4:H28	4:A:408:PX4:H56	0.74	1.59	5	1
4:A:370:PX4:H17	4:A:430:PX4:H50	0.74	1.58	8	3
4:A:373:PX4:H59	4:A:406:PX4:H26	0.73	1.59	11	1
4:A:327:PX4:H21	4:A:348:PX4:H22	0.73	1.58	4	1
4:A:369:PX4:H30	4:A:429:PX4:H66	0.73	1.60	17	1
4:A:371:PX4:H18	4:A:401:PX4:H33	0.73	1.59	17	1
4:A:313:PX4:H17	4:A:329:PX4:H48	0.73	1.58	4	1
4:A:409:PX4:H17	4:A:412:PX4:H19	0.73	1.60	4	1
4:A:333:PX4:H48	4:A:364:PX4:H53	0.73	1.61	20	1
4:A:341:PX4:H30	4:A:356:PX4:H29	0.73	1.60	17	1
4:A:330:PX4:H20	4:A:337:PX4:H16	0.73	1.59	14	2
4:A:385:PX4:H59	4:A:387:PX4:H54	0.73	1.58	18	1
4:A:306:PX4:H48	4:A:342:PX4:H22	0.73	1.59	9	2
4:A:325:PX4:H57	4:A:353:PX4:H54	0.73	1.59	7	1
4:A:372:PX4:H65	4:A:420:PX4:H69	0.73	1.61	4	1
4:A:389:PX4:H16	4:A:399:PX4:H46	0.73	1.60	5	1
4:A:382:PX4:H66	4:A:397:PX4:H40	0.73	1.59	10	1
4:A:370:PX4:H48	4:A:381:PX4:H47	0.73	1.61	12	1
4:A:365:PX4:H30	4:A:369:PX4:H41	0.72	1.59	1	1
4:A:393:PX4:H16	4:A:419:PX4:H20	0.72	1.61	16	1
4:A:323:PX4:H37	4:A:347:PX4:H20	0.72	1.58	8	1
4:A:361:PX4:H57	4:A:403:PX4:H34	0.72	1.62	12	1
4:A:417:PX4:H22	4:A:418:PX4:H26	0.72	1.59	16	1
4:A:317:PX4:H20	4:A:326:PX4:H16	0.72	1.61	16	1
4:A:316:PX4:H53	4:A:343:PX4:H26	0.72	1.62	7	1
4:A:347:PX4:H46	4:A:360:PX4:H19	0.72	1.61	12	1
4:A:344:PX4:H47	4:A:354:PX4:H9	0.72	1.61	19	1
4:A:383:PX4:H30	4:A:405:PX4:H72	0.71	1.61	1	1
4:A:311:PX4:H20	4:A:324:PX4:H69	0.71	1.63	7	1
4:A:317:PX4:H24	4:A:326:PX4:H21	0.71	1.61	8	1
4:A:366:PX4:H57	4:A:403:PX4:H50	0.71	1.61	1	1
4:A:353:PX4:H23	4:A:361:PX4:H32	0.71	1.61	7	1
4:A:375:PX4:H28	4:A:407:PX4:H29	0.71	1.63	14	1
4:A:307:PX4:H49	4:A:337:PX4:H53	0.71	1.60	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:345:PX4:H62	4:A:359:PX4:H17	0.71	1.60	3	1
4:A:338:PX4:H46	4:A:347:PX4:H57	0.71	1.63	6	1
4:A:316:PX4:H41	4:A:399:PX4:H68	0.71	1.61	6	1
4:A:316:PX4:H50	4:A:343:PX4:H24	0.70	1.62	1	1
4:A:307:PX4:H22	4:A:337:PX4:H52	0.70	1.63	15	1
4:A:397:PX4:H19	4:A:423:PX4:H61	0.70	1.63	4	1
4:A:334:PX4:H70	4:A:373:PX4:H33	0.70	1.63	8	1
4:A:308:PX4:H17	4:A:426:PX4:H45	0.70	1.62	9	1
4:A:367:PX4:H42	4:A:389:PX4:H33	0.70	1.61	14	1
4:A:324:PX4:H18	4:A:324:PX4:H1	0.70	1.63	5	1
4:A:413:PX4:H35	4:A:428:PX4:H34	0.70	1.63	6	1
4:A:333:PX4:H20	5:A:432:C3S:H443	0.70	1.61	4	1
4:A:395:PX4:H60	4:A:405:PX4:H31	0.70	1.62	2	1
4:A:332:PX4:H37	4:A:350:PX4:H22	0.70	1.64	2	1
4:A:324:PX4:H38	4:A:368:PX4:H41	0.70	1.64	11	1
4:A:360:PX4:H37	4:A:393:PX4:H72	0.70	1.61	11	1
4:A:365:PX4:H21	4:A:383:PX4:H31	0.70	1.64	12	1
4:A:312:PX4:H49	4:A:324:PX4:H26	0.70	1.62	11	1
4:A:369:PX4:H44	4:A:429:PX4:H65	0.69	1.64	14	1
4:A:397:PX4:H67	4:A:411:PX4:H42	0.69	1.64	1	1
4:A:369:PX4:H20	4:A:430:PX4:H16	0.69	1.64	8	1
4:A:373:PX4:H16	4:A:389:PX4:H49	0.69	1.64	19	1
4:A:369:PX4:H51	4:A:419:PX4:H57	0.69	1.62	8	1
4:A:397:PX4:H66	4:A:423:PX4:H68	0.69	1.64	12	1
4:A:347:PX4:H61	4:A:360:PX4:H47	0.69	1.63	20	1
4:A:371:PX4:H20	4:A:401:PX4:H41	0.69	1.65	5	1
4:A:428:PX4:H72	4:A:429:PX4:H56	0.69	1.64	5	1
4:A:391:PX4:H16	4:A:427:PX4:H14	0.69	1.63	2	1
4:A:343:PX4:H17	4:A:356:PX4:H46	0.69	1.65	17	1
4:A:308:PX4:H59	4:A:326:PX4:H26	0.69	1.62	18	1
4:A:343:PX4:H48	4:A:356:PX4:H51	0.69	1.64	4	1
4:A:370:PX4:H62	4:A:381:PX4:H60	0.68	1.65	3	1
4:A:388:PX4:H17	4:A:391:PX4:H50	0.68	1.63	18	1
4:A:369:PX4:H58	4:A:429:PX4:H21	0.68	1.64	19	1
4:A:388:PX4:H48	4:A:388:PX4:H27	0.68	1.65	7	1
4:A:386:PX4:H58	4:A:402:PX4:H25	0.68	1.64	9	1
4:A:371:PX4:H19	4:A:386:PX4:H53	0.68	1.64	19	1
4:A:394:PX4:H51	4:A:430:PX4:H59	0.68	1.66	20	1
4:A:318:PX4:H53	4:A:357:PX4:H23	0.68	1.65	6	1
4:A:388:PX4:H67	4:A:390:PX4:H58	0.68	1.65	11	1
4:A:316:PX4:H21	4:A:321:PX4:H16	0.68	1.65	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:365:PX4:H52	4:A:396:PX4:H49	0.68	1.66	6	1
4:A:408:PX4:H67	4:A:427:PX4:H62	0.68	1.66	2	1
4:A:339:PX4:H42	4:A:346:PX4:H66	0.68	1.66	20	1
4:A:322:PX4:H38	4:A:344:PX4:H41	0.68	1.65	9	1
4:A:358:PX4:H54	4:A:358:PX4:H23	0.68	1.66	11	1
4:A:365:PX4:H55	4:A:383:PX4:H23	0.68	1.66	13	1
4:A:315:PX4:H57	4:A:350:PX4:H19	0.68	1.66	20	1
4:A:352:PX4:O6	4:A:352:PX4:H7	0.68	1.89	20	1
4:A:393:PX4:H21	4:A:429:PX4:H38	0.68	1.67	4	1
4:A:366:PX4:H22	4:A:403:PX4:H32	0.68	1.64	18	1
4:A:376:PX4:H17	4:A:388:PX4:H19	0.67	1.65	4	1
4:A:307:PX4:H29	4:A:327:PX4:H56	0.67	1.64	2	1
4:A:318:PX4:H22	4:A:321:PX4:H51	0.67	1.65	7	1
4:A:316:PX4:H32	4:A:318:PX4:H40	0.67	1.67	14	1
4:A:322:PX4:H50	4:A:337:PX4:H17	0.67	1.65	13	1
4:A:365:PX4:H55	4:A:376:PX4:H55	0.67	1.64	18	1
4:A:306:PX4:H36	4:A:342:PX4:H41	0.67	1.66	13	1
4:A:312:PX4:H20	4:A:346:PX4:H19	0.67	1.64	10	1
4:A:327:PX4:H23	4:A:338:PX4:H58	0.67	1.65	12	1
4:A:320:PX4:H35	4:A:332:PX4:H38	0.67	1.64	7	1
4:A:400:PX4:H33	4:A:401:PX4:H67	0.67	1.67	20	1
4:A:320:PX4:H63	4:A:334:PX4:H59	0.67	1.66	2	1
4:A:347:PX4:H53	4:A:351:PX4:H43	0.67	1.66	3	1
4:A:309:PX4:H22	4:A:328:PX4:H24	0.67	1.65	10	1
4:A:322:PX4:H69	4:A:369:PX4:H31	0.67	1.67	15	1
4:A:365:PX4:H47	4:A:383:PX4:H16	0.67	1.65	13	1
4:A:369:PX4:H18	4:A:429:PX4:H54	0.67	1.67	17	1
4:A:374:PX4:H64	4:A:381:PX4:H69	0.66	1.66	13	1
4:A:397:PX4:H16	4:A:411:PX4:H23	0.66	1.66	19	1
4:A:347:PX4:H22	4:A:351:PX4:H30	0.66	1.66	20	1
4:A:387:PX4:H31	4:A:416:PX4:H57	0.66	1.67	4	1
4:A:400:PX4:H20	4:A:401:PX4:H14	0.66	1.67	9	1
4:A:310:PX4:H50	4:A:333:PX4:H48	0.66	1.67	15	1
4:A:328:PX4:H51	4:A:347:PX4:H16	0.66	1.67	14	1
4:A:365:PX4:O3	4:A:369:PX4:H7	0.66	1.90	8	1
4:A:383:PX4:H21	4:A:396:PX4:H50	0.66	1.65	18	1
4:A:325:PX4:H45	4:A:325:PX4:H67	0.66	1.67	3	1
4:A:345:PX4:H49	4:A:358:PX4:H16	0.66	1.67	7	1
4:A:357:PX4:H26	4:A:363:PX4:H24	0.66	1.68	3	1
4:A:376:PX4:H14	4:A:390:PX4:H9	0.66	1.67	11	1
4:A:375:PX4:H21	4:A:392:PX4:H31	0.66	1.68	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:365:PX4:H27	4:A:369:PX4:H62	0.66	1.66	4	1
4:A:372:PX4:H17	4:A:420:PX4:H55	0.66	1.66	4	1
4:A:317:PX4:H36	4:A:326:PX4:H32	0.66	1.68	14	1
4:A:305:PX4:H38	4:A:310:PX4:H33	0.66	1.68	19	1
4:A:319:PX4:H21	4:A:352:PX4:H17	0.66	1.69	6	1
4:A:336:PX4:H17	4:A:354:PX4:H15	0.66	1.65	7	1
4:A:305:PX4:H67	4:A:426:PX4:H67	0.65	1.66	11	1
4:A:386:PX4:H28	4:A:401:PX4:H44	0.65	1.69	2	1
4:A:414:PX4:O6	4:A:426:PX4:H6	0.65	1.91	9	1
4:A:397:PX4:H48	4:A:423:PX4:H60	0.65	1.67	16	1
4:A:317:PX4:H40	4:A:326:PX4:H37	0.65	1.66	7	1
4:A:315:PX4:H53	4:A:332:PX4:H21	0.65	1.69	1	1
4:A:371:PX4:H14	4:A:373:PX4:H20	0.65	1.68	5	1
4:A:330:PX4:H69	4:A:415:PX4:H67	0.65	1.68	9	1
4:A:323:PX4:H18	4:A:328:PX4:H2	0.65	1.68	11	1
4:A:309:PX4:H19	4:A:328:PX4:H31	0.65	1.69	12	1
4:A:316:PX4:H64	4:A:389:PX4:H72	0.65	1.66	16	1
4:A:305:PX4:H36	4:A:310:PX4:H34	0.65	1.69	4	1
4:A:404:PX4:H33	4:A:418:PX4:H72	0.65	1.67	11	1
4:A:305:PX4:H50	4:A:312:PX4:H47	0.65	1.69	13	1
4:A:371:PX4:H68	4:A:399:PX4:H30	0.65	1.69	6	1
4:A:369:PX4:H25	4:A:430:PX4:H24	0.65	1.67	10	1
4:A:326:PX4:H60	4:A:353:PX4:H63	0.65	1.68	13	1
4:A:384:PX4:H50	4:A:389:PX4:H23	0.65	1.66	15	1
4:A:386:PX4:H47	4:A:417:PX4:H58	0.65	1.68	17	1
4:A:369:PX4:H18	4:A:429:PX4:H49	0.65	1.69	6	1
4:A:308:PX4:H32	4:A:332:PX4:H31	0.65	1.69	8	1
4:A:329:PX4:H51	4:A:355:PX4:H46	0.65	1.69	13	1
4:A:428:PX4:H52	4:A:430:PX4:H25	0.64	1.69	11	1
4:A:335:PX4:H53	4:A:363:PX4:H54	0.64	1.67	20	1
4:A:428:PX4:H24	4:A:429:PX4:H22	0.64	1.70	9	1
4:A:387:PX4:H71	4:A:403:PX4:H35	0.64	1.67	12	1
4:A:318:PX4:H28	4:A:357:PX4:H28	0.64	1.69	15	1
4:A:394:PX4:H38	4:A:400:PX4:H69	0.64	1.69	5	1
4:A:308:PX4:H20	4:A:326:PX4:H54	0.64	1.67	2	1
4:A:373:PX4:H18	4:A:406:PX4:H49	0.64	1.69	8	1
4:A:320:PX4:H64	4:A:340:PX4:H22	0.64	1.67	3	1
4:A:317:PX4:H30	4:A:325:PX4:H25	0.64	1.69	7	1
4:A:403:PX4:H47	4:A:421:PX4:H17	0.64	1.69	16	1
4:A:341:PX4:H64	4:A:352:PX4:H56	0.64	1.68	17	1
4:A:338:PX4:H16	4:A:344:PX4:H47	0.64	1.68	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:335:PX4:H46	4:A:354:PX4:H46	0.64	1.68	3	1
4:A:376:PX4:H50	4:A:376:PX4:H20	0.64	1.68	3	1
4:A:305:PX4:H45	4:A:311:PX4:H68	0.64	1.66	4	1
4:A:415:PX4:H32	4:A:421:PX4:H29	0.64	1.69	20	1
4:A:319:PX4:O2	4:A:336:PX4:H9	0.64	1.93	8	1
4:A:335:PX4:H64	4:A:347:PX4:H68	0.64	1.70	11	1
4:A:392:PX4:H14	4:A:392:PX4:H6	0.64	1.70	4	1
4:A:383:PX4:H38	4:A:419:PX4:H60	0.64	1.68	12	1
4:A:317:PX4:H50	4:A:325:PX4:H30	0.64	1.70	8	1
4:A:377:PX4:H29	4:A:377:PX4:H59	0.64	1.68	19	1
4:A:334:PX4:H64	5:A:432:C3S:H443	0.64	1.68	2	1
5:A:436:C3S:H402	5:A:436:C3S:H501	0.64	1.70	17	2
4:A:369:PX4:H42	4:A:430:PX4:H45	0.63	1.67	11	1
4:A:365:PX4:H50	4:A:407:PX4:H47	0.63	1.68	13	1
4:A:371:PX4:H59	4:A:389:PX4:C5	0.63	2.22	15	1
4:A:366:PX4:H16	4:A:378:PX4:H20	0.63	1.69	18	2
4:A:308:PX4:H69	4:A:355:PX4:H45	0.63	1.69	20	1
4:A:370:PX4:H16	4:A:394:PX4:H15	0.63	1.68	3	2
4:A:382:PX4:H54	4:A:404:PX4:H45	0.63	1.70	12	1
4:A:383:PX4:H25	4:A:383:PX4:H52	0.63	1.69	14	1
4:A:339:PX4:H61	4:A:357:PX4:H59	0.63	1.68	9	1
4:A:328:PX4:H17	4:A:347:PX4:H20	0.63	1.69	7	1
4:A:371:PX4:H19	4:A:402:PX4:H22	0.63	1.69	7	1
4:A:324:PX4:H42	4:A:346:PX4:H33	0.63	1.70	16	1
4:A:375:PX4:H70	4:A:405:PX4:H37	0.63	1.71	3	1
4:A:380:PX4:H16	4:A:385:PX4:H10	0.63	1.69	19	1
4:A:326:PX4:H66	4:A:326:PX4:H39	0.63	1.71	1	1
1:A:222:GLN:O	4:A:317:PX4:H1	0.63	1.94	12	3
4:A:376:PX4:H61	4:A:390:PX4:H30	0.63	1.70	8	1
4:A:336:PX4:H23	4:A:354:PX4:H27	0.63	1.70	9	1
4:A:373:PX4:H28	4:A:406:PX4:H52	0.63	1.71	14	1
4:A:371:PX4:H59	4:A:389:PX4:H13	0.63	1.68	15	1
4:A:308:PX4:H24	4:A:320:PX4:H50	0.63	1.71	16	1
4:A:312:PX4:H53	4:A:346:PX4:H61	0.63	1.69	16	1
4:A:321:PX4:H59	4:A:357:PX4:H40	0.63	1.71	17	1
4:A:338:PX4:H40	4:A:344:PX4:H28	0.63	1.70	2	1
4:A:375:PX4:O6	4:A:392:PX4:H6	0.63	1.93	5	1
4:A:388:PX4:H2	4:A:391:PX4:H15	0.63	1.71	8	1
4:A:318:PX4:H17	4:A:357:PX4:H27	0.62	1.71	1	1
4:A:389:PX4:H16	4:A:399:PX4:H53	0.62	1.70	1	1
1:A:107:ARG:HG3	4:A:315:PX4:H46	0.62	1.71	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:365:PX4:H62	4:A:407:PX4:H58	0.62	1.71	9	1
4:A:376:PX4:H25	4:A:396:PX4:H26	0.62	1.70	17	1
4:A:307:PX4:H57	4:A:348:PX4:H66	0.62	1.70	2	1
4:A:318:PX4:H26	4:A:342:PX4:H18	0.62	1.69	9	2
4:A:306:PX4:H53	4:A:342:PX4:H27	0.62	1.69	11	1
4:A:311:PX4:H52	4:A:313:PX4:H52	0.62	1.68	14	1
4:A:305:PX4:H24	4:A:311:PX4:H16	0.62	1.70	15	1
4:A:318:PX4:H59	4:A:336:PX4:H34	0.62	1.71	19	1
4:A:306:PX4:H16	4:A:358:PX4:H46	0.62	1.71	9	1
4:A:410:PX4:H18	4:A:410:PX4:H2	0.62	1.70	15	1
4:A:309:PX4:H32	4:A:347:PX4:H40	0.62	1.69	3	1
4:A:341:PX4:H10	4:A:356:PX4:O6	0.62	1.94	8	1
4:A:386:PX4:H31	4:A:417:PX4:H67	0.62	1.71	19	1
4:A:380:PX4:H16	4:A:385:PX4:H23	0.62	1.71	20	1
4:A:330:PX4:H62	4:A:337:PX4:H34	0.62	1.71	11	1
4:A:307:PX4:H69	4:A:430:PX4:H66	0.62	1.71	2	1
4:A:365:PX4:H46	4:A:376:PX4:H49	0.62	1.72	2	1
4:A:361:PX4:H58	4:A:378:PX4:H42	0.62	1.70	7	1
4:A:365:PX4:H22	4:A:370:PX4:H26	0.62	1.70	10	1
4:A:397:PX4:H16	4:A:411:PX4:H21	0.62	1.71	10	1
4:A:316:PX4:H52	4:A:352:PX4:H46	0.62	1.71	8	1
4:A:306:PX4:H59	4:A:359:PX4:H56	0.62	1.72	12	1
4:A:335:PX4:H46	4:A:354:PX4:H49	0.62	1.69	16	1
4:A:396:PX4:H27	4:A:407:PX4:H21	0.62	1.72	1	1
4:A:335:PX4:H17	4:A:347:PX4:H53	0.62	1.72	5	1
4:A:306:PX4:H57	4:A:359:PX4:H46	0.62	1.71	9	1
4:A:337:PX4:H20	4:A:355:PX4:H31	0.62	1.72	13	1
4:A:383:PX4:H59	4:A:394:PX4:H30	0.62	1.71	17	1
4:A:376:PX4:H24	4:A:376:PX4:H54	0.61	1.72	3	1
4:A:310:PX4:H72	4:A:364:PX4:H69	0.61	1.72	9	1
4:A:429:PX4:H54	4:A:430:PX4:H23	0.61	1.72	14	1
4:A:386:PX4:H44	4:A:417:PX4:H66	0.61	1.71	15	1
1:A:125:ARG:HH21	4:A:359:PX4:H14	0.61	1.55	19	1
4:A:325:PX4:H10	4:A:325:PX4:H14	0.61	1.71	5	1
4:A:308:PX4:H55	4:A:403:PX4:H39	0.61	1.70	6	1
4:A:389:PX4:O1	4:A:401:PX4:H13	0.61	1.93	20	1
4:A:410:PX4:H29	4:A:424:PX4:H27	0.61	1.70	1	1
4:A:320:PX4:H44	4:A:402:PX4:H66	0.61	1.72	18	1
4:A:366:PX4:H32	4:A:402:PX4:H30	0.61	1.72	7	1
4:A:369:PX4:H55	4:A:429:PX4:H21	0.61	1.72	11	1
4:A:371:PX4:H68	4:A:375:PX4:H65	0.61	1.72	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:368:PX4:H50	4:A:414:PX4:H29	0.61	1.72	13	1
4:A:413:PX4:H60	4:A:422:PX4:H64	0.61	1.73	4	1
4:A:308:PX4:H30	4:A:320:PX4:H58	0.61	1.71	5	1
4:A:317:PX4:H54	4:A:330:PX4:H33	0.61	1.73	7	1
4:A:312:PX4:H16	4:A:346:PX4:H47	0.61	1.71	10	1
4:A:400:PX4:H3	4:A:401:PX4:O1	0.61	1.96	14	1
4:A:331:PX4:H54	4:A:344:PX4:H34	0.61	1.72	20	1
4:A:368:PX4:H8	4:A:406:PX4:O6	0.61	1.96	1	1
4:A:343:PX4:H57	4:A:350:PX4:H17	0.61	1.70	10	3
4:A:394:PX4:H43	4:A:405:PX4:H33	0.61	1.71	3	1
4:A:394:PX4:H31	4:A:400:PX4:H20	0.61	1.73	6	1
4:A:396:PX4:H31	4:A:407:PX4:H27	0.61	1.73	16	1
4:A:319:PX4:H54	4:A:341:PX4:H55	0.61	1.72	3	1
4:A:351:PX4:H42	4:A:419:PX4:H69	0.61	1.72	13	1
4:A:360:PX4:H62	4:A:429:PX4:H36	0.61	1.72	16	1
4:A:338:PX4:H20	4:A:344:PX4:H53	0.61	1.72	17	1
4:A:376:PX4:H20	4:A:396:PX4:H49	0.61	1.71	17	1
4:A:382:PX4:H46	4:A:423:PX4:H56	0.61	1.71	4	1
4:A:324:PX4:H30	4:A:346:PX4:H60	0.61	1.71	6	1
4:A:340:PX4:H9	4:A:340:PX4:H16	0.61	1.71	6	1
4:A:358:PX4:H66	4:A:407:PX4:H42	0.61	1.72	13	1
4:A:395:PX4:H33	4:A:402:PX4:H60	0.60	1.73	3	1
4:A:401:PX4:H63	4:A:405:PX4:H36	0.60	1.72	4	1
4:A:372:PX4:O2	4:A:380:PX4:H20	0.60	1.96	12	1
4:A:327:PX4:H16	4:A:351:PX4:H4	0.60	1.73	14	1
4:A:315:PX4:H57	4:A:350:PX4:H21	0.60	1.73	1	1
4:A:388:PX4:H61	4:A:403:PX4:H65	0.60	1.73	5	1
4:A:414:PX4:H50	4:A:426:PX4:H21	0.60	1.71	12	1
4:A:321:PX4:H54	4:A:342:PX4:H35	0.60	1.74	15	1
4:A:370:PX4:H17	4:A:430:PX4:H46	0.60	1.71	18	1
4:A:319:PX4:H17	4:A:352:PX4:H50	0.60	1.73	19	1
4:A:384:PX4:H62	5:A:434:C3S:H601	0.60	1.71	14	1
4:A:376:PX4:H65	4:A:390:PX4:H51	0.60	1.72	19	1
4:A:426:PX4:H15	4:A:426:PX4:H13	0.60	1.72	5	1
4:A:401:PX4:H71	4:A:405:PX4:H29	0.60	1.73	7	1
4:A:403:PX4:H17	4:A:421:PX4:H51	0.60	1.73	7	1
4:A:340:PX4:H28	5:A:432:C3S:H262	0.60	1.73	9	1
4:A:322:PX4:H65	4:A:365:PX4:H40	0.60	1.72	10	1
4:A:404:PX4:H29	4:A:417:PX4:H24	0.60	1.73	15	1
4:A:387:PX4:H20	4:A:415:PX4:H22	0.60	1.73	1	1
4:A:399:PX4:H38	5:A:435:C3S:H693	0.60	1.73	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:309:PX4:H58	4:A:345:PX4:H41	0.60	1.74	9	1
4:A:404:PX4:H23	4:A:418:PX4:H27	0.60	1.73	9	1
4:A:321:PX4:H69	4:A:427:PX4:H33	0.60	1.72	11	1
4:A:413:PX4:H31	4:A:429:PX4:H32	0.60	1.72	4	1
4:A:308:PX4:H36	4:A:332:PX4:H27	0.60	1.73	8	1
4:A:306:PX4:H22	4:A:358:PX4:H47	0.60	1.73	5	2
4:A:403:PX4:H46	4:A:421:PX4:H17	0.60	1.74	7	1
4:A:322:PX4:H32	4:A:331:PX4:H25	0.60	1.73	4	1
4:A:306:PX4:H56	4:A:342:PX4:H29	0.60	1.73	9	1
4:A:365:PX4:C24	4:A:383:PX4:H23	0.60	2.27	17	1
4:A:411:PX4:H28	4:A:423:PX4:H58	0.60	1.71	20	1
4:A:305:PX4:H57	4:A:312:PX4:H59	0.60	1.74	5	2
4:A:369:PX4:H46	4:A:419:PX4:H17	0.60	1.72	3	1
4:A:370:PX4:H17	4:A:430:PX4:C26	0.60	2.27	8	1
4:A:320:PX4:H24	4:A:326:PX4:H60	0.59	1.74	4	1
4:A:346:PX4:H38	5:A:431:C3S:H691	0.59	1.74	17	1
4:A:316:PX4:H21	4:A:352:PX4:H25	0.59	1.74	7	1
4:A:375:PX4:H68	4:A:392:PX4:H29	0.59	1.74	8	1
4:A:395:PX4:H30	4:A:401:PX4:H40	0.59	1.75	9	1
4:A:348:PX4:H34	4:A:359:PX4:H54	0.59	1.74	10	1
4:A:384:PX4:H23	4:A:405:PX4:H20	0.59	1.72	11	1
4:A:333:PX4:H22	4:A:340:PX4:H52	0.59	1.72	13	1
4:A:406:PX4:H70	4:A:426:PX4:H54	0.59	1.73	9	1
4:A:322:PX4:H72	4:A:337:PX4:H59	0.59	1.73	13	1
4:A:387:PX4:H26	4:A:416:PX4:H19	0.59	1.75	15	1
4:A:316:PX4:H16	4:A:321:PX4:H11	0.59	1.71	17	1
4:A:369:PX4:H62	4:A:430:PX4:H42	0.59	1.74	2	1
4:A:370:PX4:H50	4:A:381:PX4:H17	0.59	1.72	10	1
4:A:422:PX4:H53	4:A:425:PX4:H53	0.59	1.73	14	1
4:A:313:PX4:H29	4:A:362:PX4:H56	0.59	1.73	16	1
4:A:386:PX4:H52	4:A:402:PX4:H22	0.59	1.74	18	1
4:A:411:PX4:H64	4:A:412:PX4:H71	0.59	1.73	18	1
4:A:308:PX4:H47	4:A:361:PX4:H63	0.59	1.73	20	1
4:A:404:PX4:H40	4:A:417:PX4:H39	0.59	1.74	7	1
4:A:412:PX4:H17	4:A:424:PX4:H54	0.59	1.74	8	1
4:A:404:PX4:H21	4:A:418:PX4:H17	0.59	1.74	17	1
4:A:391:PX4:H31	4:A:407:PX4:H31	0.59	1.75	4	1
4:A:327:PX4:H71	4:A:429:PX4:H37	0.59	1.74	8	1
4:A:368:PX4:H61	4:A:426:PX4:H58	0.59	1.75	9	1
4:A:362:PX4:H67	4:A:415:PX4:H67	0.59	1.74	14	1
4:A:415:PX4:H32	4:A:418:PX4:H66	0.59	1.74	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PX4:H56	4:A:407:PX4:H23	0.59	1.73	1	1
4:A:342:PX4:H39	4:A:407:PX4:H37	0.59	1.74	2	1
4:A:336:PX4:H50	4:A:338:PX4:H28	0.59	1.74	3	1
4:A:306:PX4:H20	4:A:358:PX4:H47	0.59	1.73	4	1
4:A:310:PX4:H53	4:A:364:PX4:H55	0.59	1.75	15	1
4:A:371:PX4:H18	4:A:401:PX4:C17	0.59	2.28	17	1
4:A:371:PX4:H65	4:A:384:PX4:H19	0.59	1.73	19	1
4:A:369:PX4:H30	4:A:381:PX4:H67	0.59	1.74	2	1
4:A:397:PX4:H3	4:A:411:PX4:O6	0.59	1.98	4	1
4:A:305:PX4:H28	4:A:311:PX4:H30	0.59	1.72	5	1
4:A:387:PX4:H47	4:A:421:PX4:H16	0.59	1.72	8	1
4:A:324:PX4:H58	4:A:334:PX4:H55	0.59	1.74	10	1
4:A:404:PX4:O1	4:A:418:PX4:H3	0.59	1.98	16	1
4:A:338:PX4:H69	4:A:359:PX4:H32	0.59	1.74	3	1
4:A:312:PX4:H20	4:A:339:PX4:H22	0.59	1.75	1	1
4:A:366:PX4:H22	4:A:403:PX4:H20	0.59	1.74	7	1
4:A:369:PX4:H59	4:A:393:PX4:H29	0.59	1.74	7	1
4:A:351:PX4:H19	4:A:359:PX4:H32	0.59	1.75	16	1
4:A:382:PX4:H53	4:A:423:PX4:H39	0.58	1.75	1	1
4:A:339:PX4:H18	4:A:339:PX4:H2	0.58	1.74	7	1
4:A:321:PX4:H48	4:A:342:PX4:H35	0.58	1.73	16	1
4:A:400:PX4:H24	4:A:401:PX4:H17	0.58	1.74	8	2
4:A:325:PX4:H23	4:A:362:PX4:H55	0.58	1.74	9	1
4:A:307:PX4:H54	4:A:332:PX4:H30	0.58	1.73	13	1
4:A:386:PX4:H67	4:A:426:PX4:H64	0.58	1.73	18	1
4:A:339:PX4:H28	4:A:346:PX4:H67	0.58	1.76	4	1
4:A:359:PX4:H18	4:A:359:PX4:H6	0.58	1.74	7	1
4:A:315:PX4:H43	4:A:381:PX4:H70	0.58	1.76	8	1
4:A:341:PX4:H45	4:A:367:PX4:H35	0.58	1.73	11	1
4:A:334:PX4:H39	4:A:426:PX4:H25	0.58	1.75	3	1
4:A:409:PX4:H5	4:A:412:PX4:O6	0.58	1.98	5	1
4:A:366:PX4:H37	4:A:378:PX4:H61	0.58	1.75	7	1
4:A:370:PX4:H30	4:A:430:PX4:H60	0.58	1.75	11	1
4:A:387:PX4:H17	4:A:421:PX4:H20	0.58	1.74	2	2
4:A:354:PX4:H66	4:A:416:PX4:H70	0.58	1.73	5	1
4:A:380:PX4:H33	4:A:385:PX4:H35	0.58	1.75	8	1
4:A:329:PX4:H34	4:A:360:PX4:H33	0.58	1.75	14	1
4:A:328:PX4:H49	4:A:347:PX4:H16	0.58	1.73	5	1
4:A:399:PX4:H22	4:A:424:PX4:H24	0.58	1.75	5	1
4:A:422:PX4:H36	4:A:425:PX4:H61	0.58	1.74	5	1
4:A:314:PX4:H15	4:A:314:PX4:H13	0.58	1.76	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:H17	4:A:380:PX4:H27	0.58	1.75	7	1
4:A:396:PX4:O6	4:A:407:PX4:H9	0.58	1.97	12	1
4:A:313:PX4:H17	4:A:355:PX4:H50	0.58	1.75	20	1
4:A:325:PX4:H17	4:A:353:PX4:H20	0.58	1.74	1	1
4:A:327:PX4:H22	4:A:338:PX4:H58	0.58	1.75	2	1
4:A:392:PX4:H48	4:A:427:PX4:H47	0.58	1.75	7	1
4:A:338:PX4:O1	4:A:344:PX4:H3	0.58	1.98	9	1
4:A:308:PX4:H42	4:A:350:PX4:H26	0.58	1.76	14	1
4:A:385:PX4:H68	4:A:415:PX4:H35	0.58	1.76	14	1
4:A:409:PX4:H33	5:A:434:C3S:H403	0.58	1.75	17	1
4:A:307:PX4:H33	4:A:337:PX4:H71	0.58	1.74	20	1
4:A:406:PX4:H32	4:A:410:PX4:H61	0.58	1.76	1	1
4:A:324:PX4:O1	4:A:334:PX4:H6	0.58	1.99	16	1
4:A:387:PX4:H26	4:A:416:PX4:H17	0.58	1.75	18	1
4:A:327:PX4:H4	4:A:348:PX4:H18	0.58	1.75	19	1
4:A:375:PX4:H64	4:A:405:PX4:H66	0.58	1.76	3	1
4:A:409:PX4:H66	4:A:412:PX4:H65	0.58	1.75	8	1
4:A:367:PX4:H60	4:A:412:PX4:H52	0.58	1.76	16	1
4:A:305:PX4:H32	4:A:310:PX4:H34	0.58	1.76	18	1
4:A:316:PX4:H30	4:A:318:PX4:H47	0.58	1.74	20	1
4:A:324:PX4:H55	4:A:334:PX4:H51	0.58	1.76	4	1
4:A:337:PX4:H68	4:A:397:PX4:H43	0.58	1.76	13	1
4:A:347:PX4:H21	4:A:360:PX4:H22	0.57	1.76	5	1
4:A:365:PX4:H24	4:A:396:PX4:H49	0.57	1.76	9	1
4:A:314:PX4:H57	4:A:354:PX4:H38	0.57	1.74	13	1
4:A:323:PX4:H46	4:A:325:PX4:C6	0.57	2.29	5	1
4:A:377:PX4:H48	4:A:420:PX4:H46	0.57	1.74	5	1
4:A:375:PX4:H32	4:A:427:PX4:H27	0.57	1.76	6	1
4:A:328:PX4:H43	4:A:338:PX4:H62	0.57	1.75	12	1
4:A:316:PX4:H57	4:A:319:PX4:H45	0.57	1.73	3	1
4:A:323:PX4:H14	4:A:353:PX4:O7	0.57	1.99	7	1
4:A:319:PX4:H47	4:A:341:PX4:H65	0.57	1.75	18	1
4:A:327:PX4:H27	4:A:348:PX4:H51	0.57	1.76	18	1
4:A:423:PX4:H68	4:A:430:PX4:H36	0.57	1.76	18	1
4:A:373:PX4:H28	4:A:401:PX4:H37	0.57	1.77	5	1
4:A:310:PX4:H21	4:A:311:PX4:H17	0.57	1.76	19	1
4:A:365:PX4:H15	4:A:383:PX4:H19	0.57	1.77	4	1
4:A:364:PX4:H45	4:A:372:PX4:H44	0.57	1.75	6	1
1:A:125:ARG:CZ	4:A:306:PX4:H53	0.57	2.30	8	1
4:A:373:PX4:H47	4:A:406:PX4:H17	0.57	1.75	11	1
4:A:371:PX4:H47	4:A:373:PX4:H23	0.57	1.77	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:H55	4:A:377:PX4:H25	0.57	1.76	19	1
4:A:353:PX4:H29	4:A:355:PX4:H67	0.57	1.76	20	1
4:A:365:PX4:H53	4:A:383:PX4:H34	0.57	1.76	7	1
4:A:420:PX4:H27	4:A:422:PX4:H49	0.57	1.75	10	1
4:A:327:PX4:H30	4:A:348:PX4:H51	0.57	1.74	11	1
4:A:373:PX4:H17	4:A:406:PX4:H49	0.57	1.76	13	1
4:A:343:PX4:H28	4:A:352:PX4:H52	0.57	1.75	2	1
4:A:316:PX4:H49	4:A:321:PX4:H24	0.57	1.75	12	1
4:A:310:PX4:H44	4:A:364:PX4:H65	0.57	1.75	13	1
4:A:338:PX4:H28	4:A:344:PX4:H25	0.57	1.75	16	1
4:A:312:PX4:H47	4:A:324:PX4:H16	0.57	1.77	20	3
4:A:353:PX4:H19	4:A:361:PX4:H54	0.57	1.77	4	1
4:A:316:PX4:O1	4:A:352:PX4:H14	0.57	2.00	8	1
4:A:375:PX4:H15	4:A:405:PX4:O3	0.57	2.00	8	1
4:A:375:PX4:H59	4:A:399:PX4:H67	0.57	1.75	12	1
4:A:322:PX4:H69	4:A:327:PX4:H44	0.57	1.76	13	1
4:A:375:PX4:H22	4:A:405:PX4:H47	0.57	1.77	15	1
4:A:370:PX4:H66	4:A:381:PX4:H64	0.57	1.75	3	1
4:A:394:PX4:H33	4:A:400:PX4:H65	0.57	1.77	5	1
4:A:316:PX4:H64	4:A:350:PX4:H66	0.57	1.76	6	1
1:A:2:GLN:HE22	1:A:57:ARG:CZ	0.57	2.12	8	1
4:A:409:PX4:H51	4:A:428:PX4:H28	0.57	1.76	8	1
4:A:320:PX4:H52	4:A:334:PX4:H28	0.57	1.75	10	1
4:A:306:PX4:H56	4:A:321:PX4:H17	0.57	1.75	15	1
4:A:316:PX4:H21	4:A:321:PX4:H22	0.57	1.75	16	1
4:A:414:PX4:H25	5:A:432:C3S:H693	0.57	1.77	6	1
4:A:414:PX4:H55	4:A:426:PX4:H63	0.57	1.76	7	1
4:A:324:PX4:H71	4:A:408:PX4:H71	0.57	1.76	9	1
4:A:395:PX4:H32	4:A:402:PX4:H56	0.56	1.76	1	1
4:A:380:PX4:H38	4:A:420:PX4:H66	0.56	1.76	7	1
4:A:389:PX4:H59	4:A:401:PX4:H36	0.56	1.77	7	1
4:A:422:PX4:H13	4:A:425:PX4:O8	0.56	2.00	10	1
1:A:88:VAL:HG11	4:A:306:PX4:H46	0.56	1.75	13	1
4:A:379:PX4:H20	4:A:422:PX4:H46	0.56	1.77	15	1
4:A:331:PX4:H23	4:A:337:PX4:H25	0.56	1.77	16	1
4:A:396:PX4:H53	4:A:407:PX4:H58	0.56	1.76	20	1
4:A:343:PX4:H69	4:A:350:PX4:H29	0.56	1.77	1	1
4:A:318:PX4:H21	4:A:357:PX4:H38	0.56	1.76	2	1
4:A:412:PX4:H61	4:A:424:PX4:H58	0.56	1.77	11	1
4:A:397:PX4:H53	4:A:423:PX4:H60	0.56	1.77	13	1
4:A:331:PX4:H62	4:A:354:PX4:H28	0.56	1.77	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:409:PX4:H48	4:A:412:PX4:H19	0.56	1.77	8	1
4:A:387:PX4:H38	4:A:421:PX4:H44	0.56	1.77	9	1
4:A:313:PX4:H12	4:A:313:PX4:H14	0.56	1.76	11	1
4:A:411:PX4:H49	4:A:412:PX4:H51	0.56	1.77	12	1
4:A:369:PX4:O4	4:A:419:PX4:H5	0.56	2.01	13	1
4:A:370:PX4:H60	4:A:370:PX4:H33	0.56	1.77	13	1
4:A:336:PX4:H17	4:A:354:PX4:H50	0.56	1.76	17	1
4:A:315:PX4:H49	4:A:332:PX4:H21	0.56	1.76	1	1
4:A:368:PX4:H22	5:A:436:C3S:H571	0.56	1.78	1	1
4:A:331:PX4:O2	4:A:337:PX4:H3	0.56	2.00	7	1
4:A:409:PX4:H17	4:A:412:PX4:H22	0.56	1.77	8	1
4:A:392:PX4:H17	4:A:425:PX4:H20	0.56	1.76	10	1
4:A:327:PX4:H19	4:A:348:PX4:H29	0.56	1.77	16	1
4:A:387:PX4:H59	4:A:421:PX4:H55	0.56	1.76	16	1
4:A:371:PX4:H68	4:A:373:PX4:H59	0.56	1.77	20	1
4:A:345:PX4:H63	4:A:359:PX4:H50	0.56	1.77	4	1
4:A:384:PX4:H18	4:A:384:PX4:O3	0.56	2.01	6	1
4:A:400:PX4:H27	4:A:401:PX4:H17	0.56	1.77	10	1
4:A:338:PX4:H24	4:A:344:PX4:H21	0.56	1.77	13	1
4:A:340:PX4:H25	4:A:356:PX4:H64	0.56	1.77	3	1
4:A:352:PX4:H34	4:A:407:PX4:H35	0.56	1.76	8	1
4:A:381:PX4:H29	4:A:418:PX4:H37	0.56	1.75	9	1
4:A:372:PX4:H36	4:A:406:PX4:H33	0.56	1.77	13	1
4:A:306:PX4:H17	4:A:342:PX4:H19	0.56	1.77	6	1
4:A:409:PX4:H11	5:A:434:C3S:H92	0.56	1.78	7	1
4:A:315:PX4:H42	4:A:374:PX4:H64	0.56	1.77	15	1
4:A:380:PX4:H17	4:A:420:PX4:O2	0.56	2.00	15	1
4:A:318:PX4:H20	4:A:342:PX4:H52	0.56	1.78	16	1
4:A:415:PX4:H22	4:A:415:PX4:H51	0.56	1.76	16	1
4:A:351:PX4:H28	4:A:359:PX4:H19	0.56	1.77	19	1
4:A:396:PX4:H3	4:A:407:PX4:O1	0.56	2.01	19	1
4:A:409:PX4:H32	4:A:412:PX4:H33	0.56	1.78	4	1
1:A:23:TYR:CE1	1:A:72:VAL:HG21	0.56	2.36	10	1
4:A:406:PX4:H49	4:A:414:PX4:H26	0.56	1.77	14	1
4:A:343:PX4:H41	4:A:425:PX4:H70	0.56	1.78	5	1
4:A:338:PX4:H32	4:A:344:PX4:H23	0.56	1.76	12	1
4:A:392:PX4:H50	4:A:425:PX4:H53	0.56	1.78	17	1
4:A:376:PX4:H19	4:A:396:PX4:H25	0.56	1.76	18	1
4:A:318:PX4:H31	4:A:342:PX4:H65	0.56	1.76	19	1
4:A:322:PX4:H11	4:A:344:PX4:O1	0.56	2.01	7	1
4:A:397:PX4:H21	4:A:411:PX4:O5	0.56	2.00	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:366:PX4:H12	4:A:403:PX4:O2	0.56	2.01	12	1
4:A:305:PX4:H28	4:A:310:PX4:H56	0.56	1.78	14	1
4:A:316:PX4:H25	4:A:321:PX4:H32	0.56	1.76	14	1
4:A:315:PX4:H26	4:A:332:PX4:H24	0.56	1.78	16	1
4:A:354:PX4:H37	4:A:409:PX4:H42	0.56	1.77	18	1
4:A:330:PX4:H33	4:A:337:PX4:H47	0.55	1.77	5	1
4:A:333:PX4:H14	5:A:432:C3S:H30	0.55	1.76	17	1
4:A:400:PX4:H47	4:A:405:PX4:H16	0.55	1.78	5	2
4:A:348:PX4:H38	4:A:359:PX4:H58	0.55	1.79	7	1
4:A:377:PX4:H25	4:A:377:PX4:H58	0.55	1.77	13	1
4:A:318:PX4:H70	4:A:389:PX4:H40	0.55	1.78	14	1
4:A:388:PX4:H15	4:A:388:PX4:H13	0.55	1.77	14	1
4:A:403:PX4:O2	4:A:421:PX4:H10	0.55	2.00	15	1
4:A:311:PX4:O8	4:A:329:PX4:H10	0.55	2.01	16	1
4:A:386:PX4:H23	4:A:402:PX4:H48	0.55	1.76	18	1
4:A:406:PX4:O1	4:A:410:PX4:H15	0.55	2.01	19	1
4:A:417:PX4:H20	4:A:418:PX4:H22	0.55	1.77	20	1
4:A:306:PX4:H36	4:A:345:PX4:H64	0.55	1.77	12	1
4:A:394:PX4:H56	4:A:395:PX4:H59	0.55	1.78	14	1
4:A:403:PX4:H46	4:A:421:PX4:H49	0.55	1.78	15	1
4:A:312:PX4:H27	4:A:345:PX4:H30	0.55	1.76	17	1
4:A:322:PX4:H33	4:A:344:PX4:H34	0.55	1.76	18	1
4:A:400:PX4:O2	4:A:405:PX4:H14	0.55	2.02	20	1
4:A:343:PX4:H40	4:A:410:PX4:H45	0.55	1.77	3	1
4:A:378:PX4:H21	4:A:403:PX4:H20	0.55	1.78	3	1
4:A:393:PX4:H18	4:A:419:PX4:H16	0.55	1.78	5	1
4:A:365:PX4:H65	4:A:396:PX4:H61	0.55	1.77	7	1
4:A:382:PX4:H51	4:A:423:PX4:H20	0.55	1.78	9	1
4:A:403:PX4:H21	4:A:421:PX4:H51	0.55	1.78	10	1
4:A:413:PX4:H27	4:A:428:PX4:H41	0.55	1.77	15	1
4:A:361:PX4:H62	5:A:431:C3S:H42	0.55	1.79	18	1
4:A:383:PX4:H52	4:A:396:PX4:H50	0.55	1.77	19	1
4:A:371:PX4:H60	4:A:406:PX4:H61	0.55	1.77	20	1
4:A:317:PX4:H29	4:A:326:PX4:H50	0.55	1.77	3	1
4:A:343:PX4:H54	4:A:350:PX4:H49	0.55	1.78	3	1
4:A:403:PX4:H36	4:A:417:PX4:H34	0.55	1.78	9	1
4:A:366:PX4:H68	4:A:404:PX4:H41	0.55	1.76	13	1
4:A:383:PX4:H21	4:A:430:PX4:H57	0.55	1.79	13	1
4:A:327:PX4:O1	4:A:348:PX4:H16	0.55	2.01	14	1
4:A:306:PX4:H48	4:A:342:PX4:H21	0.55	1.78	19	1
4:A:315:PX4:H53	4:A:332:PX4:C11	0.55	2.30	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H32	4:A:399:PX4:H59	0.55	1.79	1	1
4:A:382:PX4:H51	4:A:423:PX4:H52	0.55	1.77	2	1
4:A:344:PX4:H66	4:A:419:PX4:H41	0.55	1.77	4	1
4:A:366:PX4:H64	4:A:403:PX4:H40	0.55	1.78	5	1
4:A:305:PX4:H62	4:A:363:PX4:H55	0.55	1.77	16	1
4:A:319:PX4:H10	4:A:319:PX4:H14	0.55	1.79	4	1
4:A:307:PX4:H19	4:A:327:PX4:H44	0.55	1.78	5	1
4:A:388:PX4:H31	4:A:388:PX4:H51	0.55	1.78	7	1
4:A:319:PX4:H64	4:A:384:PX4:H68	0.55	1.79	8	1
4:A:351:PX4:H50	4:A:359:PX4:H32	0.55	1.77	9	1
4:A:385:PX4:H17	5:A:433:C3S:H443	0.55	1.78	10	1
4:A:330:PX4:H51	4:A:337:PX4:H29	0.55	1.77	20	1
4:A:382:PX4:H54	4:A:423:PX4:H49	0.55	1.76	5	1
4:A:338:PX4:H56	4:A:344:PX4:H61	0.55	1.77	11	1
4:A:415:PX4:H61	4:A:418:PX4:H69	0.55	1.78	12	1
4:A:313:PX4:H45	4:A:355:PX4:H49	0.55	1.79	15	1
4:A:363:PX4:H10	4:A:363:PX4:H20	0.55	1.79	1	1
4:A:378:PX4:H34	4:A:408:PX4:H70	0.55	1.79	1	1
4:A:332:PX4:H46	4:A:348:PX4:H5	0.55	1.77	4	1
4:A:319:PX4:H63	4:A:352:PX4:H55	0.55	1.79	6	1
4:A:353:PX4:H47	4:A:361:PX4:H24	0.55	1.79	6	1
4:A:317:PX4:H47	4:A:330:PX4:H28	0.55	1.79	7	1
1:A:115:MET:HB2	4:A:315:PX4:H4	0.55	1.78	15	1
4:A:420:PX4:H36	4:A:422:PX4:H26	0.55	1.78	15	1
4:A:365:PX4:H47	4:A:383:PX4:H23	0.55	1.78	17	1
4:A:398:PX4:H67	4:A:404:PX4:H58	0.55	1.77	3	1
4:A:336:PX4:H71	4:A:409:PX4:H31	0.55	1.79	5	1
4:A:330:PX4:H17	4:A:355:PX4:H24	0.55	1.78	6	1
4:A:383:PX4:H53	4:A:407:PX4:H54	0.55	1.79	14	1
4:A:333:PX4:H25	4:A:364:PX4:H36	0.55	1.79	15	1
4:A:375:PX4:H55	4:A:384:PX4:H18	0.55	1.79	17	1
4:A:369:PX4:H48	4:A:419:PX4:H51	0.55	1.79	20	1
4:A:376:PX4:H12	4:A:390:PX4:O6	0.54	2.02	3	1
4:A:389:PX4:H64	4:A:399:PX4:H39	0.54	1.78	15	1
4:A:320:PX4:H51	4:A:334:PX4:H17	0.54	1.78	16	1
4:A:365:PX4:H48	4:A:419:PX4:H52	0.54	1.79	20	1
4:A:383:PX4:H55	4:A:394:PX4:H48	0.54	1.78	2	1
4:A:351:PX4:H50	4:A:359:PX4:H42	0.54	1.78	5	1
4:A:312:PX4:H24	4:A:324:PX4:H16	0.54	1.78	6	1
4:A:415:PX4:H24	5:A:433:C3S:H442	0.54	1.78	15	1
4:A:315:PX4:H40	4:A:350:PX4:H30	0.54	1.77	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:H36	4:A:408:PX4:H60	0.54	1.79	19	1
4:A:397:PX4:H24	4:A:411:PX4:H49	0.54	1.78	20	1
4:A:307:PX4:H16	4:A:337:PX4:H54	0.54	1.79	1	1
4:A:310:PX4:H70	4:A:424:PX4:H42	0.54	1.79	5	1
4:A:365:PX4:H58	4:A:370:PX4:H40	0.54	1.79	11	1
4:A:319:PX4:H50	4:A:356:PX4:H14	0.54	1.79	15	1
4:A:404:PX4:H35	4:A:404:PX4:H67	0.54	1.78	18	1
4:A:364:PX4:H65	4:A:364:PX4:H39	0.54	1.77	19	1
4:A:392:PX4:H57	4:A:425:PX4:H26	0.54	1.79	19	1
4:A:325:PX4:H24	4:A:355:PX4:H22	0.54	1.78	8	1
4:A:308:PX4:H69	4:A:371:PX4:H43	0.54	1.80	11	1
4:A:336:PX4:H55	4:A:344:PX4:H43	0.54	1.78	11	1
4:A:367:PX4:H21	4:A:367:PX4:H48	0.54	1.78	17	1
4:A:380:PX4:H56	4:A:380:PX4:H29	0.54	1.80	18	1
4:A:409:PX4:H49	4:A:428:PX4:H21	0.54	1.79	18	1
4:A:305:PX4:H39	4:A:333:PX4:H61	0.54	1.79	6	1
4:A:346:PX4:H40	4:A:361:PX4:H65	0.54	1.78	10	1
4:A:376:PX4:H20	4:A:383:PX4:H24	0.54	1.79	11	1
4:A:388:PX4:H60	4:A:391:PX4:H17	0.54	1.79	12	1
4:A:310:PX4:H11	4:A:333:PX4:H50	0.54	1.78	16	1
4:A:316:PX4:H65	4:A:343:PX4:H52	0.54	1.79	17	1
4:A:308:PX4:H16	4:A:320:PX4:H16	0.54	1.78	14	2
4:A:335:PX4:H62	4:A:347:PX4:H67	0.54	1.79	2	1
4:A:418:PX4:H31	4:A:423:PX4:H30	0.54	1.79	10	1
4:A:312:PX4:H3	4:A:346:PX4:O3	0.54	2.02	2	1
4:A:331:PX4:H43	4:A:398:PX4:H39	0.54	1.79	7	1
4:A:371:PX4:H24	4:A:402:PX4:H63	0.54	1.79	12	1
4:A:386:PX4:H55	4:A:417:PX4:H17	0.54	1.80	12	1
4:A:397:PX4:H16	4:A:429:PX4:H12	0.54	1.79	14	1
4:A:317:PX4:H40	4:A:361:PX4:H34	0.54	1.79	15	1
4:A:415:PX4:H45	4:A:416:PX4:H8	0.54	1.79	20	1
4:A:310:PX4:O6	4:A:313:PX4:H5	0.54	2.02	2	1
4:A:328:PX4:H44	4:A:353:PX4:H66	0.54	1.78	3	1
4:A:368:PX4:H69	4:A:426:PX4:H66	0.54	1.80	9	1
4:A:395:PX4:O2	4:A:402:PX4:H12	0.54	2.03	9	1
4:A:323:PX4:H63	4:A:328:PX4:H58	0.54	1.80	11	1
4:A:347:PX4:H52	4:A:351:PX4:H50	0.54	1.78	12	1
4:A:392:PX4:H69	4:A:425:PX4:H71	0.54	1.80	15	1
4:A:340:PX4:H35	4:A:389:PX4:H67	0.54	1.79	17	1
4:A:378:PX4:H65	4:A:414:PX4:H46	0.54	1.78	1	1
4:A:400:PX4:H30	4:A:401:PX4:H57	0.54	1.79	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:385:PX4:H50	4:A:415:PX4:H16	0.54	1.78	5	1
4:A:428:PX4:H49	4:A:430:PX4:H30	0.54	1.80	5	1
4:A:372:PX4:H34	4:A:406:PX4:H34	0.54	1.78	6	1
4:A:312:PX4:O1	4:A:324:PX4:H2	0.54	2.02	7	1
4:A:374:PX4:O7	4:A:397:PX4:H47	0.54	2.02	7	1
1:A:103:ILE:HD13	4:A:350:PX4:H46	0.54	1.78	11	1
4:A:332:PX4:H18	4:A:348:PX4:H57	0.54	1.78	16	1
4:A:375:PX4:H60	4:A:405:PX4:H63	0.54	1.80	3	1
4:A:365:PX4:H33	4:A:419:PX4:H63	0.54	1.80	7	1
4:A:310:PX4:H49	4:A:364:PX4:H61	0.54	1.80	8	1
4:A:426:PX4:H72	5:A:432:C3S:H352	0.54	1.80	16	1
4:A:305:PX4:H58	4:A:324:PX4:H64	0.54	1.80	20	1
4:A:316:PX4:H11	4:A:318:PX4:O8	0.53	2.03	3	1
4:A:376:PX4:H19	4:A:396:PX4:H17	0.53	1.79	15	1
4:A:385:PX4:H41	5:A:433:C3S:H602	0.53	1.78	15	1
1:A:131:THR:O	4:A:321:PX4:H11	0.53	2.03	5	1
4:A:317:PX4:H25	4:A:326:PX4:H16	0.53	1.80	7	1
4:A:310:PX4:H52	4:A:333:PX4:H59	0.53	1.79	9	1
4:A:322:PX4:H19	4:A:331:PX4:H26	0.53	1.80	12	1
4:A:308:PX4:H38	4:A:350:PX4:H50	0.53	1.80	16	1
4:A:308:PX4:H23	4:A:320:PX4:H25	0.53	1.81	3	1
4:A:323:PX4:H48	4:A:361:PX4:H28	0.53	1.81	5	1
4:A:323:PX4:H34	4:A:345:PX4:H37	0.53	1.80	9	1
4:A:428:PX4:H22	4:A:429:PX4:H17	0.53	1.81	10	1
4:A:333:PX4:H50	4:A:364:PX4:H46	0.53	1.78	12	1
4:A:375:PX4:H28	4:A:427:PX4:H21	0.53	1.79	13	1
4:A:341:PX4:H19	4:A:356:PX4:H25	0.53	1.79	14	1
4:A:378:PX4:H61	4:A:386:PX4:H61	0.53	1.79	3	1
4:A:359:PX4:H71	4:A:376:PX4:H26	0.53	1.79	5	1
4:A:385:PX4:H1	4:A:385:PX4:H18	0.53	1.81	7	1
4:A:381:PX4:H21	4:A:394:PX4:H51	0.53	1.81	10	1
4:A:384:PX4:O6	4:A:401:PX4:H13	0.53	2.02	12	1
4:A:316:PX4:H52	4:A:343:PX4:H47	0.53	1.80	13	1
4:A:379:PX4:H11	5:A:434:C3S:O2	0.53	2.03	14	1
4:A:397:PX4:H10	4:A:411:PX4:O6	0.53	2.03	16	1
4:A:330:PX4:H60	4:A:331:PX4:H23	0.53	1.80	17	1
4:A:362:PX4:H41	4:A:364:PX4:H61	0.53	1.80	18	1
4:A:374:PX4:H50	4:A:430:PX4:H51	0.53	1.79	18	1
4:A:323:PX4:H20	4:A:353:PX4:H53	0.53	1.81	20	1
4:A:314:PX4:H40	4:A:352:PX4:H38	0.53	1.80	4	1
4:A:330:PX4:O8	4:A:331:PX4:H3	0.53	2.04	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:370:PX4:H55	4:A:394:PX4:H52	0.53	1.81	9	1
4:A:428:PX4:O6	4:A:428:PX4:H13	0.53	2.04	9	1
4:A:376:PX4:H27	4:A:396:PX4:H26	0.53	1.79	13	1
4:A:370:PX4:H28	4:A:383:PX4:H26	0.53	1.79	19	1
4:A:314:PX4:H56	4:A:336:PX4:H35	0.53	1.79	20	1
4:A:371:PX4:H62	4:A:389:PX4:H26	0.53	1.79	2	1
4:A:386:PX4:H52	4:A:426:PX4:H50	0.53	1.80	2	1
4:A:327:PX4:H64	4:A:344:PX4:H53	0.53	1.80	3	1
4:A:325:PX4:H36	4:A:355:PX4:H32	0.53	1.79	15	1
4:A:358:PX4:H57	4:A:358:PX4:H24	0.53	1.81	2	1
4:A:367:PX4:H57	5:A:434:C3S:H12	0.53	1.80	5	1
4:A:320:PX4:H52	4:A:334:PX4:H59	0.53	1.80	6	1
4:A:334:PX4:H24	4:A:334:PX4:H57	0.53	1.79	16	1
4:A:333:PX4:H16	5:A:432:C3S:H231	0.53	1.80	19	1
4:A:318:PX4:H19	4:A:342:PX4:H42	0.53	1.80	1	1
4:A:358:PX4:H49	4:A:359:PX4:H47	0.53	1.80	1	1
4:A:395:PX4:H16	4:A:402:PX4:H47	0.53	1.80	3	1
4:A:403:PX4:H51	4:A:421:PX4:H17	0.53	1.81	5	1
4:A:393:PX4:H32	4:A:416:PX4:H34	0.53	1.80	11	1
4:A:395:PX4:H32	4:A:402:PX4:H69	0.53	1.81	12	1
4:A:357:PX4:H17	4:A:363:PX4:H22	0.53	1.80	6	1
4:A:410:PX4:H16	5:A:435:C3S:H441	0.53	1.81	11	1
4:A:415:PX4:H57	4:A:418:PX4:H51	0.53	1.81	13	1
4:A:401:PX4:H63	4:A:405:PX4:H29	0.53	1.81	4	1
4:A:411:PX4:H17	4:A:412:PX4:H48	0.53	1.81	5	1
4:A:313:PX4:H50	4:A:329:PX4:H26	0.53	1.80	7	1
4:A:327:PX4:H45	4:A:383:PX4:H64	0.53	1.79	8	1
4:A:396:PX4:H20	4:A:407:PX4:H49	0.53	1.81	11	2
4:A:373:PX4:H55	4:A:399:PX4:H19	0.53	1.79	12	1
4:A:325:PX4:O6	4:A:330:PX4:H7	0.53	2.05	13	2
4:A:350:PX4:H57	4:A:402:PX4:H43	0.53	1.79	14	1
4:A:362:PX4:H39	4:A:367:PX4:H41	0.53	1.81	19	1
4:A:391:PX4:H20	4:A:427:PX4:H16	0.52	1.80	10	1
4:A:346:PX4:H20	4:A:358:PX4:H25	0.52	1.78	12	1
4:A:366:PX4:H27	4:A:386:PX4:H58	0.52	1.80	12	1
4:A:320:PX4:H55	4:A:334:PX4:H50	0.52	1.79	13	1
4:A:365:PX4:H17	4:A:369:PX4:H9	0.52	1.79	13	1
4:A:375:PX4:H17	4:A:405:PX4:H13	0.52	1.80	18	1
4:A:370:PX4:H4	4:A:430:PX4:H15	0.52	1.82	19	1
4:A:323:PX4:H67	4:A:329:PX4:H65	0.52	1.80	20	1
4:A:404:PX4:H39	4:A:417:PX4:H29	0.52	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:380:PX4:H19	4:A:420:PX4:H22	0.52	1.81	10	1
4:A:369:PX4:H47	4:A:419:PX4:H17	0.52	1.80	13	1
4:A:393:PX4:H67	4:A:421:PX4:H45	0.52	1.81	13	1
4:A:305:PX4:H48	4:A:311:PX4:H31	0.52	1.79	15	1
4:A:392:PX4:H38	4:A:407:PX4:H30	0.52	1.81	19	1
4:A:397:PX4:H24	4:A:428:PX4:H46	0.52	1.81	3	1
4:A:381:PX4:H25	4:A:395:PX4:H23	0.52	1.81	4	1
4:A:321:PX4:H41	4:A:399:PX4:H57	0.52	1.82	9	1
4:A:333:PX4:H30	4:A:333:PX4:H60	0.52	1.79	12	1
4:A:404:PX4:H55	4:A:415:PX4:H49	0.52	1.80	12	1
4:A:343:PX4:H60	4:A:350:PX4:H48	0.52	1.80	17	1
4:A:321:PX4:H17	4:A:342:PX4:H27	0.52	1.80	1	1
4:A:399:PX4:O6	4:A:424:PX4:H3	0.52	2.04	4	1
4:A:325:PX4:H50	4:A:361:PX4:H23	0.52	1.82	6	1
4:A:400:PX4:H50	4:A:405:PX4:H16	0.52	1.81	6	1
4:A:330:PX4:H19	4:A:337:PX4:H16	0.52	1.79	11	1
4:A:376:PX4:H32	4:A:396:PX4:H30	0.52	1.82	13	1
4:A:337:PX4:H71	4:A:381:PX4:H62	0.52	1.80	17	1
4:A:391:PX4:H10	4:A:427:PX4:H1	0.52	1.80	19	1
4:A:320:PX4:H33	4:A:361:PX4:H65	0.52	1.80	20	1
4:A:385:PX4:H22	5:A:433:C3S:H403	0.52	1.80	1	1
4:A:323:PX4:H62	4:A:328:PX4:H48	0.52	1.80	2	1
4:A:351:PX4:H23	4:A:359:PX4:H38	0.52	1.81	4	1
4:A:314:PX4:H61	4:A:336:PX4:H35	0.52	1.80	16	1
4:A:428:PX4:H14	4:A:429:PX4:H51	0.52	1.80	17	1
4:A:413:PX4:H24	4:A:419:PX4:H26	0.52	1.82	18	1
4:A:383:PX4:H37	4:A:388:PX4:H42	0.52	1.79	19	1
4:A:326:PX4:H70	4:A:353:PX4:H50	0.52	1.81	6	1
4:A:325:PX4:H65	4:A:353:PX4:H60	0.52	1.82	7	1
4:A:384:PX4:H69	4:A:392:PX4:H65	0.52	1.82	9	1
4:A:397:PX4:H57	4:A:423:PX4:H61	0.52	1.81	14	1
4:A:365:PX4:H19	4:A:369:PX4:H22	0.52	1.81	1	1
4:A:375:PX4:H56	4:A:400:PX4:H69	0.52	1.81	1	1
4:A:310:PX4:H23	4:A:311:PX4:H51	0.52	1.79	4	1
4:A:374:PX4:H71	4:A:419:PX4:H70	0.52	1.81	4	1
4:A:391:PX4:H21	4:A:427:PX4:H21	0.52	1.82	5	1
4:A:308:PX4:H31	4:A:315:PX4:H42	0.52	1.80	6	1
4:A:395:PX4:H47	4:A:401:PX4:H49	0.52	1.80	10	1
4:A:315:PX4:H56	4:A:332:PX4:H17	0.52	1.81	20	2
4:A:319:PX4:H54	4:A:343:PX4:H27	0.52	1.81	12	1
4:A:323:PX4:H16	4:A:353:PX4:H49	0.52	1.81	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:365:PX4:H37	4:A:369:PX4:H36	0.52	1.81	2	1
4:A:391:PX4:H30	4:A:407:PX4:H24	0.52	1.82	2	1
4:A:416:PX4:H49	4:A:421:PX4:H27	0.52	1.80	3	1
4:A:343:PX4:H22	4:A:356:PX4:H54	0.52	1.82	14	1
4:A:373:PX4:H19	4:A:386:PX4:H56	0.52	1.81	15	1
4:A:322:PX4:H59	4:A:330:PX4:H31	0.52	1.82	16	1
4:A:386:PX4:H52	4:A:417:PX4:H32	0.52	1.82	16	1
4:A:366:PX4:H64	4:A:390:PX4:H34	0.52	1.81	19	1
4:A:373:PX4:H41	4:A:378:PX4:H62	0.52	1.81	3	1
4:A:329:PX4:H69	4:A:387:PX4:H37	0.52	1.82	9	1
4:A:374:PX4:H57	4:A:381:PX4:H58	0.52	1.80	9	1
4:A:314:PX4:H24	4:A:336:PX4:H20	0.52	1.82	18	1
4:A:394:PX4:H56	4:A:430:PX4:H58	0.52	1.82	4	1
4:A:375:PX4:H31	4:A:407:PX4:H41	0.52	1.81	6	1
4:A:339:PX4:H46	4:A:363:PX4:H17	0.52	1.82	9	1
4:A:368:PX4:H4	5:A:436:C3S:C13	0.52	2.35	9	1
4:A:355:PX4:H38	4:A:397:PX4:H44	0.52	1.82	10	1
4:A:369:PX4:H56	4:A:419:PX4:H54	0.52	1.80	12	1
4:A:347:PX4:H60	4:A:354:PX4:H34	0.51	1.81	1	1
4:A:369:PX4:H21	4:A:374:PX4:H60	0.51	1.82	4	1
4:A:395:PX4:H21	4:A:401:PX4:H57	0.51	1.82	9	1
4:A:405:PX4:H60	4:A:407:PX4:H68	0.51	1.82	15	1
4:A:351:PX4:H69	4:A:360:PX4:H47	0.51	1.80	18	1
4:A:368:PX4:H18	5:A:436:C3S:H691	0.51	1.81	18	1
4:A:351:PX4:C14	4:A:359:PX4:H19	0.51	2.34	19	1
4:A:307:PX4:H25	4:A:307:PX4:H59	0.51	1.81	1	1
4:A:331:PX4:H28	4:A:337:PX4:H28	0.51	1.81	3	2
4:A:332:PX4:H23	4:A:348:PX4:H67	0.51	1.82	4	1
4:A:326:PX4:H52	4:A:353:PX4:H45	0.51	1.82	5	1
4:A:328:PX4:O7	4:A:347:PX4:H14	0.51	2.05	5	1
4:A:385:PX4:H46	4:A:415:PX4:H14	0.51	1.81	15	2
4:A:394:PX4:H26	4:A:401:PX4:H55	0.51	1.82	5	1
4:A:310:PX4:H51	4:A:311:PX4:H20	0.51	1.82	10	1
4:A:393:PX4:H14	4:A:419:PX4:O5	0.51	2.06	11	1
4:A:330:PX4:H24	4:A:337:PX4:H22	0.51	1.83	14	1
4:A:412:PX4:H61	4:A:424:PX4:H57	0.51	1.82	16	1
4:A:388:PX4:H22	4:A:396:PX4:H44	0.51	1.81	18	1
1:A:156:LEU:HD12	1:A:178:TRP:CH2	0.51	2.41	2	1
4:A:335:PX4:H58	4:A:347:PX4:H63	0.51	1.80	2	1
4:A:316:PX4:H25	4:A:352:PX4:H27	0.51	1.82	7	1
4:A:386:PX4:H10	4:A:417:PX4:O6	0.51	2.05	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:323:PX4:H49	4:A:360:PX4:H23	0.51	1.83	9	1
4:A:357:PX4:H17	4:A:363:PX4:H25	0.51	1.82	9	1
4:A:339:PX4:H71	4:A:363:PX4:H35	0.51	1.81	11	1
4:A:396:PX4:H24	4:A:407:PX4:H17	0.51	1.81	13	1
4:A:409:PX4:H36	4:A:425:PX4:H39	0.51	1.82	16	1
4:A:307:PX4:O2	4:A:332:PX4:H8	0.51	2.05	17	1
4:A:376:PX4:H21	4:A:383:PX4:H27	0.51	1.80	17	1
4:A:387:PX4:H62	4:A:404:PX4:H35	0.51	1.82	6	1
1:A:114:ASN:OD1	4:A:348:PX4:H3	0.51	2.05	19	3
4:A:372:PX4:C2	4:A:410:PX4:H15	0.51	2.36	10	1
4:A:368:PX4:H7	4:A:368:PX4:H14	0.51	1.83	3	1
1:A:98:ARG:O	4:A:334:PX4:H6	0.51	2.06	4	1
4:A:307:PX4:H21	4:A:322:PX4:H46	0.51	1.82	4	1
4:A:321:PX4:H41	4:A:375:PX4:H39	0.51	1.81	10	1
4:A:428:PX4:H28	4:A:429:PX4:H27	0.51	1.83	10	1
4:A:322:PX4:H67	4:A:369:PX4:H43	0.51	1.81	11	1
4:A:398:PX4:H29	4:A:411:PX4:H53	0.51	1.81	11	1
4:A:409:PX4:H43	4:A:428:PX4:H53	0.51	1.83	13	1
4:A:333:PX4:H13	4:A:334:PX4:O8	0.51	2.05	15	1
4:A:307:PX4:H13	4:A:322:PX4:H15	0.51	1.81	3	1
4:A:362:PX4:H28	4:A:364:PX4:H57	0.51	1.83	4	1
4:A:385:PX4:H47	4:A:415:PX4:H21	0.51	1.82	6	1
4:A:386:PX4:H31	4:A:386:PX4:H63	0.51	1.83	7	1
4:A:322:PX4:H52	4:A:337:PX4:H52	0.51	1.82	9	1
4:A:334:PX4:H65	4:A:426:PX4:H60	0.51	1.81	9	1
4:A:309:PX4:H39	4:A:323:PX4:H41	0.51	1.82	14	1
4:A:316:PX4:C8	4:A:352:PX4:H19	0.51	2.32	17	1
4:A:306:PX4:H41	4:A:358:PX4:H68	0.51	1.82	18	1
4:A:374:PX4:H36	4:A:418:PX4:H24	0.51	1.82	18	1
4:A:404:PX4:H57	4:A:415:PX4:H53	0.51	1.82	2	1
4:A:306:PX4:H31	4:A:358:PX4:H17	0.51	1.82	7	1
4:A:334:PX4:H39	4:A:340:PX4:H32	0.51	1.81	7	1
4:A:382:PX4:H17	4:A:423:PX4:H25	0.51	1.82	7	1
4:A:318:PX4:H23	4:A:339:PX4:H29	0.51	1.82	14	1
4:A:325:PX4:H62	4:A:355:PX4:H66	0.51	1.80	17	1
4:A:328:PX4:O4	4:A:347:PX4:H14	0.51	2.06	19	1
4:A:342:PX4:H40	4:A:345:PX4:H66	0.51	1.82	19	1
4:A:340:PX4:H14	4:A:340:PX4:H7	0.51	1.80	1	1
4:A:365:PX4:H17	4:A:383:PX4:H21	0.51	1.82	1	1
4:A:373:PX4:H23	4:A:426:PX4:H47	0.51	1.83	1	1
4:A:382:PX4:H28	4:A:385:PX4:H54	0.51	1.82	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H20	4:A:398:PX4:H47	0.51	1.81	7	1
4:A:406:PX4:H53	4:A:414:PX4:H21	0.51	1.82	7	1
4:A:375:PX4:H26	4:A:392:PX4:H36	0.51	1.82	8	1
4:A:428:PX4:H28	4:A:429:PX4:H32	0.51	1.82	13	1
4:A:397:PX4:H20	4:A:411:PX4:H70	0.51	1.81	16	1
4:A:348:PX4:H45	4:A:407:PX4:H41	0.51	1.82	1	1
4:A:408:PX4:H57	4:A:414:PX4:H48	0.51	1.83	3	1
4:A:332:PX4:H16	4:A:348:PX4:H11	0.51	1.83	7	1
4:A:394:PX4:H71	4:A:402:PX4:H72	0.51	1.83	9	1
4:A:414:PX4:H46	4:A:426:PX4:H19	0.51	1.81	10	1
4:A:381:PX4:H32	4:A:394:PX4:H57	0.51	1.81	14	1
4:A:375:PX4:H10	4:A:375:PX4:H14	0.51	1.83	15	1
4:A:325:PX4:H23	4:A:355:PX4:H17	0.51	1.82	17	1
4:A:344:PX4:H71	4:A:393:PX4:H63	0.51	1.81	17	1
4:A:399:PX4:H35	4:A:424:PX4:H28	0.51	1.83	1	1
4:A:348:PX4:H23	4:A:359:PX4:H21	0.51	1.83	2	1
4:A:353:PX4:H49	4:A:361:PX4:H25	0.51	1.82	8	1
4:A:324:PX4:H33	4:A:324:PX4:H61	0.51	1.82	9	1
4:A:323:PX4:H21	4:A:353:PX4:H20	0.51	1.83	10	1
4:A:387:PX4:H57	4:A:418:PX4:H58	0.51	1.83	20	1
4:A:400:PX4:O5	4:A:401:PX4:H49	0.51	2.05	20	1
4:A:400:PX4:H1	4:A:401:PX4:O2	0.51	2.06	20	1
4:A:321:PX4:H51	4:A:342:PX4:H28	0.50	1.81	2	1
4:A:322:PX4:H17	4:A:344:PX4:H18	0.50	1.82	4	1
4:A:414:PX4:H32	5:A:432:C3S:H693	0.50	1.82	10	1
4:A:327:PX4:H43	4:A:369:PX4:H38	0.50	1.83	12	1
4:A:318:PX4:H50	4:A:363:PX4:H30	0.50	1.84	3	1
4:A:308:PX4:H52	4:A:320:PX4:H25	0.50	1.83	7	1
4:A:374:PX4:H23	4:A:423:PX4:H53	0.50	1.83	14	1
4:A:338:PX4:H33	4:A:344:PX4:H67	0.50	1.82	18	1
4:A:371:PX4:H72	4:A:373:PX4:H45	0.50	1.83	18	1
4:A:412:PX4:H47	4:A:412:PX4:H8	0.50	1.82	20	1
4:A:332:PX4:H4	4:A:348:PX4:H49	0.50	1.84	2	1
4:A:318:PX4:H56	4:A:357:PX4:H23	0.50	1.82	4	1
4:A:327:PX4:H40	4:A:348:PX4:H62	0.50	1.82	7	1
4:A:345:PX4:H32	4:A:349:PX4:H63	0.50	1.83	8	1
4:A:342:PX4:O1	4:A:358:PX4:H12	0.50	2.06	12	1
4:A:343:PX4:H56	4:A:350:PX4:H17	0.50	1.82	13	1
4:A:387:PX4:O3	4:A:416:PX4:H12	0.50	2.06	15	1
4:A:312:PX4:H22	4:A:346:PX4:H52	0.50	1.82	17	1
4:A:354:PX4:H64	4:A:419:PX4:H45	0.50	1.82	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:H45	4:A:408:PX4:H61	0.50	1.83	19	1
4:A:323:PX4:H19	4:A:349:PX4:H16	0.50	1.84	3	1
4:A:310:PX4:H59	4:A:311:PX4:H33	0.50	1.83	4	1
4:A:420:PX4:O6	4:A:422:PX4:H16	0.50	2.07	5	1
4:A:386:PX4:O8	4:A:402:PX4:H14	0.50	2.05	6	1
4:A:383:PX4:H16	4:A:396:PX4:H46	0.50	1.82	8	1
4:A:386:PX4:O5	4:A:402:PX4:H14	0.50	2.07	9	1
4:A:403:PX4:H26	4:A:421:PX4:H55	0.50	1.82	9	1
4:A:336:PX4:H26	4:A:360:PX4:H59	0.50	1.82	11	1
4:A:305:PX4:H59	4:A:339:PX4:H41	0.50	1.82	19	1
4:A:324:PX4:H61	4:A:386:PX4:H70	0.50	1.82	2	1
4:A:315:PX4:H60	4:A:332:PX4:H17	0.50	1.84	4	1
4:A:336:PX4:H49	4:A:354:PX4:H51	0.50	1.82	4	1
4:A:369:PX4:H57	4:A:419:PX4:H21	0.50	1.83	5	1
4:A:385:PX4:H17	5:A:433:C3S:C13	0.50	2.37	6	1
4:A:336:PX4:H17	4:A:352:PX4:H11	0.50	1.81	8	1
4:A:327:PX4:H69	4:A:348:PX4:H50	0.50	1.82	12	1
1:A:156:LEU:H	1:A:156:LEU:HD23	0.50	1.66	4	1
4:A:319:PX4:H25	4:A:341:PX4:H71	0.50	1.84	4	1
4:A:427:PX4:O6	4:A:427:PX4:H2	0.50	2.06	8	2
4:A:404:PX4:H36	4:A:417:PX4:H25	0.50	1.82	8	1
4:A:311:PX4:H62	4:A:329:PX4:H64	0.50	1.82	9	1
4:A:322:PX4:H69	4:A:337:PX4:H39	0.50	1.82	16	1
4:A:346:PX4:H35	4:A:349:PX4:H40	0.50	1.82	16	1
4:A:379:PX4:H18	4:A:425:PX4:O6	0.50	2.07	17	1
4:A:357:PX4:H72	4:A:363:PX4:H33	0.50	1.82	18	1
4:A:370:PX4:O6	4:A:383:PX4:H9	0.50	2.07	18	1
4:A:350:PX4:H72	4:A:402:PX4:H39	0.50	1.83	20	1
4:A:367:PX4:H30	4:A:367:PX4:H62	0.50	1.83	2	1
4:A:375:PX4:H20	4:A:427:PX4:H17	0.50	1.84	3	1
4:A:323:PX4:H14	4:A:353:PX4:O8	0.50	2.07	6	1
4:A:387:PX4:H3	4:A:416:PX4:O2	0.50	2.07	6	1
4:A:416:PX4:O6	4:A:416:PX4:H2	0.50	2.07	9	1
4:A:340:PX4:O6	4:A:350:PX4:H8	0.50	2.06	13	2
4:A:375:PX4:H57	4:A:405:PX4:H25	0.50	1.83	13	1
4:A:394:PX4:H31	4:A:400:PX4:H52	0.50	1.83	14	1
4:A:386:PX4:H49	4:A:421:PX4:H66	0.50	1.84	1	1
4:A:400:PX4:H62	4:A:405:PX4:H53	0.50	1.83	1	1
4:A:404:PX4:H48	4:A:415:PX4:H17	0.50	1.84	2	1
4:A:392:PX4:O2	4:A:425:PX4:H14	0.50	2.06	5	1
4:A:393:PX4:H2	4:A:416:PX4:H14	0.50	1.82	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:409:PX4:O8	4:A:428:PX4:H7	0.50	2.06	9	1
4:A:307:PX4:H56	4:A:348:PX4:H58	0.50	1.84	10	1
4:A:376:PX4:H61	4:A:390:PX4:H48	0.50	1.83	10	1
4:A:420:PX4:H34	4:A:422:PX4:H61	0.50	1.83	10	1
4:A:370:PX4:H23	4:A:383:PX4:H48	0.50	1.84	18	1
4:A:386:PX4:H24	4:A:402:PX4:H16	0.50	1.83	1	1
4:A:323:PX4:H41	4:A:349:PX4:H22	0.50	1.82	3	1
4:A:371:PX4:O3	4:A:373:PX4:H18	0.50	2.06	7	1
4:A:313:PX4:H15	4:A:355:PX4:H47	0.50	1.84	9	1
4:A:309:PX4:H50	4:A:347:PX4:H20	0.50	1.83	13	1
4:A:409:PX4:H29	4:A:428:PX4:H12	0.50	1.82	14	1
4:A:388:PX4:H32	4:A:396:PX4:H35	0.50	1.82	15	1
4:A:373:PX4:H47	4:A:406:PX4:H53	0.50	1.84	19	1
4:A:307:PX4:H55	4:A:307:PX4:H21	0.49	1.83	1	1
4:A:333:PX4:H42	4:A:364:PX4:H39	0.49	1.84	1	1
4:A:393:PX4:O5	4:A:419:PX4:H19	0.49	2.07	1	1
4:A:344:PX4:H9	4:A:354:PX4:O6	0.49	2.07	4	1
4:A:365:PX4:H43	4:A:413:PX4:H41	0.49	1.84	4	1
4:A:394:PX4:H16	4:A:395:PX4:H49	0.49	1.84	5	1
4:A:389:PX4:H16	4:A:399:PX4:H52	0.49	1.83	7	1
4:A:305:PX4:H60	4:A:312:PX4:H63	0.49	1.83	13	1
4:A:312:PX4:H22	4:A:346:PX4:C27	0.49	2.37	17	1
4:A:395:PX4:H48	4:A:401:PX4:H54	0.49	1.83	17	1
1:A:224:PHE:O	4:A:315:PX4:H5	0.49	2.07	1	2
4:A:408:PX4:H55	4:A:427:PX4:H50	0.49	1.82	2	1
4:A:340:PX4:H17	4:A:356:PX4:H53	0.49	1.83	4	2
4:A:378:PX4:H9	4:A:388:PX4:O1	0.49	2.07	6	1
4:A:320:PX4:H56	5:A:432:C3S:H41	0.49	1.84	8	1
4:A:366:PX4:H62	4:A:403:PX4:H57	0.49	1.85	8	1
4:A:365:PX4:H38	4:A:376:PX4:H25	0.49	1.84	9	1
4:A:367:PX4:H22	4:A:399:PX4:H15	0.49	1.84	9	1
4:A:394:PX4:H53	4:A:395:PX4:H50	0.49	1.84	9	1
4:A:341:PX4:H17	4:A:341:PX4:H6	0.49	1.85	12	1
4:A:341:PX4:H23	4:A:362:PX4:H26	0.49	1.82	16	1
4:A:306:PX4:H69	4:A:316:PX4:H28	0.49	1.82	17	1
4:A:307:PX4:H54	4:A:344:PX4:H49	0.49	1.84	20	1
4:A:429:PX4:H14	4:A:429:PX4:H13	0.49	1.83	20	1
4:A:313:PX4:H65	4:A:325:PX4:H56	0.49	1.82	1	1
4:A:310:PX4:H36	4:A:364:PX4:H38	0.49	1.84	6	1
4:A:308:PX4:H29	4:A:315:PX4:H39	0.49	1.84	13	1
4:A:376:PX4:H60	4:A:390:PX4:H64	0.49	1.83	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:322:PX4:H69	4:A:327:PX4:H63	0.49	1.82	14	1
4:A:378:PX4:H38	4:A:426:PX4:H39	0.49	1.83	17	1
4:A:326:PX4:H36	4:A:330:PX4:H32	0.49	1.83	19	1
4:A:337:PX4:H53	4:A:337:PX4:H32	0.49	1.84	19	1
4:A:382:PX4:H24	4:A:423:PX4:H31	0.49	1.83	20	1
4:A:366:PX4:H30	4:A:414:PX4:H70	0.49	1.84	5	1
4:A:369:PX4:H53	4:A:419:PX4:H48	0.49	1.84	5	1
4:A:314:PX4:H57	4:A:336:PX4:H70	0.49	1.83	6	1
4:A:406:PX4:H20	4:A:410:PX4:H49	0.49	1.83	6	1
4:A:368:PX4:H49	4:A:414:PX4:H23	0.49	1.85	9	1
4:A:420:PX4:O8	4:A:420:PX4:H4	0.49	2.08	9	1
4:A:402:PX4:H42	5:A:431:C3S:H502	0.49	1.85	11	1
4:A:341:PX4:H7	4:A:364:PX4:O8	0.49	2.07	15	1
4:A:320:PX4:H59	4:A:334:PX4:H51	0.49	1.83	16	1
4:A:370:PX4:H26	4:A:383:PX4:H17	0.49	1.84	18	1
4:A:309:PX4:H47	4:A:328:PX4:H23	0.49	1.84	2	1
4:A:397:PX4:H29	4:A:412:PX4:H58	0.49	1.85	4	1
4:A:355:PX4:H16	4:A:362:PX4:H46	0.49	1.84	6	1
4:A:381:PX4:H41	4:A:394:PX4:H69	0.49	1.84	6	1
4:A:380:PX4:H25	4:A:385:PX4:H30	0.49	1.83	7	1
4:A:396:PX4:H19	4:A:407:PX4:C6	0.49	2.37	10	1
4:A:374:PX4:H29	4:A:418:PX4:H24	0.49	1.84	11	1
4:A:414:PX4:H16	5:A:436:C3S:H652	0.49	1.84	11	1
4:A:386:PX4:H30	4:A:417:PX4:H50	0.49	1.85	20	1
4:A:390:PX4:H37	4:A:419:PX4:H29	0.49	1.84	20	1
4:A:322:PX4:H53	4:A:330:PX4:H30	0.49	1.83	7	1
4:A:389:PX4:H46	4:A:400:PX4:H19	0.49	1.85	9	1
4:A:317:PX4:H61	4:A:330:PX4:H39	0.49	1.85	14	1
4:A:307:PX4:H41	4:A:374:PX4:H29	0.49	1.85	16	1
4:A:330:PX4:H67	4:A:331:PX4:H36	0.49	1.83	1	1
4:A:305:PX4:H53	4:A:311:PX4:H26	0.49	1.85	2	1
4:A:308:PX4:H27	4:A:320:PX4:H17	0.49	1.83	3	1
4:A:308:PX4:H3	4:A:334:PX4:O6	0.49	2.08	3	1
4:A:320:PX4:H50	4:A:334:PX4:H49	0.49	1.84	3	1
4:A:368:PX4:H34	4:A:368:PX4:H69	0.49	1.85	3	2
4:A:307:PX4:H22	4:A:331:PX4:H27	0.49	1.84	4	1
4:A:316:PX4:H25	4:A:321:PX4:H20	0.49	1.84	5	1
4:A:307:PX4:H21	4:A:322:PX4:H17	0.49	1.84	7	1
4:A:428:PX4:H14	4:A:429:PX4:O3	0.49	2.08	7	1
4:A:375:PX4:H48	4:A:392:PX4:H22	0.49	1.83	13	1
4:A:375:PX4:H67	4:A:379:PX4:H41	0.49	1.83	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:308:PX4:H43	4:A:343:PX4:H67	0.49	1.83	16	1
4:A:338:PX4:H15	4:A:351:PX4:H2	0.49	1.84	20	1
4:A:343:PX4:H48	4:A:356:PX4:C26	0.49	2.38	4	1
4:A:370:PX4:H35	4:A:400:PX4:H60	0.49	1.83	6	1
4:A:388:PX4:H50	4:A:391:PX4:H47	0.49	1.83	7	1
4:A:342:PX4:H72	4:A:377:PX4:H44	0.49	1.83	11	1
4:A:409:PX4:H34	4:A:428:PX4:O6	0.49	2.08	13	1
4:A:373:PX4:H47	4:A:406:PX4:H49	0.49	1.85	19	1
4:A:394:PX4:H40	4:A:407:PX4:H28	0.49	1.85	20	1
4:A:308:PX4:H70	4:A:418:PX4:H43	0.49	1.83	1	1
4:A:308:PX4:H15	4:A:326:PX4:H46	0.49	1.85	2	1
4:A:370:PX4:H69	4:A:374:PX4:H64	0.49	1.84	2	1
4:A:309:PX4:H6	4:A:351:PX4:H20	0.49	1.85	3	1
4:A:310:PX4:H46	4:A:333:PX4:H54	0.49	1.85	3	1
4:A:353:PX4:H19	4:A:361:PX4:H49	0.49	1.84	4	1
4:A:305:PX4:O2	4:A:339:PX4:H2	0.49	2.08	8	1
4:A:394:PX4:H22	4:A:400:PX4:H46	0.49	1.83	20	2
4:A:373:PX4:H21	4:A:406:PX4:H53	0.49	1.84	18	1
4:A:374:PX4:H36	4:A:382:PX4:H54	0.49	1.82	20	1
1:A:222:GLN:O	4:A:317:PX4:H5	0.49	2.08	2	1
4:A:365:PX4:H40	4:A:430:PX4:H68	0.49	1.85	2	1
4:A:365:PX4:O6	4:A:369:PX4:H13	0.49	2.08	2	1
4:A:306:PX4:H69	4:A:342:PX4:H35	0.49	1.84	3	1
4:A:346:PX4:H25	5:A:431:C3S:H41	0.49	1.85	7	1
4:A:375:PX4:H68	4:A:392:PX4:H40	0.49	1.85	13	1
4:A:324:PX4:H66	4:A:373:PX4:H34	0.49	1.85	15	1
4:A:341:PX4:H40	4:A:362:PX4:H64	0.49	1.85	16	1
4:A:374:PX4:O2	4:A:423:PX4:H3	0.49	2.08	16	1
4:A:322:PX4:H66	4:A:430:PX4:C35	0.49	2.36	17	1
4:A:343:PX4:H47	4:A:356:PX4:H51	0.49	1.82	18	1
4:A:383:PX4:H61	4:A:405:PX4:H61	0.48	1.84	1	1
4:A:325:PX4:H8	4:A:328:PX4:H49	0.48	1.83	2	1
4:A:373:PX4:H70	4:A:399:PX4:H44	0.48	1.85	5	1
4:A:423:PX4:H69	4:A:428:PX4:H63	0.48	1.85	6	1
4:A:410:PX4:H22	4:A:414:PX4:H36	0.48	1.84	7	1
4:A:378:PX4:H17	4:A:426:PX4:O6	0.48	2.07	11	1
4:A:397:PX4:H16	4:A:411:PX4:H20	0.48	1.85	12	1
4:A:314:PX4:H65	4:A:387:PX4:H42	0.48	1.84	15	1
4:A:411:PX4:H62	4:A:424:PX4:H39	0.48	1.83	15	1
4:A:322:PX4:O6	4:A:336:PX4:H11	0.48	2.08	16	1
4:A:391:PX4:H49	4:A:427:PX4:H19	0.48	1.85	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:417:PX4:H16	4:A:418:PX4:H22	0.48	1.85	8	1
4:A:345:PX4:H40	4:A:346:PX4:H38	0.48	1.84	9	1
4:A:327:PX4:H22	4:A:348:PX4:H20	0.48	1.84	11	1
4:A:397:PX4:H62	4:A:429:PX4:H58	0.48	1.84	12	1
4:A:399:PX4:H30	4:A:414:PX4:H36	0.48	1.85	12	1
4:A:325:PX4:H50	4:A:355:PX4:H55	0.48	1.84	17	1
4:A:317:PX4:H46	4:A:330:PX4:H23	0.48	1.84	20	1
4:A:388:PX4:O2	4:A:391:PX4:H15	0.48	2.07	1	1
4:A:316:PX4:H47	4:A:321:PX4:H33	0.48	1.84	4	1
4:A:403:PX4:H31	4:A:421:PX4:H69	0.48	1.86	5	1
4:A:312:PX4:H19	4:A:346:PX4:H17	0.48	1.85	7	1
4:A:341:PX4:H52	4:A:356:PX4:H23	0.48	1.85	9	1
4:A:326:PX4:H71	4:A:371:PX4:H37	0.48	1.85	11	1
4:A:369:PX4:H36	4:A:374:PX4:H61	0.48	1.85	11	1
4:A:315:PX4:H32	4:A:350:PX4:H42	0.48	1.84	12	1
4:A:308:PX4:H44	4:A:343:PX4:H66	0.48	1.85	13	1
4:A:376:PX4:H38	4:A:427:PX4:H24	0.48	1.83	14	1
4:A:385:PX4:H49	4:A:415:PX4:H20	0.48	1.83	16	1
4:A:411:PX4:H72	4:A:411:PX4:H24	0.48	1.84	16	1
4:A:368:PX4:O6	4:A:414:PX4:H14	0.48	2.08	1	1
4:A:309:PX4:H66	4:A:351:PX4:H34	0.48	1.83	2	1
4:A:388:PX4:H67	4:A:414:PX4:H63	0.48	1.84	3	1
4:A:379:PX4:O8	4:A:425:PX4:H3	0.48	2.09	4	1
4:A:382:PX4:H6	4:A:424:PX4:O6	0.48	2.08	4	1
4:A:328:PX4:H70	4:A:390:PX4:H41	0.48	1.85	5	1
1:A:102:HIS:CE1	4:A:350:PX4:H6	0.48	2.43	8	1
4:A:327:PX4:H20	4:A:348:PX4:H16	0.48	1.85	8	1
1:A:113:LEU:HD21	1:A:196:LEU:HD22	0.48	1.83	10	1
4:A:377:PX4:H49	4:A:408:PX4:H23	0.48	1.85	10	1
4:A:414:PX4:O2	4:A:426:PX4:H10	0.48	2.07	12	1
4:A:382:PX4:O4	4:A:398:PX4:H17	0.48	2.07	14	1
4:A:374:PX4:H9	4:A:423:PX4:O2	0.48	2.08	1	1
4:A:333:PX4:H39	4:A:389:PX4:C36	0.48	2.39	2	1
4:A:395:PX4:H17	4:A:401:PX4:H49	0.48	1.85	2	1
4:A:305:PX4:H32	4:A:310:PX4:H57	0.48	1.85	3	1
4:A:393:PX4:H71	4:A:429:PX4:H43	0.48	1.83	5	1
4:A:384:PX4:H34	4:A:389:PX4:H56	0.48	1.85	6	1
4:A:397:PX4:H64	4:A:423:PX4:H62	0.48	1.85	8	1
4:A:309:PX4:H24	4:A:345:PX4:H67	0.48	1.84	9	1
4:A:405:PX4:H59	4:A:407:PX4:H60	0.48	1.85	9	1
4:A:315:PX4:H60	4:A:332:PX4:H69	0.48	1.85	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H24	4:A:351:PX4:H72	0.48	1.85	12	1
4:A:419:PX4:H31	4:A:429:PX4:H26	0.48	1.84	15	1
4:A:321:PX4:H58	4:A:342:PX4:H37	0.48	1.84	18	1
4:A:321:PX4:H50	4:A:342:PX4:H34	0.48	1.86	19	1
4:A:328:PX4:H64	4:A:360:PX4:H22	0.48	1.86	20	1
4:A:324:PX4:H52	5:A:432:C3S:H322	0.48	1.84	1	1
1:A:128:VAL:HG21	4:A:343:PX4:H63	0.48	1.84	3	1
4:A:309:PX4:H26	4:A:359:PX4:H22	0.48	1.85	8	1
4:A:312:PX4:H69	5:A:431:C3S:H693	0.48	1.85	12	1
4:A:323:PX4:H52	4:A:328:PX4:H16	0.48	1.83	12	1
4:A:389:PX4:H37	4:A:399:PX4:H66	0.48	1.84	13	1
4:A:327:PX4:H15	4:A:348:PX4:H16	0.48	1.84	16	1
4:A:365:PX4:H67	4:A:407:PX4:H61	0.48	1.86	16	1
4:A:317:PX4:H35	4:A:361:PX4:H29	0.48	1.85	17	1
4:A:337:PX4:H23	4:A:355:PX4:H27	0.48	1.84	17	1
4:A:346:PX4:H45	4:A:402:PX4:H35	0.48	1.83	17	1
4:A:352:PX4:C20	4:A:375:PX4:H44	0.48	2.33	18	1
4:A:374:PX4:H51	4:A:430:PX4:H53	0.48	1.85	19	1
4:A:325:PX4:H63	4:A:329:PX4:H52	0.48	1.84	20	1
4:A:374:PX4:H20	4:A:423:PX4:H49	0.48	1.85	20	1
4:A:367:PX4:H17	4:A:367:PX4:O8	0.48	2.07	2	1
1:A:99:ASP:O	4:A:334:PX4:H11	0.48	2.09	3	1
4:A:371:PX4:H20	4:A:400:PX4:H41	0.48	1.84	3	1
4:A:376:PX4:H63	4:A:396:PX4:H64	0.48	1.85	3	1
4:A:322:PX4:H42	4:A:331:PX4:H41	0.48	1.84	4	1
4:A:343:PX4:H20	4:A:352:PX4:H54	0.48	1.85	6	1
4:A:379:PX4:H59	4:A:413:PX4:H22	0.48	1.85	8	1
1:A:15:ALA:HB1	1:A:39:LEU:HD21	0.48	1.86	9	1
4:A:313:PX4:O7	4:A:329:PX4:H15	0.48	2.09	10	1
4:A:392:PX4:H50	4:A:425:PX4:H49	0.48	1.86	11	1
4:A:320:PX4:H42	4:A:350:PX4:H35	0.48	1.85	12	1
1:A:158:HIS:CD2	1:A:171:HIS:HB2	0.48	2.43	13	1
4:A:400:PX4:H20	4:A:401:PX4:H47	0.48	1.86	13	1
4:A:314:PX4:H14	4:A:336:PX4:O6	0.48	2.08	14	1
4:A:391:PX4:H34	4:A:408:PX4:H66	0.48	1.86	15	1
4:A:341:PX4:O8	4:A:341:PX4:H3	0.48	2.09	16	1
4:A:328:PX4:H37	4:A:345:PX4:H27	0.48	1.86	18	1
4:A:314:PX4:H19	4:A:336:PX4:H29	0.48	1.86	1	1
1:A:156:LEU:H	1:A:156:LEU:CD2	0.48	2.21	4	1
4:A:399:PX4:H35	4:A:424:PX4:H31	0.48	1.85	5	1
4:A:429:PX4:H63	4:A:430:PX4:H33	0.48	1.85	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:O8	4:A:405:PX4:H11	0.48	2.08	12	1
4:A:367:PX4:H69	4:A:389:PX4:H31	0.48	1.84	13	1
4:A:338:PX4:C10	4:A:344:PX4:H53	0.48	2.39	17	1
4:A:327:PX4:H32	4:A:332:PX4:H56	0.48	1.85	18	1
4:A:367:PX4:H18	4:A:399:PX4:O7	0.48	2.09	18	1
4:A:340:PX4:H13	5:A:432:C3S:O4	0.48	2.08	19	1
1:A:128:VAL:HG23	4:A:343:PX4:H39	0.48	1.84	1	1
4:A:396:PX4:H19	4:A:407:PX4:H17	0.48	1.85	7	2
4:A:308:PX4:H59	4:A:417:PX4:H40	0.48	1.84	3	1
4:A:376:PX4:H21	4:A:383:PX4:H30	0.48	1.86	4	1
4:A:343:PX4:H42	4:A:384:PX4:H43	0.48	1.85	7	1
4:A:381:PX4:H58	4:A:430:PX4:H65	0.48	1.86	7	1
4:A:377:PX4:H16	5:A:436:C3S:H442	0.48	1.85	9	1
4:A:373:PX4:H41	4:A:401:PX4:H34	0.48	1.86	10	1
4:A:327:PX4:H19	4:A:359:PX4:H30	0.48	1.85	13	1
4:A:377:PX4:H17	4:A:408:PX4:O1	0.48	2.08	15	1
4:A:392:PX4:H20	4:A:407:PX4:H18	0.48	1.85	15	1
1:A:104:THR:C	1:A:108:LEU:HD12	0.48	2.34	19	1
4:A:369:PX4:H23	4:A:374:PX4:H54	0.48	1.86	19	1
4:A:320:PX4:H71	4:A:350:PX4:H46	0.48	1.84	20	1
4:A:378:PX4:H54	4:A:402:PX4:H22	0.48	1.84	20	1
4:A:326:PX4:H33	4:A:404:PX4:H39	0.48	1.85	3	1
4:A:387:PX4:H6	4:A:415:PX4:O3	0.48	2.08	7	1
4:A:319:PX4:H54	4:A:356:PX4:H16	0.48	1.84	8	1
4:A:320:PX4:H8	4:A:326:PX4:H17	0.48	1.86	8	1
1:A:15:ALA:HB1	1:A:39:LEU:CD2	0.48	2.39	9	1
4:A:328:PX4:H57	4:A:347:PX4:H22	0.48	1.86	12	1
4:A:307:PX4:H36	4:A:331:PX4:H35	0.48	1.86	14	1
4:A:322:PX4:H24	4:A:331:PX4:H51	0.48	1.85	14	1
4:A:353:PX4:H20	4:A:361:PX4:H48	0.48	1.84	15	1
4:A:342:PX4:H44	4:A:405:PX4:H37	0.48	1.86	16	1
4:A:316:PX4:H63	4:A:352:PX4:H68	0.48	1.86	17	1
4:A:367:PX4:H46	4:A:384:PX4:H5	0.48	1.86	17	1
4:A:374:PX4:H23	4:A:397:PX4:H67	0.48	1.84	17	1
4:A:374:PX4:O2	4:A:397:PX4:H15	0.48	2.09	17	1
4:A:378:PX4:H35	4:A:403:PX4:H39	0.48	1.85	20	1
4:A:398:PX4:H2	5:A:435:C3S:O2	0.47	2.08	1	1
4:A:322:PX4:H50	4:A:331:PX4:H19	0.47	1.85	3	1
4:A:375:PX4:H35	4:A:391:PX4:H26	0.47	1.84	8	1
4:A:400:PX4:O4	4:A:401:PX4:H1	0.47	2.09	9	1
4:A:309:PX4:H46	4:A:349:PX4:H54	0.47	1.84	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:PHE:HB2	4:A:348:PX4:H1	0.47	1.84	12	1
4:A:334:PX4:H63	5:A:431:C3S:H48	0.47	1.86	12	1
4:A:400:PX4:H26	4:A:405:PX4:H26	0.47	1.85	15	1
4:A:348:PX4:H63	4:A:350:PX4:H40	0.47	1.85	16	1
4:A:319:PX4:H59	4:A:341:PX4:H57	0.47	1.85	17	1
4:A:383:PX4:H57	4:A:394:PX4:H37	0.47	1.85	1	1
4:A:385:PX4:H15	4:A:415:PX4:H18	0.47	1.86	1	1
4:A:399:PX4:H18	4:A:424:PX4:H13	0.47	1.86	4	1
4:A:399:PX4:H19	5:A:435:C3S:H42	0.47	1.85	4	1
4:A:326:PX4:H55	4:A:361:PX4:H57	0.47	1.84	5	1
4:A:321:PX4:H59	4:A:357:PX4:H42	0.47	1.85	8	1
4:A:305:PX4:O6	4:A:311:PX4:H12	0.47	2.09	12	1
4:A:378:PX4:H63	4:A:426:PX4:H26	0.47	1.84	16	1
4:A:407:PX4:O4	4:A:427:PX4:H1	0.47	2.09	17	1
4:A:417:PX4:H3	4:A:418:PX4:O6	0.47	2.07	19	1
4:A:383:PX4:H52	4:A:395:PX4:H59	0.47	1.86	1	1
4:A:385:PX4:H46	4:A:415:PX4:H46	0.47	1.86	1	1
4:A:310:PX4:H19	4:A:311:PX4:H47	0.47	1.86	4	1
4:A:343:PX4:H19	4:A:352:PX4:H55	0.47	1.86	5	1
4:A:387:PX4:H32	4:A:393:PX4:H50	0.47	1.85	5	1
4:A:343:PX4:H28	4:A:352:PX4:H58	0.47	1.86	8	1
4:A:370:PX4:H56	4:A:381:PX4:H47	0.47	1.84	10	1
4:A:382:PX4:H53	5:A:435:C3S:H601	0.47	1.87	12	1
4:A:366:PX4:H53	4:A:403:PX4:H49	0.47	1.86	14	1
4:A:347:PX4:H15	4:A:351:PX4:O8	0.47	2.09	1	1
4:A:409:PX4:H6	5:A:434:C3S:H91	0.47	1.84	2	1
4:A:367:PX4:H64	4:A:412:PX4:H26	0.47	1.86	9	1
4:A:368:PX4:H11	4:A:406:PX4:O1	0.47	2.10	9	1
4:A:336:PX4:H52	4:A:354:PX4:H21	0.47	1.85	10	1
4:A:340:PX4:H70	4:A:406:PX4:H68	0.47	1.86	12	1
4:A:387:PX4:H32	4:A:416:PX4:H60	0.47	1.86	12	1
4:A:346:PX4:H24	4:A:358:PX4:H24	0.47	1.86	14	1
4:A:412:PX4:H17	4:A:424:PX4:H53	0.47	1.87	19	1
4:A:397:PX4:H51	4:A:430:PX4:H20	0.47	1.87	20	1
4:A:368:PX4:C13	4:A:391:PX4:H44	0.47	2.38	1	1
4:A:327:PX4:H27	4:A:351:PX4:H6	0.47	1.85	3	1
4:A:310:PX4:H54	4:A:333:PX4:H48	0.47	1.85	5	1
4:A:384:PX4:H33	4:A:405:PX4:H37	0.47	1.85	5	1
4:A:345:PX4:H65	4:A:359:PX4:H27	0.47	1.87	6	1
4:A:316:PX4:H67	4:A:350:PX4:H55	0.47	1.86	9	1
4:A:328:PX4:H21	4:A:347:PX4:H23	0.47	1.86	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H56	4:A:405:PX4:H27	0.47	1.87	14	1
4:A:371:PX4:H10	4:A:426:PX4:H50	0.47	1.86	17	1
4:A:368:PX4:H69	4:A:372:PX4:H39	0.47	1.85	18	1
4:A:324:PX4:H61	4:A:406:PX4:H72	0.47	1.85	19	1
4:A:412:PX4:H49	4:A:424:PX4:H51	0.47	1.86	19	1
4:A:342:PX4:C22	4:A:405:PX4:H69	0.47	2.40	3	1
4:A:376:PX4:H5	4:A:390:PX4:O8	0.47	2.10	4	1
4:A:382:PX4:H37	4:A:398:PX4:H39	0.47	1.86	4	1
4:A:334:PX4:H56	4:A:334:PX4:H29	0.47	1.84	9	1
4:A:323:PX4:H63	4:A:328:PX4:C30	0.47	2.40	11	1
4:A:379:PX4:H24	4:A:384:PX4:H53	0.47	1.84	13	1
4:A:398:PX4:H20	4:A:411:PX4:H46	0.47	1.86	14	1
4:A:338:PX4:H31	4:A:354:PX4:O8	0.47	2.10	17	1
4:A:319:PX4:H71	4:A:356:PX4:H32	0.47	1.85	19	1
4:A:327:PX4:O2	4:A:351:PX4:H4	0.47	2.10	19	1
4:A:370:PX4:H49	4:A:394:PX4:H54	0.47	1.86	19	1
4:A:351:PX4:H43	4:A:392:PX4:H41	0.47	1.87	2	1
4:A:384:PX4:H30	4:A:405:PX4:H41	0.47	1.85	2	1
4:A:407:PX4:H10	4:A:427:PX4:O6	0.47	2.10	2	1
1:A:124:PHE:O	4:A:348:PX4:H2	0.47	2.10	18	3
4:A:333:PX4:H34	4:A:340:PX4:H40	0.47	1.85	4	1
4:A:412:PX4:H10	4:A:412:PX4:O2	0.47	2.10	4	1
4:A:423:PX4:H13	4:A:423:PX4:H15	0.47	1.86	4	1
1:A:134:ILE:HG23	1:A:168:GLY:O	0.47	2.09	5	1
4:A:316:PX4:H43	4:A:352:PX4:H44	0.47	1.87	6	1
4:A:398:PX4:H31	5:A:435:C3S:H502	0.47	1.85	7	1
4:A:378:PX4:H40	4:A:418:PX4:H72	0.47	1.86	8	1
4:A:387:PX4:H27	4:A:416:PX4:H52	0.47	1.87	8	1
4:A:323:PX4:H67	4:A:328:PX4:H58	0.47	1.85	11	1
4:A:309:PX4:H38	4:A:345:PX4:H57	0.47	1.86	12	1
4:A:307:PX4:H31	4:A:344:PX4:H33	0.47	1.86	14	1
4:A:317:PX4:H30	4:A:326:PX4:H20	0.47	1.84	16	1
4:A:327:PX4:H66	4:A:347:PX4:H42	0.47	1.86	17	1
4:A:318:PX4:H16	4:A:357:PX4:H35	0.47	1.87	18	1
4:A:384:PX4:H52	5:A:434:C3S:H261	0.47	1.85	20	1
4:A:335:PX4:H27	4:A:363:PX4:H57	0.47	1.85	4	1
4:A:419:PX4:H30	4:A:429:PX4:H37	0.47	1.87	4	1
4:A:348:PX4:H27	4:A:359:PX4:H16	0.47	1.87	10	2
4:A:325:PX4:H55	4:A:329:PX4:H55	0.47	1.85	7	1
4:A:385:PX4:H19	5:A:433:C3S:H91	0.47	1.85	7	1
1:A:71:ASP:OD1	1:A:198:HIS:CE1	0.47	2.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:374:PX4:H13	4:A:423:PX4:O8	0.47	2.09	14	1
4:A:392:PX4:H21	4:A:427:PX4:H60	0.47	1.86	14	1
4:A:317:PX4:H43	4:A:361:PX4:H59	0.47	1.86	16	1
4:A:319:PX4:O1	4:A:352:PX4:H3	0.47	2.09	17	1
4:A:308:PX4:H61	4:A:326:PX4:H57	0.47	1.87	20	1
4:A:343:PX4:H65	4:A:350:PX4:H25	0.47	1.85	1	1
4:A:373:PX4:H46	4:A:410:PX4:H10	0.47	1.87	5	1
4:A:380:PX4:H50	4:A:420:PX4:H22	0.47	1.87	7	1
4:A:334:PX4:H60	4:A:334:PX4:H33	0.47	1.86	9	1
4:A:312:PX4:H68	4:A:402:PX4:H38	0.47	1.87	10	1
4:A:404:PX4:H35	4:A:418:PX4:H38	0.47	1.84	10	1
4:A:306:PX4:H20	4:A:358:PX4:H15	0.47	1.87	11	1
4:A:428:PX4:H63	4:A:430:PX4:H32	0.47	1.86	11	1
4:A:372:PX4:H44	4:A:426:PX4:H70	0.47	1.85	17	1
4:A:390:PX4:H36	4:A:421:PX4:H23	0.47	1.84	18	1
4:A:347:PX4:H36	4:A:413:PX4:H40	0.47	1.85	1	1
4:A:307:PX4:H34	4:A:337:PX4:H36	0.47	1.86	3	1
4:A:375:PX4:H64	4:A:384:PX4:H28	0.47	1.85	5	1
4:A:307:PX4:H46	4:A:332:PX4:H6	0.47	1.87	7	1
4:A:327:PX4:H48	4:A:338:PX4:H58	0.47	1.87	8	1
4:A:404:PX4:H36	4:A:417:PX4:C13	0.47	2.39	8	1
4:A:368:PX4:H33	4:A:388:PX4:H65	0.47	1.85	9	1
4:A:315:PX4:O6	4:A:332:PX4:H2	0.47	2.10	12	1
4:A:321:PX4:H71	4:A:357:PX4:H29	0.47	1.86	12	1
4:A:322:PX4:H47	4:A:337:PX4:H17	0.47	1.87	16	1
4:A:377:PX4:H23	4:A:408:PX4:H23	0.47	1.87	18	1
4:A:318:PX4:H16	4:A:321:PX4:H51	0.46	1.87	1	1
4:A:404:PX4:H20	4:A:418:PX4:H58	0.46	1.85	1	1
4:A:404:PX4:H20	4:A:423:PX4:H27	0.46	1.87	6	1
4:A:395:PX4:H64	4:A:395:PX4:H37	0.46	1.86	7	1
4:A:325:PX4:H10	4:A:361:PX4:O2	0.46	2.10	8	1
4:A:351:PX4:H66	4:A:387:PX4:H45	0.46	1.86	8	1
4:A:338:PX4:H43	4:A:411:PX4:H51	0.46	1.87	9	1
4:A:372:PX4:H4	4:A:410:PX4:O2	0.46	2.09	10	1
4:A:315:PX4:H19	4:A:337:PX4:H62	0.46	1.87	12	1
4:A:317:PX4:H59	4:A:337:PX4:H59	0.46	1.87	14	1
4:A:329:PX4:C17	4:A:360:PX4:H33	0.46	2.40	14	1
4:A:418:PX4:H71	4:A:421:PX4:H23	0.46	1.87	14	1
4:A:375:PX4:H51	4:A:405:PX4:H17	0.46	1.87	16	1
4:A:345:PX4:H30	4:A:349:PX4:H58	0.46	1.86	18	1
4:A:315:PX4:H70	4:A:321:PX4:H36	0.46	1.87	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:306:PX4:O8	4:A:306:PX4:H15	0.46	2.09	20	1
4:A:397:PX4:H39	4:A:424:PX4:H42	0.46	1.85	20	1
4:A:330:PX4:H35	4:A:337:PX4:H57	0.46	1.87	3	1
1:A:71:ASP:OD1	1:A:204:HIS:CD2	0.46	2.68	4	1
1:A:118:LYS:O	4:A:351:PX4:H3	0.46	2.10	5	1
4:A:370:PX4:H27	4:A:383:PX4:H51	0.46	1.85	6	1
4:A:307:PX4:H39	4:A:338:PX4:H64	0.46	1.87	8	1
4:A:308:PX4:H33	4:A:350:PX4:H58	0.46	1.86	8	1
1:A:129:TRP:HB3	4:A:316:PX4:H55	0.46	1.87	9	1
4:A:370:PX4:H38	4:A:394:PX4:H32	0.46	1.85	9	1
4:A:395:PX4:H13	4:A:401:PX4:H49	0.46	1.88	9	1
4:A:309:PX4:H29	4:A:359:PX4:H36	0.46	1.86	12	1
4:A:384:PX4:H56	4:A:392:PX4:H56	0.46	1.87	13	1
4:A:309:PX4:H22	4:A:345:PX4:H60	0.46	1.85	16	1
4:A:413:PX4:H20	4:A:429:PX4:H21	0.46	1.86	17	1
4:A:312:PX4:H43	4:A:388:PX4:H54	0.46	1.86	1	1
4:A:399:PX4:H39	4:A:424:PX4:H32	0.46	1.87	1	1
4:A:308:PX4:H15	4:A:320:PX4:H12	0.46	1.86	4	1
4:A:376:PX4:H17	4:A:388:PX4:C10	0.46	2.40	4	1
4:A:308:PX4:H41	4:A:350:PX4:H27	0.46	1.87	7	1
4:A:330:PX4:H54	4:A:362:PX4:H30	0.46	1.87	9	1
4:A:340:PX4:H13	5:A:432:C3S:H91	0.46	1.87	13	1
4:A:404:PX4:O3	4:A:404:PX4:H9	0.46	2.10	13	1
4:A:321:PX4:H58	4:A:352:PX4:H38	0.46	1.87	19	1
4:A:371:PX4:H57	4:A:389:PX4:H17	0.46	1.87	2	1
4:A:307:PX4:H3	4:A:322:PX4:O3	0.46	2.10	3	1
4:A:409:PX4:H22	4:A:412:PX4:H20	0.46	1.88	3	1
4:A:371:PX4:H47	4:A:389:PX4:H46	0.46	1.87	8	1
4:A:325:PX4:H34	4:A:362:PX4:H68	0.46	1.87	9	1
4:A:370:PX4:H34	4:A:383:PX4:H33	0.46	1.86	13	1
4:A:325:PX4:H37	4:A:430:PX4:H43	0.46	1.87	15	1
4:A:400:PX4:H21	4:A:405:PX4:H19	0.46	1.87	15	1
4:A:366:PX4:H17	4:A:403:PX4:H28	0.46	1.86	18	1
4:A:328:PX4:H43	4:A:358:PX4:H36	0.46	1.88	19	1
4:A:369:PX4:H52	4:A:419:PX4:H54	0.46	1.87	20	1
4:A:350:PX4:H44	4:A:395:PX4:H29	0.46	1.86	2	1
4:A:394:PX4:H59	4:A:396:PX4:H67	0.46	1.85	2	1
4:A:313:PX4:H68	4:A:323:PX4:H57	0.46	1.85	3	1
4:A:376:PX4:H57	4:A:388:PX4:H35	0.46	1.86	4	1
4:A:371:PX4:H3	4:A:373:PX4:O1	0.46	2.10	11	1
4:A:375:PX4:H53	4:A:384:PX4:H55	0.46	1.87	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:325:PX4:H19	4:A:355:PX4:H17	0.46	1.86	16	1
4:A:328:PX4:H8	4:A:349:PX4:O8	0.46	2.10	16	1
4:A:328:PX4:H36	4:A:361:PX4:H34	0.46	1.88	16	1
4:A:417:PX4:H21	4:A:418:PX4:H32	0.46	1.86	17	1
4:A:313:PX4:H55	4:A:325:PX4:H55	0.46	1.86	20	1
4:A:338:PX4:O1	4:A:351:PX4:H7	0.46	2.11	20	1
4:A:371:PX4:H14	4:A:373:PX4:H18	0.46	1.87	20	1
4:A:306:PX4:H22	4:A:342:PX4:H15	0.46	1.88	2	1
4:A:311:PX4:H40	4:A:339:PX4:H51	0.46	1.88	2	1
4:A:327:PX4:H20	4:A:348:PX4:H20	0.46	1.87	2	1
4:A:377:PX4:H54	4:A:422:PX4:H25	0.46	1.86	3	1
4:A:313:PX4:H46	4:A:329:PX4:H17	0.46	1.88	12	1
1:A:7:MET:SD	1:A:54:LEU:HD22	0.46	2.51	13	1
4:A:370:PX4:H31	4:A:383:PX4:H51	0.46	1.87	16	1
4:A:386:PX4:H27	4:A:402:PX4:H53	0.46	1.88	18	1
4:A:398:PX4:H33	4:A:411:PX4:H54	0.46	1.88	20	1
4:A:306:PX4:H54	4:A:359:PX4:C27	0.46	2.40	4	1
4:A:325:PX4:H39	4:A:326:PX4:H25	0.46	1.88	5	1
4:A:396:PX4:H16	4:A:407:PX4:H52	0.46	1.88	5	1
4:A:316:PX4:O2	4:A:321:PX4:H11	0.46	2.11	6	1
4:A:404:PX4:O2	4:A:404:PX4:H13	0.46	2.11	6	1
4:A:306:PX4:H58	4:A:342:PX4:H36	0.46	1.88	11	1
4:A:384:PX4:O3	4:A:401:PX4:H5	0.46	2.10	12	1
4:A:340:PX4:H12	5:A:432:C3S:H91	0.46	1.88	14	1
4:A:319:PX4:H36	4:A:425:PX4:H70	0.46	1.88	17	1
4:A:336:PX4:H68	4:A:412:PX4:H37	0.46	1.87	17	1
4:A:388:PX4:H47	4:A:391:PX4:H51	0.46	1.88	17	1
4:A:429:PX4:H53	4:A:430:PX4:H20	0.46	1.88	18	1
4:A:366:PX4:H55	4:A:403:PX4:H47	0.46	1.87	20	1
4:A:320:PX4:H51	4:A:334:PX4:H15	0.46	1.87	1	1
4:A:365:PX4:H30	4:A:430:PX4:H33	0.46	1.87	2	1
4:A:366:PX4:H52	4:A:378:PX4:H26	0.46	1.87	6	1
4:A:386:PX4:O6	4:A:402:PX4:H20	0.46	2.11	7	1
4:A:318:PX4:H28	4:A:321:PX4:H54	0.46	1.87	9	1
4:A:400:PX4:H16	4:A:401:PX4:H46	0.46	1.88	10	1
4:A:324:PX4:H49	4:A:324:PX4:H24	0.46	1.88	16	1
4:A:336:PX4:H14	4:A:336:PX4:H2	0.46	1.87	16	1
4:A:338:PX4:H28	4:A:354:PX4:H48	0.46	1.88	17	1
4:A:305:PX4:H55	4:A:311:PX4:H39	0.46	1.88	18	1
1:A:222:GLN:O	4:A:317:PX4:H11	0.46	2.10	19	1
4:A:417:PX4:H7	4:A:418:PX4:H21	0.46	1.87	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PX4:O1	4:A:410:PX4:H10	0.46	2.11	10	2
4:A:305:PX4:H51	4:A:324:PX4:H72	0.46	1.88	7	1
4:A:387:PX4:H67	4:A:421:PX4:H35	0.46	1.87	8	1
1:A:111:LYS:HE3	4:A:315:PX4:H15	0.46	1.88	9	1
4:A:393:PX4:H50	4:A:419:PX4:H19	0.46	1.87	12	1
4:A:413:PX4:H49	4:A:429:PX4:H23	0.46	1.86	16	1
4:A:322:PX4:H8	4:A:337:PX4:H2	0.46	1.88	18	1
4:A:399:PX4:H26	4:A:410:PX4:H32	0.46	1.88	1	1
4:A:357:PX4:H3	4:A:363:PX4:O6	0.46	2.11	2	1
4:A:414:PX4:H9	4:A:426:PX4:O6	0.46	2.11	3	1
4:A:424:PX4:O8	4:A:424:PX4:H15	0.46	2.11	5	1
4:A:340:PX4:H63	4:A:364:PX4:H38	0.46	1.88	7	1
4:A:329:PX4:H51	4:A:355:PX4:H60	0.46	1.88	12	1
4:A:320:PX4:H59	4:A:334:PX4:H54	0.46	1.87	13	1
4:A:348:PX4:H31	4:A:359:PX4:H31	0.46	1.88	13	1
4:A:393:PX4:H27	4:A:419:PX4:H54	0.46	1.87	17	1
4:A:327:PX4:H24	4:A:348:PX4:H26	0.46	1.88	18	1
4:A:370:PX4:H60	4:A:381:PX4:H35	0.46	1.87	18	1
4:A:406:PX4:H44	4:A:410:PX4:H65	0.46	1.86	20	1
4:A:391:PX4:H60	4:A:427:PX4:H40	0.45	1.88	2	1
1:A:184:LEU:HD21	4:A:349:PX4:H12	0.45	1.87	3	1
4:A:365:PX4:H26	4:A:369:PX4:H23	0.45	1.86	3	1
4:A:367:PX4:H33	4:A:389:PX4:H30	0.45	1.88	5	1
4:A:377:PX4:H29	4:A:377:PX4:H54	0.45	1.88	5	1
4:A:322:PX4:H50	4:A:331:PX4:H20	0.45	1.86	6	1
4:A:325:PX4:H23	4:A:355:PX4:H48	0.45	1.88	6	1
4:A:389:PX4:H62	4:A:394:PX4:H42	0.45	1.88	6	1
4:A:311:PX4:H69	4:A:364:PX4:H69	0.45	1.87	7	1
4:A:333:PX4:H27	4:A:340:PX4:H30	0.45	1.89	7	1
4:A:352:PX4:H35	4:A:392:PX4:H65	0.45	1.87	10	1
4:A:308:PX4:H36	4:A:373:PX4:H43	0.45	1.87	16	1
4:A:337:PX4:H30	4:A:341:PX4:H25	0.45	1.87	16	1
4:A:377:PX4:H27	4:A:408:PX4:H28	0.45	1.87	18	1
4:A:308:PX4:H26	4:A:326:PX4:H58	0.45	1.88	19	1
4:A:384:PX4:O4	4:A:405:PX4:H5	0.45	2.10	19	1
4:A:382:PX4:H62	4:A:397:PX4:H40	0.45	1.88	2	1
4:A:306:PX4:C9	4:A:342:PX4:H14	0.45	2.41	3	1
4:A:376:PX4:H16	4:A:390:PX4:H47	0.45	1.87	3	1
4:A:420:PX4:H20	4:A:422:PX4:H16	0.45	1.89	15	1
4:A:342:PX4:H38	4:A:357:PX4:H37	0.45	1.88	17	1
4:A:392:PX4:H9	4:A:405:PX4:H15	0.45	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:342:PX4:H54	4:A:357:PX4:H37	0.45	1.89	18	1
1:A:90:THR:HG21	4:A:321:PX4:H1	0.45	1.87	20	1
4:A:318:PX4:H11	4:A:321:PX4:O8	0.45	2.12	2	1
4:A:312:PX4:H26	4:A:324:PX4:H22	0.45	1.89	4	1
4:A:375:PX4:H22	4:A:407:PX4:H19	0.45	1.88	7	1
4:A:382:PX4:H17	4:A:423:PX4:H20	0.45	1.88	7	1
4:A:375:PX4:H17	4:A:392:PX4:O1	0.45	2.12	9	1
4:A:309:PX4:H6	4:A:328:PX4:O6	0.45	2.11	19	2
4:A:404:PX4:H26	4:A:418:PX4:H20	0.45	1.89	10	1
4:A:386:PX4:H27	4:A:417:PX4:H55	0.45	1.88	11	1
4:A:379:PX4:H26	5:A:434:C3S:H152	0.45	1.87	14	1
4:A:320:PX4:H61	4:A:334:PX4:H67	0.45	1.88	15	1
4:A:397:PX4:H21	4:A:411:PX4:H16	0.45	1.88	15	1
4:A:316:PX4:H35	4:A:321:PX4:H53	0.45	1.88	16	1
4:A:375:PX4:H61	4:A:379:PX4:H42	0.45	1.86	17	1
4:A:370:PX4:O1	4:A:383:PX4:H11	0.45	2.12	18	1
4:A:371:PX4:H32	4:A:395:PX4:H27	0.45	1.89	1	1
4:A:316:PX4:O2	4:A:318:PX4:H4	0.45	2.12	2	1
4:A:375:PX4:H68	4:A:384:PX4:H31	0.45	1.86	2	1
4:A:368:PX4:H43	4:A:426:PX4:H29	0.45	1.86	5	1
4:A:368:PX4:H57	4:A:426:PX4:H55	0.45	1.87	9	1
4:A:377:PX4:H23	4:A:408:PX4:H54	0.45	1.87	10	1
4:A:345:PX4:H63	4:A:358:PX4:H56	0.45	1.88	11	1
4:A:327:PX4:H35	4:A:327:PX4:H55	0.45	1.89	13	1
4:A:336:PX4:H27	4:A:354:PX4:H34	0.45	1.89	13	1
4:A:382:PX4:H64	4:A:415:PX4:H59	0.45	1.88	13	1
4:A:374:PX4:H34	4:A:397:PX4:H69	0.45	1.88	18	1
4:A:365:PX4:O6	4:A:369:PX4:H10	0.45	2.11	19	1
4:A:345:PX4:H71	4:A:419:PX4:H66	0.45	1.87	20	1
4:A:369:PX4:H5	4:A:370:PX4:O6	0.45	2.11	20	1
4:A:383:PX4:H71	4:A:407:PX4:H30	0.45	1.89	1	1
4:A:397:PX4:H31	4:A:398:PX4:H36	0.45	1.88	1	1
4:A:368:PX4:H3	4:A:372:PX4:O1	0.45	2.12	5	2
4:A:307:PX4:O2	4:A:322:PX4:H9	0.45	2.12	6	1
4:A:350:PX4:H40	4:A:371:PX4:H44	0.45	1.89	7	1
4:A:373:PX4:H59	4:A:414:PX4:H32	0.45	1.89	7	1
1:A:123:HIS:CE1	4:A:348:PX4:H21	0.45	2.46	15	2
4:A:374:PX4:H25	4:A:423:PX4:H21	0.45	1.88	11	1
4:A:350:PX4:H70	4:A:402:PX4:H70	0.45	1.87	12	1
4:A:391:PX4:H19	4:A:408:PX4:H53	0.45	1.88	12	1
4:A:323:PX4:H42	4:A:345:PX4:H37	0.45	1.89	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:O2	4:A:427:PX4:H2	0.45	2.12	14	1
4:A:384:PX4:O3	4:A:384:PX4:H12	0.45	2.10	14	1
4:A:351:PX4:H67	4:A:429:PX4:H38	0.45	1.89	20	1
4:A:322:PX4:H67	4:A:322:PX4:H29	0.45	1.88	1	1
4:A:373:PX4:H37	4:A:400:PX4:H44	0.45	1.88	2	1
4:A:403:PX4:H3	4:A:417:PX4:O6	0.45	2.12	3	1
4:A:391:PX4:H27	4:A:407:PX4:H27	0.45	1.89	4	1
4:A:370:PX4:H32	4:A:383:PX4:H25	0.45	1.87	5	1
4:A:409:PX4:H43	4:A:429:PX4:H37	0.45	1.89	9	1
4:A:350:PX4:H60	4:A:395:PX4:H44	0.45	1.87	10	1
4:A:310:PX4:H50	4:A:333:PX4:H53	0.45	1.88	14	1
4:A:316:PX4:H70	4:A:340:PX4:H60	0.45	1.87	1	1
4:A:331:PX4:H40	4:A:337:PX4:H17	0.45	1.88	2	1
4:A:318:PX4:H24	4:A:342:PX4:H48	0.45	1.89	5	1
4:A:362:PX4:H41	4:A:424:PX4:H42	0.45	1.88	8	1
4:A:401:PX4:H67	4:A:401:PX4:H38	0.45	1.89	8	1
4:A:338:PX4:H16	4:A:344:PX4:H48	0.45	1.88	9	1
4:A:308:PX4:H17	4:A:326:PX4:H51	0.45	1.88	10	1
4:A:326:PX4:H63	5:A:431:C3S:H442	0.45	1.88	11	1
4:A:378:PX4:H53	4:A:426:PX4:H14	0.45	1.89	13	1
4:A:317:PX4:H43	4:A:361:PX4:C30	0.45	2.42	16	1
4:A:366:PX4:H19	4:A:417:PX4:H20	0.45	1.88	16	1
4:A:305:PX4:H42	4:A:372:PX4:H40	0.45	1.88	18	1
4:A:324:PX4:H40	4:A:426:PX4:H31	0.45	1.87	19	1
4:A:308:PX4:H61	4:A:326:PX4:C29	0.45	2.41	20	1
4:A:335:PX4:H37	4:A:360:PX4:H36	0.45	1.88	20	1
4:A:341:PX4:H8	4:A:356:PX4:O6	0.45	2.12	20	1
4:A:326:PX4:H69	4:A:361:PX4:H41	0.45	1.87	3	1
4:A:327:PX4:H21	4:A:348:PX4:C11	0.45	2.36	4	1
4:A:333:PX4:O6	4:A:340:PX4:H4	0.45	2.12	4	1
4:A:389:PX4:H45	4:A:405:PX4:H34	0.45	1.88	4	1
4:A:428:PX4:H21	4:A:428:PX4:H54	0.45	1.88	4	1
4:A:411:PX4:H46	4:A:424:PX4:H47	0.45	1.88	8	1
4:A:328:PX4:H40	4:A:360:PX4:H35	0.45	1.89	9	1
4:A:368:PX4:H40	4:A:391:PX4:H35	0.45	1.87	9	1
1:A:42:MET:HE1	1:A:62:MET:SD	0.45	2.52	10	1
4:A:323:PX4:H48	4:A:361:PX4:H19	0.45	1.88	10	1
4:A:365:PX4:H62	4:A:376:PX4:H28	0.45	1.88	16	1
4:A:391:PX4:O2	4:A:414:PX4:H8	0.45	2.11	18	1
4:A:308:PX4:H28	4:A:334:PX4:H34	0.45	1.88	2	1
4:A:370:PX4:H12	4:A:397:PX4:H46	0.45	1.88	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:H17	4:A:405:PX4:H4	0.45	1.89	10	1
4:A:333:PX4:H33	4:A:340:PX4:H34	0.45	1.89	12	1
4:A:386:PX4:H31	4:A:417:PX4:H51	0.45	1.89	12	1
4:A:386:PX4:O6	4:A:417:PX4:H17	0.45	2.12	14	1
4:A:346:PX4:H32	4:A:361:PX4:H65	0.45	1.87	18	1
4:A:375:PX4:C11	4:A:400:PX4:H62	0.45	2.42	19	1
1:A:96:TYR:CD2	1:A:102:HIS:HA	0.45	2.47	6	1
4:A:353:PX4:H56	4:A:378:PX4:C22	0.45	2.42	8	1
4:A:366:PX4:H40	4:A:368:PX4:H40	0.45	1.89	8	1
4:A:420:PX4:O8	4:A:420:PX4:H10	0.45	2.11	9	1
4:A:310:PX4:H22	4:A:311:PX4:H17	0.45	1.89	10	1
4:A:324:PX4:H55	4:A:334:PX4:H55	0.45	1.88	11	1
4:A:315:PX4:H37	4:A:327:PX4:H66	0.45	1.89	12	1
4:A:367:PX4:H29	4:A:399:PX4:H25	0.45	1.89	13	1
4:A:369:PX4:H58	4:A:428:PX4:H36	0.45	1.89	14	1
4:A:392:PX4:H62	4:A:422:PX4:H56	0.45	1.88	14	1
4:A:305:PX4:H47	4:A:312:PX4:H61	0.45	1.89	15	1
4:A:309:PX4:O6	4:A:351:PX4:H18	0.45	2.11	15	1
4:A:365:PX4:H6	4:A:383:PX4:O2	0.45	2.12	15	1
4:A:320:PX4:H25	4:A:332:PX4:H42	0.45	1.88	18	1
4:A:405:PX4:H17	4:A:405:PX4:H7	0.44	1.89	1	1
4:A:306:PX4:H59	4:A:321:PX4:H17	0.44	1.89	8	1
4:A:395:PX4:O4	4:A:401:PX4:H16	0.44	2.12	11	1
4:A:308:PX4:H16	4:A:320:PX4:H17	0.44	1.90	15	1
4:A:316:PX4:H25	4:A:342:PX4:H38	0.44	1.89	16	1
4:A:384:PX4:H47	4:A:389:PX4:H26	0.44	1.89	17	1
4:A:400:PX4:O6	4:A:405:PX4:H10	0.44	2.13	18	1
4:A:400:PX4:H59	4:A:405:PX4:H21	0.44	1.89	19	1
4:A:369:PX4:H24	4:A:374:PX4:H51	0.44	1.88	20	1
4:A:307:PX4:H11	4:A:337:PX4:O2	0.44	2.12	3	1
4:A:371:PX4:H23	4:A:402:PX4:H23	0.44	1.89	3	1
4:A:338:PX4:H46	4:A:351:PX4:H48	0.44	1.89	10	1
4:A:391:PX4:H35	4:A:427:PX4:H65	0.44	1.89	10	1
4:A:343:PX4:H16	4:A:343:PX4:O6	0.44	2.12	11	1
4:A:378:PX4:H55	4:A:386:PX4:H30	0.44	1.89	11	1
4:A:328:PX4:H58	4:A:347:PX4:H26	0.44	1.89	12	1
4:A:366:PX4:O6	4:A:417:PX4:H5	0.44	2.11	14	1
4:A:395:PX4:O1	4:A:402:PX4:H4	0.44	2.12	14	1
4:A:391:PX4:H31	4:A:408:PX4:H61	0.44	1.89	15	1
4:A:333:PX4:H17	4:A:333:PX4:H51	0.44	1.89	16	1
4:A:317:PX4:H21	4:A:326:PX4:H20	0.44	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:398:PX4:H38	4:A:411:PX4:H67	0.44	1.89	20	1
4:A:342:PX4:O4	4:A:358:PX4:H10	0.44	2.12	1	1
4:A:382:PX4:H17	4:A:415:PX4:H46	0.44	1.88	2	1
4:A:369:PX4:O8	4:A:419:PX4:H8	0.44	2.12	4	1
4:A:396:PX4:H20	4:A:407:PX4:H14	0.44	1.89	4	1
4:A:412:PX4:H54	4:A:424:PX4:H51	0.44	1.89	6	1
4:A:340:PX4:H62	4:A:356:PX4:H34	0.44	1.89	8	1
4:A:409:PX4:H69	4:A:411:PX4:H27	0.44	1.89	8	1
4:A:411:PX4:H9	4:A:411:PX4:H14	0.44	1.89	8	1
4:A:309:PX4:H22	4:A:345:PX4:H57	0.44	1.89	9	1
4:A:380:PX4:H39	4:A:422:PX4:H66	0.44	1.87	10	1
4:A:318:PX4:H31	4:A:321:PX4:H49	0.44	1.89	14	1
4:A:323:PX4:H21	4:A:328:PX4:H23	0.44	1.88	14	1
4:A:307:PX4:O2	4:A:322:PX4:H7	0.44	2.12	16	1
4:A:361:PX4:H52	4:A:402:PX4:H43	0.44	1.89	17	1
4:A:320:PX4:H41	4:A:381:PX4:H61	0.44	1.88	18	1
4:A:367:PX4:O6	4:A:399:PX4:H17	0.44	2.12	18	1
4:A:375:PX4:H19	4:A:392:PX4:H10	0.44	1.90	18	1
4:A:345:PX4:H16	4:A:349:PX4:H51	0.44	1.88	19	1
4:A:393:PX4:H57	4:A:413:PX4:H32	0.44	1.89	1	1
4:A:327:PX4:H25	4:A:338:PX4:H62	0.44	1.89	2	1
4:A:309:PX4:H59	4:A:359:PX4:H34	0.44	1.89	7	1
4:A:341:PX4:H48	4:A:356:PX4:H23	0.44	1.87	9	1
4:A:368:PX4:H54	4:A:406:PX4:H29	0.44	1.90	11	1
4:A:328:PX4:H47	4:A:347:PX4:H14	0.44	1.88	13	2
4:A:331:PX4:O2	4:A:337:PX4:H11	0.44	2.11	13	1
4:A:404:PX4:H16	4:A:418:PX4:H47	0.44	1.89	15	1
4:A:330:PX4:H59	4:A:337:PX4:H31	0.44	1.89	17	1
4:A:312:PX4:H66	4:A:363:PX4:H72	0.44	1.90	1	1
4:A:306:PX4:H62	4:A:348:PX4:H37	0.44	1.88	7	1
1:A:181:GLY:O	4:A:361:PX4:H10	0.44	2.13	9	1
4:A:323:PX4:H58	4:A:347:PX4:H31	0.44	1.90	9	1
4:A:334:PX4:H27	4:A:414:PX4:H66	0.44	1.89	9	1
4:A:371:PX4:H39	4:A:373:PX4:H32	0.44	1.89	9	1
4:A:411:PX4:H25	4:A:424:PX4:H60	0.44	1.88	9	1
4:A:372:PX4:H54	4:A:398:PX4:H71	0.44	1.89	12	1
4:A:308:PX4:H51	4:A:326:PX4:H62	0.44	1.89	13	1
4:A:314:PX4:H23	4:A:352:PX4:O6	0.44	2.13	13	1
4:A:390:PX4:H49	4:A:403:PX4:H52	0.44	1.89	14	1
4:A:310:PX4:H64	4:A:356:PX4:H44	0.44	1.90	15	1
4:A:307:PX4:H64	4:A:327:PX4:H36	0.44	1.88	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:371:PX4:H48	4:A:373:PX4:H16	0.44	1.87	16	1
4:A:389:PX4:H16	4:A:399:PX4:H50	0.44	1.89	16	1
4:A:408:PX4:H69	4:A:426:PX4:H20	0.44	1.90	16	1
4:A:394:PX4:H29	4:A:395:PX4:H54	0.44	1.87	17	1
4:A:328:PX4:H26	4:A:347:PX4:H24	0.44	1.90	19	1
4:A:354:PX4:H48	4:A:357:PX4:H49	0.44	1.90	3	1
4:A:387:PX4:H28	4:A:418:PX4:C30	0.44	2.43	3	1
4:A:305:PX4:H32	4:A:310:PX4:H30	0.44	1.89	4	1
4:A:393:PX4:H22	4:A:416:PX4:H23	0.44	1.89	4	1
4:A:326:PX4:H62	4:A:361:PX4:H30	0.44	1.88	6	1
4:A:343:PX4:O1	4:A:356:PX4:H5	0.44	2.13	6	1
4:A:371:PX4:H17	4:A:401:PX4:O6	0.44	2.13	6	1
4:A:371:PX4:H35	4:A:395:PX4:H35	0.44	1.89	9	1
4:A:402:PX4:H8	4:A:417:PX4:O1	0.44	2.12	11	1
4:A:423:PX4:H72	4:A:429:PX4:H65	0.44	1.88	12	1
4:A:374:PX4:H34	4:A:423:PX4:H58	0.44	1.90	13	1
4:A:385:PX4:H17	4:A:415:PX4:H20	0.44	1.88	13	1
4:A:388:PX4:H8	4:A:391:PX4:O6	0.44	2.12	13	1
4:A:320:PX4:H36	4:A:334:PX4:H40	0.44	1.88	14	1
4:A:384:PX4:H62	5:A:434:C3S:C60	0.44	2.42	14	1
4:A:400:PX4:H14	4:A:401:PX4:O2	0.44	2.12	14	1
4:A:387:PX4:O6	4:A:421:PX4:H20	0.44	2.13	16	1
4:A:330:PX4:H16	4:A:337:PX4:H19	0.44	1.90	19	1
4:A:428:PX4:H16	4:A:429:PX4:H50	0.44	1.89	19	1
4:A:338:PX4:H6	4:A:344:PX4:O6	0.44	2.13	20	1
4:A:389:PX4:H66	4:A:400:PX4:H38	0.44	1.88	20	1
4:A:307:PX4:H29	4:A:307:PX4:H62	0.44	1.88	1	1
4:A:397:PX4:H54	4:A:430:PX4:H21	0.44	1.90	1	1
1:A:83:LYS:HG2	1:A:238:TYR:CE1	0.44	2.48	2	1
1:A:101:PRO:HG3	4:A:334:PX4:H1	0.44	1.88	2	1
4:A:326:PX4:H72	4:A:417:PX4:H64	0.44	1.90	4	1
4:A:383:PX4:H68	4:A:396:PX4:H60	0.44	1.87	4	1
4:A:323:PX4:H46	4:A:325:PX4:H15	0.44	1.88	5	1
4:A:336:PX4:C36	4:A:409:PX4:H31	0.44	2.42	5	1
4:A:395:PX4:H68	4:A:405:PX4:H37	0.44	1.88	11	1
4:A:314:PX4:H27	4:A:352:PX4:H22	0.44	1.90	13	1
4:A:382:PX4:H61	4:A:423:PX4:H36	0.44	1.88	13	1
4:A:428:PX4:H28	4:A:429:PX4:H36	0.44	1.89	14	1
4:A:381:PX4:H20	4:A:394:PX4:H53	0.44	1.88	17	1
4:A:399:PX4:H48	4:A:399:PX4:H22	0.44	1.88	19	1
4:A:306:PX4:H34	4:A:358:PX4:H52	0.44	1.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:H56	4:A:398:PX4:H57	0.44	1.90	1	1
4:A:397:PX4:H36	4:A:404:PX4:H70	0.44	1.89	3	1
4:A:377:PX4:H50	4:A:408:PX4:H23	0.44	1.88	5	1
4:A:404:PX4:O1	4:A:418:PX4:H12	0.44	2.12	6	1
4:A:333:PX4:H34	4:A:340:PX4:H57	0.44	1.89	7	1
4:A:332:PX4:H72	4:A:388:PX4:H43	0.44	1.88	8	1
4:A:359:PX4:H69	4:A:383:PX4:H61	0.44	1.90	8	1
4:A:394:PX4:H21	4:A:401:PX4:H50	0.44	1.90	8	1
4:A:317:PX4:H59	4:A:332:PX4:H25	0.44	1.90	9	1
4:A:343:PX4:H59	4:A:350:PX4:H66	0.44	1.89	9	1
1:A:128:VAL:CG2	4:A:315:PX4:H72	0.44	2.41	10	1
4:A:322:PX4:H62	4:A:369:PX4:H38	0.44	1.89	10	1
4:A:369:PX4:H65	4:A:429:PX4:H65	0.44	1.90	10	1
4:A:337:PX4:H36	4:A:355:PX4:H36	0.44	1.89	12	1
4:A:398:PX4:H10	5:A:435:C3S:O2	0.44	2.12	12	1
4:A:428:PX4:H33	4:A:429:PX4:H35	0.44	1.88	12	1
4:A:317:PX4:H65	4:A:330:PX4:H45	0.44	1.89	14	1
4:A:327:PX4:H68	4:A:338:PX4:H24	0.44	1.88	15	1
4:A:336:PX4:H36	4:A:354:PX4:H64	0.44	1.90	1	1
4:A:322:PX4:H50	4:A:331:PX4:C10	0.44	2.42	6	1
4:A:308:PX4:H32	4:A:315:PX4:H34	0.44	1.89	9	1
4:A:370:PX4:H57	4:A:374:PX4:H48	0.44	1.88	10	1
4:A:389:PX4:H38	4:A:389:PX4:H31	0.44	1.48	10	1
4:A:388:PX4:H47	4:A:390:PX4:H51	0.44	1.89	11	1
4:A:312:PX4:H21	4:A:324:PX4:H9	0.44	1.88	13	1
4:A:404:PX4:H32	4:A:423:PX4:H35	0.44	1.89	13	1
4:A:349:PX4:H33	4:A:361:PX4:H56	0.44	1.90	14	1
4:A:306:PX4:H61	4:A:332:PX4:H61	0.44	1.90	16	1
4:A:340:PX4:H32	4:A:389:PX4:H71	0.44	1.90	17	1
4:A:365:PX4:H66	4:A:388:PX4:H42	0.44	1.90	18	1
4:A:306:PX4:H57	4:A:342:PX4:H26	0.43	1.90	1	1
4:A:338:PX4:O3	4:A:347:PX4:H5	0.43	2.13	3	1
4:A:343:PX4:O4	4:A:350:PX4:H9	0.43	2.12	3	1
4:A:328:PX4:H53	4:A:347:PX4:H54	0.43	1.90	6	1
4:A:385:PX4:H63	4:A:415:PX4:H38	0.43	1.88	6	1
4:A:404:PX4:H69	4:A:423:PX4:H36	0.43	1.90	7	1
4:A:368:PX4:H24	5:A:436:C3S:H502	0.43	1.89	8	1
4:A:320:PX4:H30	4:A:326:PX4:H41	0.43	1.89	9	1
4:A:386:PX4:H36	4:A:386:PX4:H60	0.43	1.89	9	1
4:A:314:PX4:H16	4:A:336:PX4:H22	0.43	1.88	11	1
4:A:321:PX4:H29	4:A:343:PX4:H40	0.43	1.89	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:PX4:H14	4:A:411:PX4:H7	0.43	1.90	11	1
4:A:365:PX4:H48	4:A:370:PX4:H34	0.43	1.89	15	1
4:A:416:PX4:H25	4:A:416:PX4:H32	0.43	1.62	17	1
4:A:329:PX4:H31	4:A:355:PX4:H63	0.43	1.88	18	1
4:A:316:PX4:H15	4:A:352:PX4:H20	0.43	1.89	19	1
4:A:367:PX4:H16	4:A:399:PX4:H50	0.43	1.89	19	1
4:A:305:PX4:H49	4:A:324:PX4:H59	0.43	1.90	1	1
4:A:335:PX4:H8	4:A:360:PX4:H18	0.43	1.90	1	1
4:A:321:PX4:H46	4:A:342:PX4:H23	0.43	1.89	4	1
4:A:305:PX4:H40	5:A:432:C3S:H693	0.43	1.89	5	1
4:A:376:PX4:H14	4:A:396:PX4:O1	0.43	2.13	5	1
4:A:375:PX4:H38	4:A:427:PX4:H50	0.43	1.90	6	1
4:A:326:PX4:H68	4:A:326:PX4:H42	0.43	1.90	7	1
4:A:366:PX4:H13	4:A:403:PX4:H13	0.43	1.90	8	1
4:A:375:PX4:H39	4:A:427:PX4:H72	0.43	1.90	15	1
1:A:84:TRP:CE2	1:A:162:PRO:HB3	0.43	2.47	16	1
4:A:346:PX4:H6	4:A:346:PX4:O2	0.43	2.13	17	1
4:A:423:PX4:H10	4:A:423:PX4:O3	0.43	2.12	2	1
4:A:338:PX4:H64	4:A:351:PX4:H51	0.43	1.89	3	1
4:A:343:PX4:H31	4:A:352:PX4:H64	0.43	1.90	3	1
1:A:96:TYR:OH	4:A:340:PX4:H3	0.43	2.13	7	1
4:A:309:PX4:H72	4:A:390:PX4:H40	0.43	1.90	7	1
4:A:322:PX4:H43	4:A:362:PX4:H37	0.43	1.90	7	1
4:A:308:PX4:H68	4:A:397:PX4:H66	0.43	1.90	8	1
4:A:371:PX4:H59	4:A:402:PX4:H45	0.43	1.89	8	1
4:A:345:PX4:H17	4:A:358:PX4:H20	0.43	1.89	9	1
4:A:372:PX4:H3	4:A:410:PX4:H15	0.43	1.89	10	1
4:A:374:PX4:H49	4:A:397:PX4:H50	0.43	1.90	13	1
4:A:310:PX4:H24	4:A:311:PX4:H17	0.43	1.89	15	1
4:A:328:PX4:H46	4:A:347:PX4:H48	0.43	1.89	15	1
4:A:325:PX4:H16	4:A:355:PX4:H48	0.43	1.90	18	1
4:A:343:PX4:H26	4:A:343:PX4:H31	0.43	1.53	18	1
4:A:374:PX4:H57	4:A:381:PX4:H54	0.43	1.89	20	1
4:A:334:PX4:H47	5:A:432:C3S:H7	0.43	1.90	1	1
4:A:345:PX4:H66	4:A:383:PX4:H45	0.43	1.89	1	1
4:A:411:PX4:H28	4:A:423:PX4:H56	0.43	1.90	2	1
4:A:383:PX4:H53	4:A:407:PX4:H50	0.43	1.90	3	1
4:A:327:PX4:H55	4:A:348:PX4:H69	0.43	1.89	6	1
4:A:370:PX4:H8	4:A:394:PX4:O2	0.43	2.13	6	1
4:A:305:PX4:H39	4:A:368:PX4:H71	0.43	1.90	10	1
4:A:313:PX4:O6	4:A:355:PX4:H3	0.43	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:314:PX4:H25	4:A:352:PX4:H22	0.43	1.90	12	1
4:A:328:PX4:H30	4:A:328:PX4:H35	0.43	1.50	12	1
4:A:340:PX4:H25	4:A:340:PX4:H20	0.43	1.56	12	1
4:A:385:PX4:C8	4:A:415:PX4:H20	0.43	2.43	13	1
4:A:383:PX4:H49	4:A:407:PX4:H50	0.43	1.90	14	1
4:A:318:PX4:H25	4:A:321:PX4:H55	0.43	1.90	16	1
4:A:351:PX4:H29	4:A:351:PX4:H36	0.43	1.55	16	1
4:A:390:PX4:H33	4:A:390:PX4:H62	0.43	1.90	16	1
4:A:306:PX4:H56	4:A:342:PX4:H23	0.43	1.90	19	1
4:A:324:PX4:H22	5:A:431:C3S:H262	0.43	1.90	20	1
4:A:342:PX4:H30	4:A:358:PX4:H56	0.43	1.89	20	1
4:A:344:PX4:H38	4:A:354:PX4:H41	0.43	1.90	2	1
4:A:320:PX4:H66	4:A:373:PX4:H44	0.43	1.89	4	1
4:A:324:PX4:H48	5:A:431:C3S:H501	0.43	1.89	4	1
4:A:388:PX4:O6	4:A:407:PX4:H5	0.43	2.14	4	1
4:A:315:PX4:H36	4:A:395:PX4:H45	0.43	1.90	5	1
4:A:312:PX4:H19	4:A:346:PX4:H66	0.43	1.89	6	1
4:A:384:PX4:H15	5:A:434:C3S:H42	0.43	1.89	7	1
4:A:382:PX4:H70	4:A:404:PX4:H45	0.43	1.90	9	1
4:A:393:PX4:H4	4:A:416:PX4:H16	0.43	1.90	10	1
4:A:306:PX4:H52	4:A:359:PX4:H46	0.43	1.89	16	1
4:A:380:PX4:H58	4:A:416:PX4:H51	0.43	1.88	16	1
4:A:335:PX4:O4	4:A:347:PX4:H51	0.43	2.12	17	1
4:A:369:PX4:H35	4:A:370:PX4:H42	0.43	1.89	18	1
4:A:309:PX4:H7	4:A:328:PX4:O1	0.43	2.13	19	1
4:A:389:PX4:H44	4:A:399:PX4:H72	0.43	1.90	1	1
4:A:371:PX4:H29	4:A:401:PX4:H41	0.43	1.91	2	1
4:A:326:PX4:H42	4:A:418:PX4:H33	0.43	1.88	3	1
4:A:316:PX4:H48	4:A:316:PX4:H55	0.43	1.66	4	1
4:A:398:PX4:H25	4:A:411:PX4:H53	0.43	1.89	4	1
4:A:403:PX4:H67	4:A:416:PX4:H40	0.43	1.90	6	1
4:A:389:PX4:H3	4:A:401:PX4:O2	0.43	2.12	7	1
4:A:365:PX4:H17	4:A:383:PX4:H19	0.43	1.90	10	1
4:A:306:PX4:H21	4:A:342:PX4:H19	0.43	1.89	12	1
4:A:316:PX4:C13	4:A:321:PX4:H32	0.43	2.43	14	1
4:A:325:PX4:H32	4:A:353:PX4:H36	0.43	1.89	16	1
4:A:399:PX4:H70	4:A:405:PX4:H45	0.43	1.88	16	1
4:A:312:PX4:H18	4:A:346:PX4:H17	0.43	1.89	17	1
4:A:340:PX4:H47	4:A:356:PX4:H46	0.43	1.91	18	1
4:A:419:PX4:H66	4:A:419:PX4:H60	0.43	1.64	18	1
4:A:335:PX4:H65	4:A:363:PX4:H66	0.43	1.91	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:355:PX4:H71	4:A:421:PX4:H40	0.43	1.89	20	1
4:A:307:PX4:H68	4:A:369:PX4:H70	0.43	1.90	1	1
1:A:118:LYS:O	4:A:351:PX4:H4	0.43	2.13	2	1
4:A:328:PX4:H67	4:A:335:PX4:H41	0.43	1.90	2	1
4:A:367:PX4:H14	4:A:389:PX4:O4	0.43	2.13	2	1
4:A:377:PX4:H26	4:A:408:PX4:H24	0.43	1.89	2	1
4:A:374:PX4:H3	4:A:397:PX4:H18	0.43	1.91	3	1
4:A:400:PX4:H44	4:A:401:PX4:H18	0.43	1.91	3	1
4:A:381:PX4:H25	4:A:395:PX4:H24	0.43	1.89	5	1
4:A:346:PX4:H42	4:A:376:PX4:H43	0.43	1.90	7	1
4:A:370:PX4:H41	4:A:394:PX4:H48	0.43	1.89	7	1
4:A:408:PX4:H56	4:A:408:PX4:H63	0.43	1.50	9	1
4:A:368:PX4:H54	4:A:406:PX4:H30	0.43	1.90	10	1
4:A:376:PX4:O8	4:A:390:PX4:H7	0.43	2.14	11	1
4:A:308:PX4:O6	4:A:308:PX4:H1	0.43	2.14	12	1
4:A:365:PX4:O8	4:A:396:PX4:H10	0.43	2.13	16	1
1:A:114:ASN:ND2	4:A:332:PX4:H1	0.43	2.29	17	1
4:A:368:PX4:H56	4:A:426:PX4:H66	0.43	1.89	18	1
4:A:317:PX4:H68	4:A:418:PX4:H42	0.43	1.89	19	1
4:A:382:PX4:H19	4:A:398:PX4:H54	0.43	1.91	19	1
4:A:308:PX4:H46	4:A:326:PX4:H48	0.43	1.89	20	1
4:A:354:PX4:H8	4:A:360:PX4:O4	0.43	2.14	1	1
4:A:387:PX4:H22	4:A:416:PX4:H17	0.43	1.90	1	1
4:A:417:PX4:O6	4:A:418:PX4:H49	0.43	2.14	2	1
4:A:371:PX4:H68	4:A:424:PX4:H35	0.43	1.89	3	1
4:A:307:PX4:H53	4:A:338:PX4:H72	0.43	1.89	4	1
4:A:308:PX4:H36	4:A:332:PX4:H40	0.43	1.90	5	1
4:A:351:PX4:H23	4:A:359:PX4:H25	0.43	1.90	5	1
4:A:365:PX4:H22	4:A:419:PX4:H56	0.43	1.91	6	1
4:A:380:PX4:H47	4:A:385:PX4:H23	0.43	1.91	6	1
4:A:319:PX4:H28	4:A:336:PX4:H18	0.43	1.89	8	1
4:A:307:PX4:H43	4:A:411:PX4:H58	0.43	1.89	9	1
4:A:317:PX4:H71	4:A:417:PX4:H45	0.43	1.91	9	1
4:A:428:PX4:H24	4:A:429:PX4:H17	0.43	1.91	15	2
4:A:371:PX4:H4	4:A:373:PX4:H18	0.43	1.90	12	1
4:A:379:PX4:H59	4:A:422:PX4:H65	0.43	1.88	13	1
4:A:371:PX4:H55	4:A:373:PX4:H57	0.43	1.90	14	1
4:A:322:PX4:H71	4:A:429:PX4:H56	0.43	1.90	15	1
1:A:223:ASN:O	4:A:315:PX4:H8	0.43	2.13	18	1
4:A:357:PX4:H49	4:A:363:PX4:H24	0.43	1.91	18	1
4:A:382:PX4:H55	4:A:423:PX4:H22	0.43	1.89	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:320:PX4:H28	4:A:320:PX4:H21	0.43	1.41	3	1
4:A:389:PX4:H72	4:A:389:PX4:H64	0.43	1.46	4	1
4:A:317:PX4:H22	4:A:326:PX4:H16	0.43	1.91	6	1
4:A:357:PX4:H51	4:A:363:PX4:H49	0.43	1.91	6	1
4:A:307:PX4:H46	4:A:332:PX4:C3	0.43	2.44	7	1
4:A:354:PX4:H72	4:A:425:PX4:H37	0.43	1.90	7	1
4:A:331:PX4:H22	4:A:337:PX4:H21	0.43	1.90	8	1
4:A:345:PX4:O6	4:A:345:PX4:H3	0.43	2.14	10	1
4:A:404:PX4:H37	4:A:417:PX4:H28	0.43	1.89	11	1
4:A:320:PX4:H29	4:A:332:PX4:H28	0.43	1.91	12	1
4:A:389:PX4:H25	4:A:399:PX4:H51	0.43	1.91	13	1
4:A:371:PX4:H57	4:A:389:PX4:H48	0.43	1.91	15	1
4:A:316:PX4:H67	4:A:401:PX4:H41	0.43	1.91	16	1
4:A:367:PX4:H7	4:A:367:PX4:O2	0.43	2.13	18	1
4:A:416:PX4:H60	4:A:416:PX4:H67	0.43	1.49	18	1
4:A:377:PX4:H57	4:A:377:PX4:H62	0.43	1.60	2	1
4:A:395:PX4:H41	4:A:401:PX4:H65	0.43	1.91	2	1
4:A:305:PX4:H38	4:A:324:PX4:H70	0.43	1.91	3	1
4:A:309:PX4:H48	4:A:347:PX4:H24	0.43	1.90	3	1
4:A:344:PX4:H26	4:A:344:PX4:H31	0.43	1.65	3	1
4:A:406:PX4:H32	5:A:435:C3S:H443	0.43	1.90	3	1
4:A:355:PX4:H45	4:A:412:PX4:H64	0.43	1.90	4	1
4:A:367:PX4:H55	4:A:424:PX4:H50	0.43	1.89	5	1
4:A:378:PX4:H55	4:A:426:PX4:H53	0.43	1.90	5	1
4:A:349:PX4:H24	4:A:361:PX4:H19	0.43	1.90	6	1
4:A:344:PX4:H28	4:A:344:PX4:H33	0.43	1.60	7	1
4:A:351:PX4:H40	4:A:393:PX4:H37	0.43	1.90	7	1
4:A:370:PX4:H16	4:A:383:PX4:H49	0.43	1.91	10	1
4:A:403:PX4:H44	4:A:403:PX4:H38	0.43	1.53	10	1
4:A:385:PX4:H51	4:A:415:PX4:H16	0.43	1.91	11	1
4:A:370:PX4:H52	4:A:381:PX4:H50	0.43	1.89	12	1
4:A:315:PX4:H57	4:A:332:PX4:H17	0.43	1.90	13	1
4:A:309:PX4:H38	4:A:345:PX4:H38	0.43	1.90	14	1
4:A:410:PX4:H59	5:A:435:C3S:H151	0.43	1.91	14	1
4:A:318:PX4:H28	4:A:357:PX4:C14	0.43	2.42	15	1
4:A:313:PX4:H60	4:A:353:PX4:H58	0.43	1.90	16	1
4:A:327:PX4:H25	4:A:332:PX4:H68	0.43	1.90	18	1
4:A:306:PX4:H19	4:A:358:PX4:H47	0.43	1.91	19	1
4:A:416:PX4:O6	4:A:416:PX4:H10	0.43	2.13	19	1
4:A:317:PX4:H36	4:A:361:PX4:H22	0.43	1.91	20	1
1:A:30:LYS:O	1:A:31:ASN:HB3	0.42	2.13	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:381:PX4:H26	4:A:417:PX4:H58	0.42	1.91	1	1
1:A:156:LEU:CD2	1:A:156:LEU:N	0.42	2.82	4	1
4:A:349:PX4:H57	4:A:349:PX4:H62	0.42	1.49	4	1
4:A:338:PX4:H26	4:A:344:PX4:H17	0.42	1.91	7	1
4:A:318:PX4:H63	4:A:412:PX4:H44	0.42	1.90	9	1
4:A:403:PX4:H60	4:A:403:PX4:H67	0.42	1.57	10	1
4:A:330:PX4:H66	4:A:330:PX4:H61	0.42	1.65	12	1
4:A:403:PX4:H17	4:A:421:PX4:H47	0.42	1.90	13	1
4:A:307:PX4:H26	4:A:374:PX4:H70	0.42	1.90	15	1
4:A:312:PX4:H53	4:A:312:PX4:H46	0.42	1.53	15	1
4:A:316:PX4:O6	4:A:318:PX4:H11	0.42	2.14	15	1
4:A:324:PX4:H42	4:A:346:PX4:H42	0.42	1.90	15	1
4:A:374:PX4:H30	4:A:397:PX4:H69	0.42	1.91	18	1
4:A:400:PX4:H8	4:A:407:PX4:H48	0.42	1.90	18	1
1:A:128:VAL:CG2	4:A:343:PX4:H50	0.42	2.44	19	1
4:A:322:PX4:H46	4:A:337:PX4:H17	0.42	1.90	20	1
4:A:417:PX4:H19	4:A:418:PX4:H49	0.42	1.91	20	1
4:A:316:PX4:H15	4:A:352:PX4:O5	0.42	2.14	5	1
4:A:325:PX4:O6	4:A:361:PX4:H6	0.42	2.14	5	1
4:A:393:PX4:H17	4:A:416:PX4:H22	0.42	1.91	5	1
4:A:414:PX4:H69	4:A:426:PX4:H72	0.42	1.91	6	1
1:A:71:ASP:OD2	1:A:198:HIS:CE1	0.42	2.72	7	1
4:A:352:PX4:H40	4:A:375:PX4:H63	0.42	1.91	7	1
4:A:369:PX4:H63	4:A:393:PX4:H34	0.42	1.90	7	1
4:A:348:PX4:H9	4:A:348:PX4:H15	0.42	1.90	9	1
1:A:57:ARG:CZ	1:A:217:GLY:HA3	0.42	2.44	10	1
4:A:386:PX4:H22	4:A:402:PX4:H20	0.42	1.91	10	1
4:A:334:PX4:H47	5:A:432:C3S:H232	0.42	1.91	11	1
4:A:371:PX4:H46	4:A:389:PX4:H51	0.42	1.90	11	1
4:A:308:PX4:H52	4:A:326:PX4:H19	0.42	1.91	12	1
4:A:379:PX4:H22	4:A:425:PX4:H25	0.42	1.91	12	1
4:A:395:PX4:H66	4:A:402:PX4:H61	0.42	1.90	14	1
4:A:428:PX4:H10	4:A:428:PX4:H1	0.42	1.58	14	1
4:A:325:PX4:H48	4:A:325:PX4:H55	0.42	1.43	16	1
4:A:380:PX4:H49	4:A:385:PX4:H26	0.42	1.91	16	1
4:A:384:PX4:H16	4:A:405:PX4:H9	0.42	1.91	18	1
4:A:397:PX4:H18	4:A:411:PX4:H1	0.42	1.91	18	1
4:A:409:PX4:H48	4:A:409:PX4:H55	0.42	1.59	18	1
4:A:309:PX4:H59	4:A:328:PX4:H45	0.42	1.90	19	1
4:A:330:PX4:H40	4:A:337:PX4:H45	0.42	1.90	19	1
4:A:389:PX4:H4	4:A:401:PX4:O1	0.42	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:320:PX4:H54	4:A:334:PX4:H72	0.42	1.91	2	1
4:A:323:PX4:H61	4:A:328:PX4:H61	0.42	1.90	3	1
4:A:383:PX4:H11	4:A:400:PX4:O8	0.42	2.14	7	1
4:A:340:PX4:O8	4:A:341:PX4:H11	0.42	2.14	15	1
4:A:353:PX4:H59	4:A:361:PX4:H28	0.42	1.90	15	1
4:A:379:PX4:H21	4:A:425:PX4:H20	0.42	1.92	17	1
4:A:313:PX4:H30	4:A:362:PX4:H48	0.42	1.91	18	1
4:A:375:PX4:H70	4:A:405:PX4:H48	0.42	1.90	18	1
4:A:324:PX4:H31	4:A:324:PX4:H38	0.42	1.55	19	1
4:A:372:PX4:H16	4:A:410:PX4:H53	0.42	1.91	20	1
4:A:404:PX4:H23	4:A:418:PX4:H24	0.42	1.90	20	1
4:A:411:PX4:H54	4:A:411:PX4:H49	0.42	1.62	1	1
1:A:127:VAL:HG12	1:A:129:TRP:CZ2	0.42	2.49	2	1
4:A:362:PX4:H29	4:A:362:PX4:H36	0.42	1.66	2	1
4:A:376:PX4:H61	4:A:388:PX4:H35	0.42	1.90	2	1
4:A:428:PX4:H39	4:A:429:PX4:H34	0.42	1.91	2	1
4:A:338:PX4:H25	4:A:344:PX4:H21	0.42	1.91	3	1
4:A:369:PX4:H28	4:A:383:PX4:H27	0.42	1.91	3	1
4:A:417:PX4:H33	4:A:418:PX4:H36	0.42	1.91	3	1
4:A:329:PX4:H50	4:A:355:PX4:H61	0.42	1.90	4	1
4:A:324:PX4:H46	4:A:346:PX4:H67	0.42	1.90	6	1
4:A:327:PX4:H41	4:A:338:PX4:H34	0.42	1.92	6	1
4:A:331:PX4:H62	4:A:331:PX4:H69	0.42	1.69	11	1
4:A:403:PX4:H20	4:A:403:PX4:H18	0.42	1.47	11	1
4:A:397:PX4:C34	4:A:423:PX4:H68	0.42	2.41	12	1
4:A:354:PX4:H39	4:A:354:PX4:H34	0.42	1.54	14	1
4:A:305:PX4:O6	4:A:311:PX4:H5	0.42	2.14	15	1
4:A:353:PX4:H60	4:A:353:PX4:H55	0.42	1.46	18	1
4:A:308:PX4:H14	4:A:320:PX4:O3	0.42	2.14	19	1
4:A:380:PX4:H44	4:A:420:PX4:H68	0.42	1.91	20	1
4:A:317:PX4:H60	4:A:337:PX4:H60	0.42	1.92	1	1
4:A:353:PX4:O6	4:A:361:PX4:H1	0.42	2.14	3	1
4:A:371:PX4:H60	4:A:399:PX4:H54	0.42	1.89	3	1
4:A:317:PX4:H65	4:A:320:PX4:H35	0.42	1.91	5	1
4:A:317:PX4:H39	4:A:415:PX4:H43	0.42	1.92	7	1
4:A:339:PX4:H41	4:A:368:PX4:H65	0.42	1.92	8	1
4:A:334:PX4:H45	4:A:426:PX4:H20	0.42	1.90	9	1
4:A:419:PX4:H45	4:A:419:PX4:H37	0.42	1.48	9	1
1:A:114:ASN:OD1	4:A:348:PX4:H1	0.42	2.14	11	1
4:A:377:PX4:H60	4:A:408:PX4:H31	0.42	1.92	11	1
4:A:395:PX4:H47	4:A:401:PX4:H16	0.42	1.91	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H25	4:A:430:PX4:H25	0.42	1.91	17	1
4:A:316:PX4:H30	4:A:316:PX4:H35	0.42	1.67	5	1
4:A:338:PX4:C24	4:A:347:PX4:H57	0.42	2.41	6	1
4:A:374:PX4:H63	4:A:430:PX4:H63	0.42	1.90	7	1
4:A:338:PX4:H65	4:A:374:PX4:H72	0.42	1.90	9	1
4:A:351:PX4:H69	4:A:360:PX4:H50	0.42	1.90	11	1
4:A:428:PX4:H28	4:A:428:PX4:H33	0.42	1.60	11	1
4:A:370:PX4:H7	4:A:430:PX4:H15	0.42	1.91	13	1
4:A:397:PX4:H56	4:A:430:PX4:H23	0.42	1.90	13	1
1:A:120:ILE:O	4:A:327:PX4:H9	0.42	2.14	15	1
4:A:407:PX4:O4	4:A:427:PX4:H3	0.42	2.14	15	1
4:A:322:PX4:H39	4:A:322:PX4:H34	0.42	1.53	17	1
4:A:375:PX4:H72	4:A:384:PX4:H26	0.42	1.91	17	1
4:A:391:PX4:H34	4:A:391:PX4:H27	0.42	1.46	20	1
4:A:340:PX4:H52	4:A:340:PX4:H31	0.42	1.90	3	1
4:A:366:PX4:H56	4:A:421:PX4:H63	0.42	1.91	5	1
4:A:393:PX4:H65	4:A:393:PX4:H58	0.42	1.53	8	1
4:A:322:PX4:H17	4:A:344:PX4:H24	0.42	1.90	10	1
4:A:399:PX4:H32	4:A:399:PX4:H60	0.42	1.90	10	1
4:A:336:PX4:H55	4:A:344:PX4:C22	0.42	2.43	11	1
4:A:333:PX4:H24	4:A:333:PX4:H29	0.42	1.60	12	1
4:A:347:PX4:H19	4:A:351:PX4:H25	0.42	1.90	12	1
4:A:310:PX4:H28	4:A:364:PX4:H41	0.42	1.90	14	1
4:A:314:PX4:H35	4:A:336:PX4:H68	0.42	1.92	14	1
4:A:397:PX4:H59	4:A:423:PX4:H51	0.42	1.90	15	1
4:A:408:PX4:H28	4:A:422:PX4:H28	0.42	1.91	15	1
4:A:344:PX4:H29	4:A:344:PX4:H24	0.42	1.69	17	1
4:A:393:PX4:H12	4:A:416:PX4:C23	0.42	2.44	17	1
4:A:307:PX4:H41	4:A:327:PX4:H26	0.42	1.90	18	1
4:A:374:PX4:H29	4:A:397:PX4:H69	0.42	1.90	20	1
4:A:428:PX4:H26	4:A:428:PX4:H19	0.42	1.54	20	1
4:A:358:PX4:H72	4:A:383:PX4:H70	0.42	1.92	1	1
4:A:377:PX4:H16	4:A:377:PX4:H46	0.42	1.57	1	3
4:A:396:PX4:H63	4:A:396:PX4:H68	0.42	1.64	2	1
4:A:356:PX4:H62	4:A:356:PX4:H57	0.42	1.66	3	1
4:A:312:PX4:O6	4:A:324:PX4:H12	0.42	2.15	4	1
4:A:332:PX4:H69	4:A:348:PX4:H33	0.42	1.91	4	1
4:A:410:PX4:H38	5:A:435:C3S:H402	0.42	1.91	5	1
4:A:383:PX4:H46	4:A:405:PX4:H48	0.42	1.91	6	1
4:A:327:PX4:H52	4:A:327:PX4:H58	0.42	1.62	8	1
4:A:402:PX4:H33	4:A:426:PX4:H52	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:317:PX4:O1	4:A:320:PX4:H11	0.42	2.15	11	1
4:A:416:PX4:H51	5:A:433:C3S:H152	0.42	1.92	11	1
4:A:393:PX4:H13	4:A:416:PX4:H16	0.42	1.91	13	1
1:A:119:GLU:O	1:A:120:ILE:HG23	0.42	2.14	15	1
4:A:314:PX4:H24	4:A:314:PX4:H30	0.42	1.62	15	1
4:A:332:PX4:H20	4:A:332:PX4:H25	0.42	1.48	15	1
4:A:397:PX4:H33	4:A:412:PX4:H63	0.42	1.92	15	1
1:A:120:ILE:O	4:A:327:PX4:H8	0.42	2.14	17	1
1:A:128:VAL:CG2	4:A:343:PX4:H53	0.42	2.45	17	1
4:A:309:PX4:H31	4:A:309:PX4:H37	0.42	1.57	17	1
4:A:373:PX4:H41	4:A:373:PX4:H35	0.42	1.33	17	1
4:A:404:PX4:H25	4:A:418:PX4:H58	0.42	1.92	19	1
4:A:425:PX4:H42	4:A:425:PX4:H35	0.42	1.59	19	1
4:A:411:PX4:H32	4:A:423:PX4:H61	0.42	1.91	2	1
4:A:318:PX4:H18	4:A:318:PX4:H13	0.42	1.91	3	1
4:A:407:PX4:H68	4:A:407:PX4:H63	0.42	1.69	3	1
4:A:306:PX4:H37	4:A:345:PX4:H30	0.42	1.90	4	1
4:A:313:PX4:H39	4:A:362:PX4:H26	0.42	1.92	4	1
4:A:307:PX4:H18	4:A:331:PX4:H36	0.42	1.92	5	1
4:A:313:PX4:H15	4:A:313:PX4:O8	0.42	2.14	5	1
4:A:387:PX4:H49	4:A:418:PX4:H69	0.42	1.92	6	1
4:A:413:PX4:H35	4:A:428:PX4:C17	0.42	2.41	6	1
4:A:308:PX4:H48	4:A:320:PX4:H22	0.42	1.92	7	1
4:A:365:PX4:O6	4:A:369:PX4:H3	0.42	2.13	7	1
4:A:309:PX4:H67	4:A:309:PX4:H60	0.42	1.62	8	1
4:A:411:PX4:H33	4:A:412:PX4:H62	0.42	1.91	8	1
4:A:364:PX4:H57	4:A:364:PX4:H51	0.42	1.45	10	1
4:A:332:PX4:H14	4:A:348:PX4:H50	0.42	1.90	11	1
4:A:345:PX4:H54	4:A:359:PX4:H15	0.42	1.90	11	1
4:A:319:PX4:H62	4:A:321:PX4:H41	0.42	1.92	12	1
4:A:319:PX4:O2	4:A:341:PX4:H13	0.42	2.15	13	1
4:A:349:PX4:H63	4:A:349:PX4:H56	0.42	1.68	14	1
4:A:396:PX4:H24	4:A:407:PX4:H48	0.42	1.92	14	1
4:A:323:PX4:H40	4:A:323:PX4:H33	0.42	1.62	16	1
4:A:373:PX4:H17	4:A:406:PX4:H46	0.42	1.92	16	1
4:A:410:PX4:H29	4:A:414:PX4:H26	0.42	1.90	16	1
4:A:324:PX4:H52	4:A:324:PX4:H59	0.42	1.72	17	1
4:A:342:PX4:H18	4:A:357:PX4:H43	0.42	1.92	17	1
4:A:367:PX4:H17	4:A:399:PX4:H4	0.42	1.92	17	1
4:A:347:PX4:H36	4:A:347:PX4:H29	0.42	1.51	18	1
4:A:351:PX4:H36	4:A:419:PX4:H65	0.42	1.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:350:PX4:H62	4:A:426:PX4:H70	0.42	1.90	1	1
4:A:375:PX4:H45	4:A:375:PX4:H37	0.42	1.63	1	1
4:A:381:PX4:H28	4:A:417:PX4:H62	0.42	1.91	1	1
4:A:376:PX4:H50	4:A:390:PX4:H15	0.42	1.90	2	1
4:A:318:PX4:H46	4:A:352:PX4:H22	0.42	1.92	5	1
4:A:413:PX4:H25	4:A:413:PX4:H32	0.42	1.48	5	1
4:A:428:PX4:H6	4:A:429:PX4:O4	0.42	2.15	5	1
4:A:312:PX4:H33	4:A:346:PX4:H17	0.42	1.92	6	1
4:A:384:PX4:H20	4:A:405:PX4:H23	0.42	1.92	10	1
4:A:398:PX4:H21	4:A:398:PX4:H28	0.42	1.79	11	1
4:A:305:PX4:H18	4:A:311:PX4:H2	0.42	1.92	12	1
4:A:305:PX4:H58	4:A:312:PX4:H56	0.42	1.92	13	1
4:A:335:PX4:H26	4:A:360:PX4:H48	0.42	1.91	13	1
4:A:376:PX4:H60	4:A:390:PX4:H17	0.42	1.92	17	1
4:A:317:PX4:H20	4:A:326:PX4:H14	0.42	1.91	18	1
4:A:345:PX4:H12	4:A:349:PX4:H17	0.42	1.90	18	1
4:A:367:PX4:H59	4:A:424:PX4:H62	0.42	1.91	18	1
4:A:374:PX4:H20	4:A:423:PX4:H12	0.42	1.91	19	1
4:A:389:PX4:O3	4:A:401:PX4:H6	0.42	2.15	20	1
4:A:331:PX4:H67	4:A:331:PX4:H60	0.41	1.41	2	1
4:A:369:PX4:H24	4:A:430:PX4:H58	0.41	1.91	2	1
4:A:333:PX4:H55	4:A:333:PX4:H24	0.41	1.91	3	1
1:A:161:ALA:HB1	1:A:162:PRO:HD2	0.41	1.92	4	1
4:A:391:PX4:H49	4:A:427:PX4:H40	0.41	1.93	4	1
4:A:359:PX4:H59	4:A:407:PX4:H43	0.41	1.91	5	1
4:A:377:PX4:O2	4:A:408:PX4:H9	0.41	2.15	6	1
4:A:395:PX4:H29	4:A:395:PX4:H36	0.41	1.59	6	1
4:A:374:PX4:H35	4:A:397:PX4:H67	0.41	1.92	7	1
4:A:348:PX4:H44	4:A:348:PX4:H38	0.41	1.58	9	1
4:A:366:PX4:H64	4:A:387:PX4:H55	0.41	1.92	9	1
4:A:404:PX4:H40	4:A:404:PX4:H33	0.41	1.36	9	1
4:A:422:PX4:H10	4:A:425:PX4:O2	0.41	2.15	9	1
4:A:315:PX4:H32	4:A:317:PX4:H46	0.41	1.91	10	1
4:A:366:PX4:H69	4:A:390:PX4:H66	0.41	1.90	14	1
4:A:314:PX4:H70	4:A:416:PX4:H72	0.41	1.91	15	1
4:A:416:PX4:H40	4:A:418:PX4:C36	0.41	2.45	16	1
4:A:319:PX4:C26	4:A:356:PX4:H16	0.41	2.45	17	1
4:A:391:PX4:H49	4:A:427:PX4:H27	0.41	1.91	19	1
4:A:379:PX4:O4	4:A:425:PX4:H3	0.41	2.15	1	1
4:A:313:PX4:H61	4:A:360:PX4:H23	0.41	1.93	3	1
4:A:406:PX4:H67	4:A:406:PX4:H60	0.41	1.46	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H8	4:A:395:PX4:O2	0.41	2.15	4	1
1:A:104:THR:CG2	4:A:320:PX4:H46	0.41	2.45	5	1
4:A:362:PX4:H21	4:A:362:PX4:H48	0.41	1.91	5	1
4:A:409:PX4:H64	4:A:411:PX4:H32	0.41	1.92	6	1
4:A:359:PX4:H72	4:A:376:PX4:H33	0.41	1.93	8	1
4:A:381:PX4:H44	4:A:402:PX4:H72	0.41	1.92	8	1
4:A:379:PX4:H18	4:A:425:PX4:O5	0.41	2.15	9	1
4:A:315:PX4:H59	4:A:332:PX4:O8	0.41	2.15	10	1
4:A:348:PX4:H67	4:A:396:PX4:H72	0.41	1.92	11	1
4:A:359:PX4:H30	4:A:359:PX4:H24	0.41	1.70	11	1
4:A:345:PX4:H58	4:A:345:PX4:H53	0.41	1.60	12	1
4:A:382:PX4:H54	4:A:404:PX4:C22	0.41	2.42	12	1
4:A:382:PX4:H24	4:A:404:PX4:H56	0.41	1.91	16	1
4:A:369:PX4:H27	4:A:374:PX4:H58	0.41	1.91	18	1
4:A:408:PX4:H11	4:A:414:PX4:O1	0.41	2.15	18	1
4:A:399:PX4:H23	4:A:424:PX4:H28	0.41	1.92	19	1
4:A:385:PX4:H52	4:A:415:PX4:H58	0.41	1.91	20	1
4:A:309:PX4:H19	4:A:345:PX4:H57	0.41	1.92	3	1
4:A:376:PX4:C12	4:A:396:PX4:H50	0.41	2.44	3	1
4:A:312:PX4:H64	4:A:333:PX4:H55	0.41	1.92	4	1
4:A:305:PX4:H33	4:A:305:PX4:H68	0.41	1.91	5	1
4:A:312:PX4:H21	4:A:324:PX4:H6	0.41	1.91	6	1
4:A:374:PX4:H5	4:A:411:PX4:O8	0.41	2.14	6	1
4:A:363:PX4:H65	4:A:363:PX4:H58	0.41	1.62	8	1
4:A:373:PX4:H26	4:A:402:PX4:H25	0.41	1.91	8	1
4:A:390:PX4:H27	4:A:416:PX4:H19	0.41	1.91	8	1
4:A:339:PX4:H71	4:A:339:PX4:H65	0.41	1.70	9	1
4:A:375:PX4:H34	4:A:396:PX4:H37	0.41	1.91	9	1
4:A:331:PX4:H53	4:A:331:PX4:H58	0.41	1.52	12	1
4:A:307:PX4:H39	4:A:344:PX4:H33	0.41	1.92	13	1
4:A:345:PX4:H58	4:A:359:PX4:H17	0.41	1.91	13	1
4:A:309:PX4:H63	4:A:309:PX4:H32	0.41	1.92	14	1
4:A:403:PX4:H30	4:A:417:PX4:H27	0.41	1.91	14	1
4:A:365:PX4:H34	4:A:369:PX4:H28	0.41	1.92	15	1
4:A:408:PX4:H18	4:A:427:PX4:H46	0.41	1.91	15	1
4:A:428:PX4:O5	4:A:429:PX4:H54	0.41	2.15	19	1
4:A:320:PX4:C36	4:A:350:PX4:H46	0.41	2.45	20	1
4:A:323:PX4:H60	4:A:360:PX4:H22	0.41	1.92	3	1
4:A:322:PX4:H54	4:A:344:PX4:H22	0.41	1.93	4	1
4:A:342:PX4:H40	4:A:358:PX4:H67	0.41	1.91	4	1
4:A:379:PX4:H45	4:A:384:PX4:H35	0.41	1.92	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:400:PX4:H15	4:A:405:PX4:O2	0.41	2.15	5	1
4:A:308:PX4:H67	4:A:326:PX4:H35	0.41	1.91	8	1
4:A:375:PX4:H20	4:A:392:PX4:H32	0.41	1.92	8	1
4:A:330:PX4:O8	4:A:337:PX4:H3	0.41	2.15	9	1
4:A:373:PX4:H37	4:A:401:PX4:H33	0.41	1.91	9	1
4:A:387:PX4:H33	4:A:387:PX4:H40	0.41	1.60	10	1
4:A:400:PX4:H53	4:A:401:PX4:H55	0.41	1.91	10	1
4:A:310:PX4:H41	4:A:313:PX4:H64	0.41	1.92	11	1
4:A:327:PX4:H32	4:A:359:PX4:H60	0.41	1.91	11	1
4:A:372:PX4:H59	4:A:372:PX4:H53	0.41	1.74	11	1
4:A:372:PX4:H72	4:A:410:PX4:H31	0.41	1.92	11	1
4:A:402:PX4:H42	5:A:431:C3S:C50	0.41	2.45	11	1
4:A:338:PX4:H31	4:A:344:PX4:H58	0.41	1.92	14	1
4:A:324:PX4:H3	5:A:431:C3S:O4	0.41	2.15	15	1
4:A:386:PX4:H52	4:A:417:PX4:C16	0.41	2.45	16	1
4:A:350:PX4:H7	4:A:356:PX4:H51	0.41	1.92	17	1
4:A:400:PX4:H21	4:A:405:PX4:O6	0.41	2.15	17	1
4:A:332:PX4:H34	4:A:332:PX4:H27	0.41	1.69	20	1
4:A:315:PX4:H70	4:A:332:PX4:H63	0.41	1.91	1	1
4:A:384:PX4:H8	4:A:389:PX4:O6	0.41	2.14	2	1
4:A:387:PX4:H62	4:A:421:PX4:H57	0.41	1.92	2	1
4:A:392:PX4:H13	4:A:405:PX4:O1	0.41	2.13	2	1
4:A:381:PX4:H34	4:A:381:PX4:H27	0.41	1.76	3	1
4:A:329:PX4:H63	4:A:329:PX4:H68	0.41	1.78	5	1
4:A:400:PX4:H18	4:A:405:PX4:O2	0.41	2.16	5	1
4:A:421:PX4:H38	4:A:421:PX4:H31	0.41	1.64	6	1
4:A:336:PX4:H30	4:A:357:PX4:H18	0.41	1.92	8	1
4:A:424:PX4:H23	5:A:435:C3S:C44	0.41	2.45	8	1
4:A:321:PX4:H38	4:A:367:PX4:H44	0.41	1.92	9	1
4:A:395:PX4:H28	4:A:402:PX4:C27	0.41	2.45	10	1
4:A:335:PX4:H39	4:A:387:PX4:H41	0.41	1.92	11	1
4:A:305:PX4:H52	4:A:312:PX4:H56	0.41	1.93	12	1
4:A:324:PX4:H17	5:A:431:C3S:H30	0.41	1.91	12	1
4:A:387:PX4:C36	4:A:403:PX4:H35	0.41	2.42	12	1
4:A:375:PX4:H32	4:A:427:PX4:H25	0.41	1.93	16	1
4:A:382:PX4:H50	4:A:404:PX4:H17	0.41	1.92	16	1
4:A:382:PX4:H63	4:A:382:PX4:H69	0.41	1.56	17	1
4:A:321:PX4:H35	4:A:332:PX4:H65	0.41	1.92	19	1
4:A:333:PX4:H15	4:A:333:PX4:H12	0.41	1.91	19	1
4:A:353:PX4:H33	4:A:361:PX4:H63	0.41	1.91	19	1
4:A:380:PX4:H20	4:A:420:PX4:H53	0.41	1.92	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:349:PX4:H16	4:A:361:PX4:H10	0.41	1.92	20	1
4:A:373:PX4:H62	4:A:414:PX4:H35	0.41	1.91	20	1
4:A:307:PX4:O2	4:A:322:PX4:H4	0.41	2.16	1	1
4:A:311:PX4:H43	4:A:377:PX4:H62	0.41	1.91	1	1
4:A:342:PX4:H29	4:A:342:PX4:H35	0.41	1.72	1	1
4:A:346:PX4:H31	4:A:346:PX4:H38	0.41	1.57	1	1
4:A:377:PX4:H17	4:A:408:PX4:H18	0.41	1.91	1	1
4:A:406:PX4:H40	4:A:410:PX4:H39	0.41	1.92	2	1
4:A:356:PX4:H28	4:A:356:PX4:H21	0.41	1.60	4	1
4:A:308:PX4:O4	4:A:320:PX4:H17	0.41	2.16	5	1
4:A:393:PX4:H52	4:A:419:PX4:H28	0.41	1.92	5	1
4:A:313:PX4:H26	4:A:313:PX4:H19	0.41	1.64	6	1
4:A:324:PX4:H47	4:A:333:PX4:H14	0.41	1.93	6	1
4:A:334:PX4:H55	4:A:334:PX4:H48	0.41	1.61	6	1
4:A:414:PX4:H28	4:A:414:PX4:H33	0.41	1.71	8	1
4:A:359:PX4:H41	4:A:430:PX4:H42	0.41	1.90	9	1
4:A:328:PX4:H41	4:A:328:PX4:H36	0.41	1.66	13	1
4:A:342:PX4:H29	4:A:358:PX4:H52	0.41	1.91	15	1
1:A:221:PRO:O	4:A:317:PX4:H5	0.41	2.16	18	1
4:A:362:PX4:H14	4:A:362:PX4:H13	0.41	1.91	18	1
4:A:369:PX4:H53	4:A:419:PX4:H47	0.41	1.92	18	1
4:A:335:PX4:H33	4:A:360:PX4:H31	0.41	1.93	20	1
4:A:334:PX4:H48	5:A:432:C3S:H20	0.41	1.91	1	1
4:A:370:PX4:H35	4:A:370:PX4:H30	0.41	1.61	2	1
4:A:428:PX4:H35	4:A:428:PX4:H42	0.41	1.35	3	1
4:A:306:PX4:H60	4:A:321:PX4:H17	0.41	1.92	4	1
4:A:308:PX4:H32	4:A:320:PX4:H17	0.41	1.92	4	1
4:A:370:PX4:H22	4:A:394:PX4:O7	0.41	2.16	4	1
4:A:398:PX4:H68	4:A:415:PX4:H51	0.41	1.93	4	1
4:A:366:PX4:H51	4:A:403:PX4:H53	0.41	1.92	5	1
4:A:372:PX4:H56	4:A:372:PX4:H63	0.41	1.70	5	1
4:A:380:PX4:H60	4:A:416:PX4:H46	0.41	1.92	6	1
4:A:406:PX4:H34	4:A:406:PX4:H39	0.41	1.43	8	1
1:A:36:GLU:OE2	1:A:40:LYS:NZ	0.41	2.48	9	1
4:A:368:PX4:H25	4:A:408:PX4:H52	0.41	1.92	9	1
4:A:324:PX4:H41	4:A:414:PX4:H52	0.41	1.93	10	1
4:A:379:PX4:H34	4:A:379:PX4:H27	0.41	1.67	10	1
4:A:374:PX4:H37	4:A:374:PX4:H32	0.41	1.51	11	1
4:A:318:PX4:H33	4:A:318:PX4:H28	0.41	1.62	12	1
4:A:389:PX4:H51	4:A:400:PX4:H23	0.41	1.93	12	1
4:A:347:PX4:H17	4:A:351:PX4:O6	0.41	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:382:PX4:H25	4:A:382:PX4:H20	0.41	1.53	13	1
4:A:322:PX4:H41	4:A:331:PX4:C20	0.41	2.46	16	1
4:A:338:PX4:H57	4:A:338:PX4:H50	0.41	1.71	16	1
4:A:315:PX4:H25	4:A:320:PX4:H20	0.41	1.92	19	1
4:A:315:PX4:H43	4:A:423:PX4:H41	0.41	1.91	19	1
4:A:374:PX4:H32	4:A:374:PX4:H37	0.41	1.56	19	1
4:A:315:PX4:H59	4:A:315:PX4:H52	0.41	1.65	1	1
4:A:316:PX4:H30	4:A:321:PX4:H52	0.41	1.92	1	1
4:A:382:PX4:H27	4:A:415:PX4:H61	0.41	1.92	1	1
4:A:306:PX4:H19	4:A:306:PX4:H26	0.41	1.60	5	1
4:A:375:PX4:H34	4:A:427:PX4:H46	0.41	1.92	6	1
4:A:338:PX4:O3	4:A:344:PX4:H4	0.41	2.16	7	1
4:A:429:PX4:H36	4:A:429:PX4:H41	0.41	1.71	7	1
4:A:307:PX4:H25	4:A:322:PX4:H48	0.41	1.92	8	1
4:A:428:PX4:O3	4:A:429:PX4:H15	0.41	2.15	8	1
4:A:417:PX4:H16	4:A:418:PX4:H20	0.41	1.92	9	1
4:A:415:PX4:H66	4:A:421:PX4:H30	0.41	1.91	12	1
4:A:340:PX4:O2	4:A:343:PX4:H12	0.41	2.16	14	1
4:A:394:PX4:H40	4:A:401:PX4:H61	0.41	1.92	16	1
4:A:400:PX4:H65	4:A:405:PX4:H25	0.41	1.92	16	1
4:A:321:PX4:H66	4:A:342:PX4:H72	0.41	1.91	18	1
4:A:386:PX4:H9	4:A:417:PX4:H49	0.41	1.92	18	1
4:A:371:PX4:H14	4:A:373:PX4:C8	0.41	2.45	20	1
4:A:400:PX4:H55	4:A:405:PX4:H49	0.41	1.92	20	1
4:A:415:PX4:H44	4:A:421:PX4:H19	0.41	1.93	20	1
4:A:371:PX4:H26	4:A:395:PX4:H27	0.41	1.93	1	1
4:A:373:PX4:H66	4:A:406:PX4:H67	0.41	1.92	1	1
4:A:383:PX4:H53	4:A:383:PX4:H59	0.41	1.68	1	1
4:A:413:PX4:H18	4:A:429:PX4:H26	0.41	1.92	1	1
4:A:413:PX4:H33	4:A:419:PX4:H31	0.41	1.93	1	1
4:A:319:PX4:O6	4:A:352:PX4:H47	0.41	2.16	2	1
4:A:386:PX4:O3	4:A:402:PX4:H13	0.41	2.15	2	1
1:A:102:HIS:CD2	4:A:350:PX4:H14	0.41	2.51	3	1
4:A:313:PX4:H54	4:A:360:PX4:H45	0.41	1.92	3	1
4:A:397:PX4:H38	4:A:397:PX4:H32	0.41	1.69	3	1
4:A:406:PX4:H26	4:A:410:PX4:H21	0.41	1.92	3	1
4:A:313:PX4:H10	4:A:362:PX4:O1	0.41	2.15	4	1
4:A:402:PX4:O8	4:A:402:PX4:H6	0.41	2.15	4	1
4:A:332:PX4:H61	4:A:376:PX4:H36	0.41	1.93	5	1
4:A:318:PX4:H19	4:A:321:PX4:H50	0.41	1.93	6	1
4:A:322:PX4:H67	4:A:337:PX4:H40	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:371:PX4:H28	4:A:371:PX4:H21	0.41	1.65	6	1
4:A:374:PX4:O8	4:A:423:PX4:H9	0.41	2.16	6	1
4:A:402:PX4:H38	4:A:402:PX4:H32	0.41	1.69	6	1
4:A:316:PX4:H28	4:A:316:PX4:H33	0.41	1.69	7	1
4:A:330:PX4:H59	4:A:330:PX4:H52	0.41	1.40	7	1
4:A:382:PX4:H51	5:A:435:C3S:H653	0.41	1.92	7	1
4:A:401:PX4:H65	4:A:405:PX4:H29	0.41	1.93	7	1
4:A:329:PX4:H71	4:A:329:PX4:H65	0.41	1.60	9	1
4:A:354:PX4:H60	4:A:354:PX4:H55	0.41	1.52	9	1
4:A:386:PX4:H60	4:A:386:PX4:H40	0.41	1.92	9	1
4:A:336:PX4:H66	4:A:429:PX4:H43	0.41	1.91	10	1
4:A:393:PX4:H71	4:A:393:PX4:H65	0.41	1.63	10	1
4:A:399:PX4:H55	4:A:424:PX4:H33	0.41	1.92	10	1
1:A:126:LYS:NZ	4:A:350:PX4:H17	0.41	2.31	11	1
4:A:325:PX4:H25	4:A:325:PX4:H20	0.41	1.63	12	1
4:A:326:PX4:H46	4:A:361:PX4:H47	0.41	1.92	12	1
4:A:413:PX4:H18	4:A:419:PX4:H22	0.41	1.92	12	1
4:A:414:PX4:H53	4:A:414:PX4:H46	0.41	1.65	12	1
4:A:359:PX4:H32	4:A:359:PX4:H37	0.41	1.71	13	1
4:A:377:PX4:H45	4:A:391:PX4:H35	0.41	1.92	13	1
4:A:412:PX4:H15	4:A:412:PX4:H13	0.41	1.93	13	1
4:A:365:PX4:H53	4:A:383:PX4:H20	0.41	1.92	14	1
4:A:374:PX4:H4	4:A:397:PX4:O6	0.41	2.16	14	1
4:A:338:PX4:H4	4:A:360:PX4:H46	0.41	1.93	15	1
4:A:391:PX4:H48	4:A:391:PX4:H55	0.41	1.60	15	1
4:A:400:PX4:O7	4:A:405:PX4:H16	0.41	2.16	15	1
4:A:383:PX4:H58	4:A:405:PX4:H50	0.41	1.92	16	1
4:A:310:PX4:H28	4:A:310:PX4:H21	0.41	1.76	17	1
4:A:353:PX4:H32	4:A:353:PX4:H37	0.41	1.50	17	1
4:A:392:PX4:H29	4:A:405:PX4:H48	0.41	1.93	17	1
4:A:316:PX4:H48	4:A:321:PX4:H24	0.41	1.93	18	1
4:A:369:PX4:H21	4:A:429:PX4:H52	0.41	1.92	18	1
4:A:317:PX4:H30	4:A:317:PX4:H35	0.41	1.59	19	1
4:A:318:PX4:H59	4:A:336:PX4:C17	0.41	2.45	19	1
4:A:340:PX4:H6	5:A:432:C3S:O3	0.41	2.16	19	1
4:A:352:PX4:H62	4:A:352:PX4:H57	0.41	1.51	19	1
4:A:368:PX4:H14	4:A:368:PX4:H13	0.41	1.92	19	1
4:A:394:PX4:O6	4:A:400:PX4:H10	0.41	2.16	19	1
4:A:363:PX4:H56	4:A:363:PX4:H63	0.41	1.71	20	1
4:A:370:PX4:C22	4:A:383:PX4:H64	0.41	2.45	20	1
4:A:392:PX4:H63	4:A:392:PX4:H56	0.41	1.63	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H6	4:A:430:PX4:O8	0.41	2.15	1	1
4:A:318:PX4:H27	4:A:342:PX4:H57	0.41	1.92	2	1
4:A:320:PX4:H63	4:A:320:PX4:H68	0.41	1.79	2	1
4:A:374:PX4:O2	4:A:423:PX4:H7	0.41	2.16	2	1
4:A:397:PX4:H29	4:A:398:PX4:C15	0.41	2.45	2	1
4:A:325:PX4:O6	4:A:330:PX4:H10	0.41	2.15	3	1
4:A:385:PX4:H65	4:A:415:PX4:H55	0.41	1.93	3	1
4:A:409:PX4:H29	4:A:409:PX4:H23	0.41	1.67	3	1
4:A:308:PX4:H53	4:A:326:PX4:H19	0.41	1.91	4	1
4:A:365:PX4:H30	4:A:369:PX4:H53	0.41	1.93	4	1
4:A:306:PX4:H56	4:A:321:PX4:H24	0.41	1.92	6	1
4:A:323:PX4:H37	4:A:323:PX4:H32	0.41	1.50	6	1
4:A:406:PX4:H18	4:A:414:PX4:H26	0.41	1.92	9	1
4:A:430:PX4:H31	4:A:430:PX4:H66	0.41	1.93	9	1
4:A:335:PX4:H55	4:A:335:PX4:H48	0.41	1.80	10	1
4:A:312:PX4:H21	4:A:346:PX4:H47	0.41	1.93	11	1
4:A:323:PX4:H41	4:A:325:PX4:H63	0.41	1.92	11	1
4:A:366:PX4:H19	4:A:378:PX4:H20	0.41	1.92	14	1
4:A:369:PX4:H52	4:A:419:PX4:H59	0.41	1.93	14	1
4:A:307:PX4:H65	4:A:348:PX4:H65	0.41	1.92	15	1
4:A:322:PX4:H24	4:A:330:PX4:H60	0.41	1.93	15	1
4:A:409:PX4:H45	4:A:409:PX4:H38	0.41	1.76	15	1
4:A:366:PX4:H59	4:A:378:PX4:H22	0.41	1.92	16	1
4:A:367:PX4:H56	4:A:412:PX4:H48	0.41	1.93	16	1
4:A:407:PX4:H17	4:A:427:PX4:O4	0.41	2.15	17	1
4:A:366:PX4:H54	4:A:378:PX4:H27	0.41	1.92	18	1
4:A:379:PX4:H22	5:A:434:C3S:C13	0.41	2.45	19	1
4:A:317:PX4:O2	4:A:330:PX4:H4	0.41	2.15	20	1
4:A:330:PX4:H21	4:A:337:PX4:H20	0.41	1.93	20	1
4:A:406:PX4:H19	4:A:414:PX4:H33	0.41	1.91	20	1
4:A:366:PX4:H36	4:A:403:PX4:H25	0.40	1.91	1	1
4:A:375:PX4:H66	4:A:405:PX4:H42	0.40	1.92	1	1
4:A:363:PX4:H34	4:A:363:PX4:H39	0.40	1.74	2	1
4:A:307:PX4:C17	4:A:337:PX4:H36	0.40	2.46	3	1
4:A:318:PX4:H19	4:A:342:PX4:H18	0.40	1.91	3	1
4:A:338:PX4:C35	4:A:359:PX4:H32	0.40	2.42	3	1
4:A:408:PX4:H19	4:A:408:PX4:H26	0.40	1.68	3	1
4:A:383:PX4:H54	4:A:394:PX4:H26	0.40	1.92	4	1
4:A:422:PX4:H50	4:A:425:PX4:H17	0.40	1.92	4	1
4:A:392:PX4:H47	4:A:425:PX4:H50	0.40	1.92	5	1
4:A:330:PX4:O8	4:A:337:PX4:H13	0.40	2.16	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H29	4:A:389:PX4:H24	0.40	1.67	9	1
4:A:382:PX4:H30	4:A:398:PX4:H59	0.40	1.93	10	1
4:A:394:PX4:H21	4:A:407:PX4:H54	0.40	1.92	10	1
4:A:305:PX4:H45	4:A:333:PX4:H63	0.40	1.93	11	1
4:A:311:PX4:H56	4:A:311:PX4:H62	0.40	1.74	11	1
4:A:332:PX4:H55	4:A:332:PX4:H60	0.40	1.72	11	1
4:A:323:PX4:H34	4:A:353:PX4:H25	0.40	1.92	12	1
4:A:350:PX4:H61	4:A:350:PX4:H54	0.40	1.48	12	1
4:A:403:PX4:H32	4:A:417:PX4:H32	0.40	1.92	13	1
4:A:322:PX4:H63	4:A:337:PX4:H36	0.40	1.92	14	1
4:A:369:PX4:H31	4:A:383:PX4:H23	0.40	1.93	14	1
4:A:402:PX4:H63	4:A:402:PX4:H68	0.40	1.76	14	1
4:A:404:PX4:H21	4:A:418:PX4:H22	0.40	1.93	14	1
4:A:329:PX4:H59	4:A:329:PX4:H52	0.40	1.68	17	1
4:A:328:PX4:H34	4:A:351:PX4:H31	0.40	1.92	18	1
4:A:429:PX4:O6	4:A:429:PX4:H4	0.40	2.16	18	1
4:A:333:PX4:H68	4:A:333:PX4:H62	0.40	1.67	1	1
4:A:317:PX4:H52	4:A:326:PX4:H27	0.40	1.93	2	1
4:A:336:PX4:H45	4:A:413:PX4:H63	0.40	1.92	3	1
4:A:409:PX4:H27	4:A:412:PX4:H29	0.40	1.93	4	1
4:A:349:PX4:H26	4:A:353:PX4:H50	0.40	1.93	5	1
4:A:397:PX4:H55	4:A:423:PX4:H55	0.40	1.93	6	1
4:A:343:PX4:H59	4:A:350:PX4:H59	0.40	1.94	7	1
4:A:365:PX4:H29	4:A:419:PX4:H60	0.40	1.92	7	1
4:A:400:PX4:H36	4:A:401:PX4:H62	0.40	1.92	7	1
4:A:404:PX4:H33	4:A:417:PX4:H31	0.40	1.94	7	1
4:A:351:PX4:H30	4:A:359:PX4:H39	0.40	1.93	8	1
4:A:306:PX4:H30	4:A:306:PX4:H35	0.40	1.72	9	1
4:A:361:PX4:H19	4:A:361:PX4:H25	0.40	1.56	9	1
4:A:370:PX4:H45	4:A:383:PX4:H67	0.40	1.93	9	1
4:A:322:PX4:H20	4:A:322:PX4:H25	0.40	1.72	11	1
4:A:388:PX4:H13	4:A:388:PX4:H2	0.40	1.72	11	1
4:A:417:PX4:H64	4:A:418:PX4:H31	0.40	1.93	12	1
4:A:307:PX4:H35	4:A:307:PX4:H41	0.40	1.45	15	1
4:A:343:PX4:H64	4:A:343:PX4:H72	0.40	1.30	16	1
4:A:334:PX4:H59	4:A:334:PX4:H52	0.40	1.73	17	1
4:A:374:PX4:H8	4:A:428:PX4:O1	0.40	2.17	17	1
4:A:370:PX4:H67	4:A:374:PX4:H69	0.40	1.93	18	1
4:A:325:PX4:H70	4:A:403:PX4:H72	0.40	1.92	19	1
4:A:408:PX4:H38	4:A:422:PX4:H44	0.40	1.94	19	1
4:A:324:PX4:H66	4:A:333:PX4:H53	0.40	1.92	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:375:PX4:H51	4:A:384:PX4:C13	0.40	2.46	20	1
4:A:370:PX4:O8	4:A:381:PX4:H1	0.40	2.16	2	1
4:A:391:PX4:H71	4:A:414:PX4:H59	0.40	1.92	2	1
4:A:306:PX4:H56	4:A:342:PX4:H24	0.40	1.93	3	1
4:A:305:PX4:H69	4:A:324:PX4:H31	0.40	1.93	6	1
4:A:308:PX4:H30	4:A:320:PX4:H17	0.40	1.91	6	1
4:A:386:PX4:H27	4:A:386:PX4:H21	0.40	1.81	7	1
4:A:413:PX4:H65	4:A:413:PX4:H58	0.40	1.65	7	1
4:A:340:PX4:H40	4:A:340:PX4:H33	0.40	1.51	8	1
4:A:355:PX4:H20	4:A:362:PX4:H17	0.40	1.93	9	1
4:A:415:PX4:H46	4:A:415:PX4:H53	0.40	1.69	9	1
4:A:310:PX4:H62	4:A:310:PX4:H57	0.40	1.66	10	1
4:A:349:PX4:H65	4:A:358:PX4:H36	0.40	1.91	10	1
4:A:313:PX4:H27	4:A:362:PX4:H62	0.40	1.93	12	1
4:A:375:PX4:H7	4:A:392:PX4:O6	0.40	2.16	12	1
4:A:417:PX4:H26	4:A:418:PX4:H46	0.40	1.93	12	1
4:A:305:PX4:H57	4:A:305:PX4:H62	0.40	1.67	13	1
4:A:323:PX4:H34	4:A:328:PX4:H37	0.40	1.93	13	1
4:A:348:PX4:H39	4:A:383:PX4:H42	0.40	1.92	13	1
4:A:373:PX4:H57	4:A:406:PX4:H52	0.40	1.93	13	1
4:A:373:PX4:H49	4:A:406:PX4:H17	0.40	1.93	15	1
4:A:314:PX4:H62	4:A:354:PX4:H29	0.40	1.92	16	1
4:A:371:PX4:H27	4:A:395:PX4:H30	0.40	1.92	16	1
4:A:401:PX4:H37	4:A:401:PX4:H32	0.40	1.58	19	1
4:A:319:PX4:H57	4:A:343:PX4:H19	0.40	1.93	20	1
4:A:351:PX4:H71	4:A:351:PX4:H65	0.40	1.70	20	1
4:A:401:PX4:H25	4:A:401:PX4:H32	0.40	1.64	20	1
4:A:384:PX4:H38	4:A:405:PX4:H27	0.40	1.92	1	1
4:A:411:PX4:H63	4:A:423:PX4:H51	0.40	1.92	3	1
4:A:338:PX4:H55	4:A:359:PX4:H35	0.40	1.93	5	1
4:A:354:PX4:H26	4:A:354:PX4:H31	0.40	1.66	6	1
4:A:322:PX4:H35	4:A:337:PX4:H42	0.40	1.92	8	1
4:A:369:PX4:O6	4:A:429:PX4:H49	0.40	2.16	9	1
4:A:374:PX4:H25	4:A:417:PX4:H68	0.40	1.92	9	1
4:A:368:PX4:H33	4:A:368:PX4:H28	0.40	1.69	10	1
1:A:26:ASP:OD2	1:A:38:LYS:NZ	0.40	2.52	13	1
4:A:343:PX4:H66	4:A:343:PX4:H61	0.40	1.70	13	1
1:A:57:ARG:NH2	1:A:60:GLU:OE2	0.40	2.45	14	1
4:A:383:PX4:H38	4:A:383:PX4:H31	0.40	1.80	14	1
1:A:221:PRO:CG	1:A:224:PHE:HB2	0.40	2.46	15	1
4:A:322:PX4:H47	4:A:344:PX4:H19	0.40	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:H1	4:A:427:PX4:O2	0.40	2.17	15	1
4:A:306:PX4:H21	4:A:342:PX4:H25	0.40	1.93	16	1
4:A:391:PX4:H6	4:A:391:PX4:H2	0.40	1.82	16	1
4:A:409:PX4:H51	4:A:409:PX4:H56	0.40	1.59	16	1
4:A:321:PX4:H72	4:A:321:PX4:H64	0.40	1.78	17	1
4:A:328:PX4:H37	4:A:345:PX4:H23	0.40	1.93	18	1
4:A:330:PX4:H31	4:A:330:PX4:H38	0.40	1.56	19	1
4:A:317:PX4:H69	4:A:330:PX4:H44	0.40	1.93	20	1
4:A:306:PX4:H71	4:A:306:PX4:H65	0.40	1.73	1	1
4:A:345:PX4:H32	4:A:345:PX4:H37	0.40	1.78	2	1
4:A:363:PX4:H43	4:A:408:PX4:H43	0.40	1.92	2	1
4:A:365:PX4:H21	4:A:365:PX4:H27	0.40	1.69	2	1
4:A:426:PX4:H7	4:A:426:PX4:H15	0.40	1.94	3	1
4:A:367:PX4:H8	4:A:389:PX4:O1	0.40	2.17	5	1
4:A:397:PX4:H31	4:A:397:PX4:H26	0.40	1.65	5	1
4:A:370:PX4:H35	4:A:394:PX4:H20	0.40	1.93	7	1
4:A:371:PX4:H62	4:A:402:PX4:H40	0.40	1.93	8	1
4:A:368:PX4:H47	5:A:436:C3S:H322	0.40	1.92	9	1
4:A:409:PX4:H63	4:A:411:PX4:H22	0.40	1.94	9	1
4:A:330:PX4:H58	4:A:330:PX4:H53	0.40	1.70	10	1
4:A:376:PX4:H49	4:A:390:PX4:H4	0.40	1.93	10	1
4:A:379:PX4:O1	4:A:409:PX4:H25	0.40	2.15	12	1
4:A:377:PX4:H30	4:A:408:PX4:H30	0.40	1.94	13	1
4:A:378:PX4:H44	4:A:378:PX4:H38	0.40	1.70	16	1
4:A:395:PX4:H47	4:A:395:PX4:H11	0.40	1.92	16	1
4:A:331:PX4:H69	4:A:331:PX4:H63	0.40	1.72	17	1
4:A:314:PX4:H19	4:A:336:PX4:H24	0.40	1.94	18	1
4:A:314:PX4:H72	4:A:314:PX4:H64	0.40	1.73	19	1
4:A:344:PX4:H34	4:A:344:PX4:H27	0.40	1.46	19	1
4:A:362:PX4:H29	4:A:364:PX4:H48	0.40	1.92	19	1
4:A:400:PX4:H59	4:A:405:PX4:C11	0.40	2.46	19	1
4:A:313:PX4:C28	4:A:325:PX4:H55	0.40	2.46	20	1
4:A:324:PX4:H54	4:A:324:PX4:H49	0.40	1.53	20	1
4:A:339:PX4:H20	4:A:339:PX4:H26	0.40	1.73	20	1
4:A:366:PX4:H51	4:A:403:PX4:C23	0.40	2.47	20	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/250 (95%)	211±3 (89±1%)	20±3 (8±1%)	6±1 (3±1%)	6	42
All	All	4740/5000 (95%)	4216 (89%)	401 (8%)	123 (3%)	6	42

All 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	31	ASN	18
1	A	147	TYR	18
1	A	150	ASP	16
1	A	25	TYR	11
1	A	224	PHE	11
1	A	155	THR	9
1	A	57	ARG	6
1	A	55	ASN	5
1	A	130	GLY	4
1	A	166	LEU	4
1	A	154	ASN	4
1	A	24	LEU	3
1	A	58	VAL	2
1	A	83	LYS	2
1	A	143	HIS	2
1	A	162	PRO	2
1	A	214	PRO	1
1	A	7	MET	1
1	A	49	PRO	1
1	A	117	GLY	1
1	A	141	GLY	1
1	A	183	SER	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/208 (94%)	187±3 (96±1%)	8±3 (4±1%)	29	79
All	All	3900/4160 (94%)	3745 (96%)	155 (4%)	29	79

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

Mol	Chain	Res	Type	Models (Total)
1	A	150	ASP	20
1	A	155	THR	12
1	A	177	ARG	7
1	A	75	TYR	6
1	A	179	THR	6
1	A	122	LEU	5
1	A	26	ASP	5
1	A	97	THR	5
1	A	156	LEU	5
1	A	45	PHE	4
1	A	10	LEU	4
1	A	158	HIS	4
1	A	166	LEU	4
1	A	171	HIS	3
1	A	174	GLU	3
1	A	202	MET	3
1	A	60	GLU	2
1	A	126	LYS	2
1	A	9	GLU	2
1	A	110	SER	2
1	A	63	GLN	2
1	A	180	ASP	2
1	A	38	LYS	2
1	A	3	GLU	2
1	A	120	ILE	2
1	A	2	GLN	2
1	A	115	MET	2
1	A	71	ASP	1
1	A	36	GLU	1
1	A	211	VAL	1
1	A	127	VAL	1
1	A	19	LEU	1
1	A	94	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	125	ARG	1
1	A	54	LEU	1
1	A	119	GLU	1
1	A	99	ASP	1
1	A	100	LEU	1
1	A	183	SER	1
1	A	215	THR	1
1	A	242	SER	1
1	A	34	SER	1
1	A	189	LEU	1
1	A	149	PHE	1
1	A	16	GLN	1
1	A	83	LYS	1
1	A	86	SER	1
1	A	128	VAL	1
1	A	198	HIS	1
1	A	72	VAL	1
1	A	145	ASP	1
1	A	164	THR	1
1	A	235	GLN	1
1	A	93	ILE	1
1	A	209	ASN	1
1	A	74	GLU	1
1	A	33	ASN	1
1	A	67	CYS	1
1	A	98	ARG	1
1	A	143	HIS	1
1	A	96	TYR	1
1	A	105	VAL	1
1	A	114	ASN	1
1	A	162	PRO	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 136 ligands modelled in this entry, 4 are monoatomic - leaving 132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	318	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	432	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	388	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	435	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	383	-	45,45,45	0.64±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	355	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	436	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	376	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.64±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
5	C3S	A	434	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	391	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	431	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	392	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.64±0.00	0±0 (0±0%)
5	C3S	A	433	-	35,35,35	1.29±0.01	2±0 (5±0%)
4	PX4	A	340	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	305	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.64±0.00	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.00	0±0 (0±0%)

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

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	318	-	51,53,53	1.51±0.15	9±3 (18±5%)
4	PX4	A	344	-	51,53,53	1.46±0.18	9±3 (16±6%)
4	PX4	A	405	-	51,53,53	1.57±0.14	10±3 (19±5%)
4	PX4	A	408	-	51,53,53	1.51±0.21	9±3 (16±6%)
4	PX4	A	386	-	51,53,53	1.52±0.12	10±2 (18±3%)
4	PX4	A	353	-	51,53,53	1.55±0.19	10±3 (19±6%)
4	PX4	A	361	-	51,53,53	1.49±0.18	9±3 (17±5%)
4	PX4	A	428	-	51,53,53	1.46±0.16	9±3 (17±5%)
4	PX4	A	345	-	51,53,53	1.51±0.16	9±2 (16±3%)
4	PX4	A	365	-	51,53,53	1.50±0.14	9±2 (17±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	379	-	51,53,53	1.51±0.14	9±2 (17±4%)
4	PX4	A	308	-	51,53,53	1.50±0.16	8±2 (15±3%)
4	PX4	A	347	-	51,53,53	1.54±0.15	10±2 (19±4%)
4	PX4	A	368	-	51,53,53	1.49±0.12	8±2 (16±4%)
4	PX4	A	380	-	51,53,53	1.48±0.12	9±2 (16±3%)
4	PX4	A	413	-	51,53,53	1.52±0.16	10±3 (19±5%)
4	PX4	A	343	-	51,53,53	1.58±0.14	11±2 (20±4%)
4	PX4	A	373	-	51,53,53	1.49±0.17	9±2 (16±3%)
4	PX4	A	414	-	51,53,53	1.51±0.12	9±3 (18±5%)
4	PX4	A	315	-	51,53,53	1.47±0.12	9±2 (17±4%)
4	PX4	A	381	-	51,53,53	1.59±0.17	10±3 (20±5%)
5	C3S	A	432	-	51,55,55	2.46±0.22	20±4 (39±6%)
4	PX4	A	388	-	51,53,53	1.48±0.11	8±2 (16±4%)
4	PX4	A	335	-	51,53,53	1.56±0.14	10±3 (19±5%)
4	PX4	A	341	-	51,53,53	1.50±0.19	9±3 (17±5%)
5	C3S	A	435	-	51,55,55	2.39±0.27	21±4 (41±7%)
4	PX4	A	383	-	51,53,53	1.49±0.17	9±3 (17±6%)
4	PX4	A	355	-	51,53,53	1.51±0.16	9±3 (18±5%)
4	PX4	A	317	-	51,53,53	1.45±0.15	8±2 (16±4%)
4	PX4	A	332	-	51,53,53	1.52±0.14	8±2 (16±4%)
4	PX4	A	423	-	51,53,53	1.48±0.14	9±2 (17±3%)
4	PX4	A	427	-	51,53,53	1.52±0.18	9±3 (18±6%)
4	PX4	A	310	-	51,53,53	1.53±0.17	9±3 (17±5%)
4	PX4	A	333	-	51,53,53	1.50±0.19	9±3 (18±5%)
4	PX4	A	403	-	51,53,53	1.49±0.11	8±2 (16±4%)
4	PX4	A	377	-	51,53,53	1.53±0.14	9±2 (18±4%)
4	PX4	A	348	-	51,53,53	1.52±0.12	9±2 (17±4%)
4	PX4	A	357	-	51,53,53	1.60±0.15	10±2 (19±4%)
4	PX4	A	396	-	51,53,53	1.46±0.14	9±2 (17±4%)
4	PX4	A	407	-	51,53,53	1.52±0.16	9±3 (17±5%)
4	PX4	A	410	-	51,53,53	1.47±0.11	8±2 (16±4%)
4	PX4	A	336	-	51,53,53	1.56±0.18	9±3 (18±4%)
4	PX4	A	400	-	51,53,53	1.49±0.14	9±2 (17±4%)
4	PX4	A	351	-	51,53,53	1.45±0.15	8±2 (15±4%)
4	PX4	A	382	-	51,53,53	1.51±0.11	8±2 (16±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	387	-	51,53,53	1.56±0.12	10±2 (18±3%)
4	PX4	A	384	-	51,53,53	1.53±0.16	10±3 (19±5%)
4	PX4	A	337	-	51,53,53	1.49±0.16	8±3 (15±5%)
4	PX4	A	417	-	51,53,53	1.53±0.13	10±2 (18±4%)
4	PX4	A	324	-	51,53,53	1.51±0.17	10±2 (18±4%)
4	PX4	A	378	-	51,53,53	1.51±0.19	9±3 (18±6%)
4	PX4	A	358	-	51,53,53	1.48±0.18	9±3 (17±6%)
4	PX4	A	375	-	51,53,53	1.55±0.15	10±2 (19±4%)
4	PX4	A	429	-	51,53,53	1.51±0.14	9±2 (18±4%)
4	PX4	A	362	-	51,53,53	1.46±0.13	8±2 (15±4%)
5	C3S	A	436	-	51,55,55	2.39±0.26	18±3 (35±6%)
4	PX4	A	376	-	51,53,53	1.56±0.21	10±2 (19±4%)
4	PX4	A	409	-	51,53,53	1.56±0.15	10±3 (20±4%)
4	PX4	A	314	-	51,53,53	1.52±0.14	10±3 (18±5%)
4	PX4	A	339	-	51,53,53	1.44±0.14	8±2 (15±4%)
4	PX4	A	334	-	51,53,53	1.50±0.13	9±2 (17±3%)
4	PX4	A	309	-	51,53,53	1.55±0.15	9±2 (18±3%)
4	PX4	A	319	-	51,53,53	1.54±0.17	9±3 (18±5%)
4	PX4	A	425	-	51,53,53	1.49±0.14	9±2 (17±4%)
4	PX4	A	395	-	51,53,53	1.55±0.17	10±3 (18±5%)
4	PX4	A	390	-	51,53,53	1.49±0.12	9±2 (16±4%)
4	PX4	A	352	-	51,53,53	1.51±0.12	9±2 (17±3%)
4	PX4	A	416	-	51,53,53	1.55±0.16	10±3 (19±5%)
4	PX4	A	411	-	51,53,53	1.52±0.16	10±3 (19±5%)
4	PX4	A	398	-	51,53,53	1.50±0.14	9±3 (18±5%)
5	C3S	A	434	-	51,55,55	2.36±0.26	19±3 (37±5%)
4	PX4	A	391	-	51,53,53	1.49±0.12	9±2 (17±4%)
4	PX4	A	397	-	51,53,53	1.55±0.14	10±3 (19±6%)
5	C3S	A	431	-	51,55,55	2.37±0.33	20±4 (38±8%)
4	PX4	A	392	-	51,53,53	1.52±0.13	8±2 (16±4%)
4	PX4	A	326	-	51,53,53	1.53±0.13	9±2 (18±4%)
4	PX4	A	404	-	51,53,53	1.45±0.15	9±2 (16±4%)
4	PX4	A	313	-	51,53,53	1.51±0.14	9±2 (17±3%)
4	PX4	A	415	-	51,53,53	1.53±0.14	9±2 (18±4%)
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Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	311	-	51,53,53	1.52±0.16	9±3 (18±6%)
4	PX4	A	364	-	51,53,53	1.53±0.14	9±3 (18±5%)
4	PX4	A	307	-	51,53,53	1.51±0.14	9±3 (17±5%)
4	PX4	A	360	-	51,53,53	1.51±0.16	9±2 (17±4%)
4	PX4	A	323	-	51,53,53	1.53±0.10	10±3 (19±5%)
4	PX4	A	327	-	51,53,53	1.42±0.17	8±3 (14±5%)
4	PX4	A	349	-	51,53,53	1.51±0.11	9±2 (17±3%)
4	PX4	A	363	-	51,53,53	1.47±0.15	9±3 (18±4%)
4	PX4	A	316	-	51,53,53	1.51±0.14	9±2 (17±4%)
4	PX4	A	367	-	51,53,53	1.53±0.14	9±3 (17±5%)
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4	PX4	A	385	-	51,53,53	1.52±0.13	9±2 (17±3%)
4	PX4	A	424	-	51,53,53	1.47±0.19	9±2 (17±3%)
4	PX4	A	370	-	51,53,53	1.52±0.13	9±2 (17±4%)
4	PX4	A	359	-	51,53,53	1.53±0.13	9±2 (18±4%)
5	C3S	A	433	-	51,55,55	2.37±0.21	20±3 (38±6%)
4	PX4	A	340	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	350	-	51,53,53	1.49±0.12	9±2 (16±4%)
4	PX4	A	369	-	51,53,53	1.47±0.09	9±2 (17±3%)
4	PX4	A	354	-	51,53,53	1.53±0.19	9±2 (17±3%)
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4	PX4	A	422	-	51,53,53	1.47±0.13	8±2 (16±4%)
4	PX4	A	325	-	51,53,53	1.54±0.17	10±2 (18±4%)
4	PX4	A	426	-	51,53,53	1.45±0.16	8±2 (15±4%)
4	PX4	A	342	-	51,53,53	1.51±0.17	9±2 (18±4%)
4	PX4	A	356	-	51,53,53	1.58±0.15	10±2 (20±3%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
5	C3S	A	434	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	377	-	-	1±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
5	C3S	A	432	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
5	C3S	A	435	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	1±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-

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

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
5	A	433	C3S	O6-S1	6.36	1.76	1.57	12	20
5	A	431	C3S	O6-S1	6.36	1.76	1.57	14	20
5	A	433	C3S	O6-C7	2.45	1.43	1.48	19	20
5	A	435	C3S	O6-C7	2.44	1.43	1.48	19	20
5	A	431	C3S	O6-C7	2.43	1.43	1.48	6	20
5	A	434	C3S	O6-C7	2.43	1.43	1.48	3	20
5	A	436	C3S	O6-C7	2.40	1.43	1.48	7	20
5	A	432	C3S	O6-C7	2.39	1.43	1.48	19	20

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
5	A	432	C3S	C29-C38-C48	10.43	135.60	119.50	14	20
5	A	434	C3S	C29-C38-C48	9.47	134.12	119.50	15	16
5	A	433	C3S	O6-C7-C4	9.27	121.32	107.61	20	12
5	A	436	C3S	C50-C48-C38	8.98	126.36	112.88	16	17
5	A	431	C3S	C9-C12-C22	8.79	127.67	116.42	1	14
5	A	431	C3S	C29-C38-C48	8.78	133.05	119.50	8	16
5	A	434	C3S	C23-C20-C22	8.73	123.85	113.08	13	13
5	A	433	C3S	C29-C38-C48	8.60	132.78	119.50	18	19
5	A	436	C3S	O6-C7-C4	8.32	119.91	107.61	6	12
5	A	434	C3S	C40-C29-C30	8.28	126.70	111.68	12	15
5	A	436	C3S	C35-C38-C48	8.23	124.63	112.18	8	10
4	A	375	PX4	C8-C7-C6	8.18	92.71	111.78	11	14
5	A	434	C3S	C40-C29-C26	8.17	98.57	110.61	16	12
4	A	308	PX4	C8-C7-C6	8.02	93.09	111.78	4	13
5	A	431	C3S	O6-C7-C4	7.89	119.26	107.61	12	11
5	A	435	C3S	C9-C12-C22	7.78	126.38	116.42	13	19
5	A	434	C3S	C9-C12-C22	7.75	126.34	116.42	15	18
5	A	436	C3S	C29-C38-C48	7.72	131.41	119.50	12	15
5	A	435	C3S	C20-C18-C30	7.68	119.12	109.09	10	9
5	A	432	C3S	C9-C12-C22	7.49	126.01	116.42	18	17
5	A	435	C3S	C29-C38-C48	7.46	131.02	119.50	14	19
5	A	434	C3S	O6-C7-C4	7.44	118.60	107.61	2	11
4	A	381	PX4	O7-C23-C24	7.43	127.55	111.48	17	9
5	A	435	C3S	C7-C9-C12	7.35	122.30	111.45	11	9
4	A	354	PX4	C8-C7-C6	7.32	94.73	111.78	15	10
5	A	435	C3S	C44-C22-C20	7.31	119.87	111.66	1	11
5	A	432	C3S	C44-C22-C20	7.30	119.85	111.66	18	12
4	A	391	PX4	C8-C7-C6	7.27	94.84	111.78	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	337	PX4	C8-C7-C6	7.26	94.87	111.78	2	15
5	A	432	C3S	O6-C7-C4	7.23	118.29	107.61	19	11
4	A	424	PX4	C7-O7-C23	7.20	135.03	117.80	18	9
5	A	436	C3S	C9-C12-C22	7.18	125.61	116.42	9	14
5	A	436	C3S	C50-C48-C54	7.17	99.24	110.34	9	8
5	A	433	C3S	C54-C48-C38	7.16	125.18	110.33	14	16
4	A	406	PX4	C8-C7-C6	7.15	95.12	111.78	12	10
5	A	435	C3S	O3-S1-O6	7.10	90.06	106.37	19	9
4	A	353	PX4	O7-C23-C24	7.10	126.83	111.48	17	11
5	A	432	C3S	C50-C48-C54	7.10	99.36	110.34	12	11
5	A	431	C3S	C35-C38-C29	7.07	95.53	103.84	8	16
5	A	431	C3S	C15-C18-C20	7.04	101.58	109.72	18	10
4	A	426	PX4	O5-C8-C7	6.91	128.32	108.40	6	13
4	A	376	PX4	O5-C8-C7	6.87	128.20	108.40	7	13
5	A	434	C3S	C44-C22-C20	6.83	119.33	111.66	14	6
4	A	376	PX4	C8-C7-C6	6.83	95.86	111.78	3	14
4	A	325	PX4	O7-C23-C24	6.82	126.24	111.48	8	11
4	A	376	PX4	C7-O7-C23	6.82	134.12	117.80	7	8
5	A	434	C3S	C4-C7-C9	6.79	101.54	110.97	20	8
5	A	435	C3S	C40-C29-C26	6.70	100.72	110.61	7	15
4	A	367	PX4	O7-C23-C24	6.70	125.98	111.48	8	7
5	A	432	C3S	C40-C29-C30	6.67	123.77	111.68	13	15
4	A	407	PX4	C8-C7-C6	6.66	96.25	111.78	3	10
4	A	317	PX4	C8-C7-C6	6.65	96.27	111.78	17	9
4	A	356	PX4	C7-O7-C23	6.64	133.68	117.80	7	15
4	A	324	PX4	O5-C8-C7	6.60	127.42	108.40	19	13
4	A	389	PX4	C8-C7-C6	6.60	96.40	111.78	6	11
4	A	423	PX4	O5-C8-C7	6.59	127.39	108.40	4	14
5	A	435	C3S	C4-C7-C9	6.57	120.11	110.97	2	7
4	A	376	PX4	O7-C23-C24	6.54	125.64	111.48	3	13
5	A	431	C3S	C44-C22-C12	6.52	98.42	108.38	2	10
4	A	345	PX4	O7-C23-C24	6.51	125.57	111.48	1	9
5	A	436	C3S	C40-C29-C26	6.50	101.02	110.61	10	16
5	A	436	C3S	C9-C12-C13	6.49	111.77	120.57	9	9
5	A	433	C3S	C44-C22-C12	6.47	98.49	108.38	10	10
5	A	431	C3S	C40-C29-C26	6.43	101.12	110.61	17	15
4	A	335	PX4	O7-C23-C24	6.40	125.32	111.48	5	9
5	A	436	C3S	C23-C20-C22	6.40	120.97	113.08	7	9
4	A	378	PX4	C8-C7-C6	6.39	96.88	111.78	17	10
4	A	392	PX4	C7-O7-C23	6.37	133.05	117.80	16	4
4	A	406	PX4	O7-C23-O8	6.37	108.80	123.70	8	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	433	C3S	C1-C4-C7	6.37	120.72	110.33	1	6
4	A	413	PX4	C8-C7-C6	6.36	96.95	111.78	16	13
4	A	333	PX4	C8-C7-C6	6.34	97.01	111.78	7	13
5	A	434	C3S	C44-C22-C12	6.32	98.73	108.38	7	12
4	A	421	PX4	C8-C7-C6	6.31	97.07	111.78	9	10
5	A	432	C3S	C40-C29-C26	6.30	101.31	110.61	17	17
5	A	436	C3S	C44-C22-C20	6.30	118.73	111.66	4	7
4	A	328	PX4	O5-C8-C7	6.29	126.53	108.40	1	15
4	A	403	PX4	C8-C7-C6	6.28	97.14	111.78	3	15
4	A	395	PX4	O7-C23-O8	6.27	109.04	123.70	7	8
4	A	405	PX4	C8-C7-C6	6.27	97.17	111.78	10	14
5	A	432	C3S	C44-C22-C12	6.26	98.82	108.38	7	13
4	A	347	PX4	C7-O7-C23	6.25	132.76	117.80	18	6
4	A	345	PX4	C8-C7-C6	6.24	97.23	111.78	10	14
5	A	436	C3S	C44-C22-C12	6.24	98.85	108.38	13	11
4	A	411	PX4	C8-C7-C6	6.23	97.27	111.78	17	16
4	A	400	PX4	C8-C7-C6	6.22	97.28	111.78	10	11
5	A	432	C3S	C15-C13-C12	6.21	114.53	125.02	3	8
4	A	401	PX4	C8-C7-C6	6.21	97.32	111.78	17	13
4	A	336	PX4	C8-C7-C6	6.17	97.39	111.78	8	15
4	A	312	PX4	C7-O7-C23	6.17	132.57	117.80	9	6
4	A	417	PX4	C8-C7-C6	6.17	97.40	111.78	5	12
4	A	361	PX4	C8-C7-C6	6.16	97.43	111.78	8	10
5	A	434	C3S	C20-C18-C30	6.14	117.11	109.09	13	6
4	A	414	PX4	O5-C8-C7	6.14	126.09	108.40	19	13
4	A	372	PX4	C8-C7-C6	6.13	97.48	111.78	13	13
5	A	434	C3S	C35-C38-C29	6.12	96.65	103.84	11	13
5	A	431	C3S	C44-C22-C1	6.10	118.72	109.43	13	9
4	A	309	PX4	O7-C23-C24	6.08	124.64	111.48	7	11
5	A	435	C3S	C35-C38-C29	6.07	96.70	103.84	10	15
5	A	436	C3S	C20-C18-C30	6.06	117.00	109.09	18	12
4	A	407	PX4	O7-C23-O8	6.06	109.54	123.70	14	12
4	A	408	PX4	C8-C7-C6	6.06	97.66	111.78	4	9
4	A	336	PX4	O7-C23-C24	6.06	124.59	111.48	5	9
4	A	374	PX4	C7-O7-C23	6.04	132.25	117.80	14	15
4	A	421	PX4	C7-O7-C23	6.03	132.22	117.80	17	6
5	A	435	C3S	C9-C12-C13	6.02	112.40	120.57	17	15
4	A	336	PX4	O7-C23-O8	6.01	109.65	123.70	6	5
4	A	418	PX4	O5-C8-C7	6.01	125.72	108.40	13	11
4	A	373	PX4	C7-O7-C23	6.00	132.16	117.80	4	8
4	A	343	PX4	O7-C23-C24	5.98	124.42	111.48	6	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	431	C3S	C1-C22-C20	5.98	116.65	108.74	9	6
4	A	310	PX4	C7-O7-C23	5.98	132.10	117.80	18	5
5	A	431	C3S	C50-C48-C38	5.98	121.86	112.88	5	8
4	A	388	PX4	C8-C7-C6	5.98	97.85	111.78	10	10
4	A	310	PX4	C5-N1-C4	5.96	93.31	108.98	5	6
4	A	382	PX4	C8-C7-C6	5.96	97.90	111.78	2	14
4	A	321	PX4	C8-C7-C6	5.95	97.91	111.78	17	13
4	A	307	PX4	C8-C7-C6	5.95	97.91	111.78	1	14
4	A	355	PX4	O7-C23-C24	5.95	124.35	111.48	19	8
4	A	371	PX4	C8-C7-C6	5.94	97.93	111.78	2	16
4	A	401	PX4	O5-C8-C7	5.94	125.53	108.40	17	12
5	A	433	C3S	C20-C18-C30	5.93	116.84	109.09	18	10
4	A	378	PX4	C7-O7-C23	5.93	131.99	117.80	9	8
5	A	432	C3S	C23-C20-C22	5.93	120.40	113.08	13	10
5	A	432	C3S	C22-C12-C13	5.93	114.27	122.93	17	12
5	A	433	C3S	C9-C12-C22	5.93	124.02	116.42	1	15
4	A	330	PX4	C7-O7-C23	5.92	131.97	117.80	7	4
4	A	311	PX4	O5-C8-C7	5.92	125.45	108.40	6	11
5	A	433	C3S	O3-S1-O6	5.90	92.83	106.37	7	10
4	A	418	PX4	C1-C2-N1	5.89	134.74	115.82	15	9
4	A	313	PX4	O7-C23-O8	5.87	109.98	123.70	4	7
4	A	336	PX4	O5-C8-C7	5.87	125.31	108.40	16	12
4	A	385	PX4	O5-C8-C7	5.87	125.31	108.40	15	9
4	A	394	PX4	O5-C8-C7	5.87	125.31	108.40	2	10
4	A	324	PX4	C7-O7-C23	5.85	131.80	117.80	15	8
4	A	365	PX4	O5-C8-C7	5.84	125.22	108.40	4	9
4	A	312	PX4	C8-C7-C6	5.83	98.19	111.78	15	12
5	A	432	C3S	C54-C48-C38	5.83	122.42	110.33	4	17
4	A	365	PX4	C8-C7-C6	5.82	98.22	111.78	5	12
4	A	412	PX4	C8-C7-C6	5.80	98.27	111.78	2	10
4	A	404	PX4	O7-C23-C24	5.79	124.02	111.48	18	13
4	A	421	PX4	O5-C8-C7	5.79	125.08	108.40	3	12
4	A	383	PX4	O5-C8-C7	5.78	125.07	108.40	6	12
4	A	415	PX4	C5-N1-C4	5.78	93.79	108.98	2	7
5	A	433	C3S	C40-C29-C30	5.77	122.14	111.68	6	11
4	A	390	PX4	O7-C23-C24	5.77	123.96	111.48	11	9
4	A	346	PX4	O5-C8-C7	5.76	124.99	108.40	18	9
5	A	433	C3S	C20-C22-C12	5.75	118.08	109.65	20	11
4	A	430	PX4	C4-N1-C3	5.74	93.90	108.98	11	8
4	A	405	PX4	O5-C8-C7	5.74	124.94	108.40	6	16
4	A	324	PX4	C8-C7-C6	5.74	98.41	111.78	10	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	337	PX4	O7-C23-C24	5.74	123.89	111.48	14	9
5	A	432	C3S	C20-C22-C12	5.73	118.05	109.65	8	7
4	A	349	PX4	O3-P1-O2	5.73	86.22	108.94	3	3
4	A	402	PX4	C8-C7-C6	5.73	98.43	111.78	9	12
4	A	343	PX4	O5-C8-C7	5.73	124.91	108.40	17	15
4	A	427	PX4	O7-C23-C24	5.73	123.87	111.48	18	12
4	A	408	PX4	C7-O7-C23	5.72	131.48	117.80	17	5
4	A	352	PX4	O7-C23-C24	5.71	123.84	111.48	12	12
4	A	316	PX4	O7-C23-O8	5.69	110.40	123.70	12	5
4	A	326	PX4	C8-C7-C6	5.69	98.53	111.78	11	12
4	A	410	PX4	O5-C8-C7	5.68	124.78	108.40	6	13
4	A	323	PX4	C5-N1-C4	5.68	94.05	108.98	4	5
4	A	394	PX4	C8-C7-C6	5.68	98.54	111.78	9	11
4	A	331	PX4	C8-C7-C6	5.68	98.55	111.78	19	11
4	A	316	PX4	O5-C8-C7	5.67	124.75	108.40	3	11
4	A	354	PX4	O5-C8-C7	5.67	124.75	108.40	17	12
4	A	370	PX4	O5-C8-C7	5.67	124.73	108.40	19	13
4	A	381	PX4	C5-N1-C4	5.67	94.09	108.98	9	13
4	A	388	PX4	C4-N1-C3	5.66	94.12	108.98	1	3
4	A	330	PX4	C8-C7-C6	5.65	98.62	111.78	3	14
4	A	418	PX4	O7-C23-C24	5.64	123.69	111.48	14	15
4	A	360	PX4	C8-C7-C6	5.64	98.63	111.78	2	13
4	A	306	PX4	C8-C7-C6	5.63	98.65	111.78	1	13
4	A	342	PX4	O5-C8-C7	5.63	124.62	108.40	6	11
4	A	349	PX4	O7-C23-C24	5.62	123.65	111.48	11	11
4	A	327	PX4	O7-C23-C24	5.62	123.64	111.48	19	8
4	A	419	PX4	C8-C7-C6	5.61	98.69	111.78	10	7
4	A	346	PX4	C7-O7-C23	5.61	131.22	117.80	15	8
4	A	309	PX4	O5-C8-C7	5.61	124.56	108.40	19	16
4	A	427	PX4	O5-C8-C7	5.61	124.56	108.40	9	14
4	A	371	PX4	O7-C23-C24	5.60	123.60	111.48	13	11
4	A	402	PX4	C1-C2-N1	5.60	133.79	115.82	4	4
4	A	404	PX4	C7-O7-C23	5.60	131.19	117.80	13	7
5	A	431	C3S	C23-C20-C22	5.59	119.98	113.08	15	13
4	A	385	PX4	P1-O3-C1	5.59	94.64	121.26	16	15
4	A	311	PX4	C8-C7-C6	5.59	98.75	111.78	12	11
4	A	426	PX4	O7-C23-C24	5.58	123.56	111.48	14	12
4	A	387	PX4	O5-C8-C7	5.58	124.49	108.40	19	9
4	A	393	PX4	C8-C7-C6	5.58	98.78	111.78	3	14
4	A	393	PX4	O7-C23-C24	5.58	123.55	111.48	3	11
4	A	417	PX4	O7-C7-C8	5.58	128.35	108.34	1	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	377	PX4	O7-C23-C24	5.57	123.54	111.48	18	14
4	A	413	PX4	O7-C23-C24	5.57	123.53	111.48	1	14
4	A	313	PX4	O7-C23-C24	5.55	123.50	111.48	17	10
4	A	386	PX4	P1-O3-C1	5.55	94.84	121.26	20	16
4	A	321	PX4	O5-C8-C7	5.55	124.39	108.40	17	9
4	A	353	PX4	C8-C7-C6	5.54	98.87	111.78	16	13
4	A	368	PX4	O5-C8-C7	5.54	124.35	108.40	1	11
4	A	397	PX4	O5-C8-C7	5.54	124.35	108.40	13	13
4	A	403	PX4	C7-O7-C23	5.53	131.04	117.80	4	7
5	A	434	C3S	C50-C48-C54	5.54	101.77	110.34	8	15
5	A	435	C3S	C40-C29-C30	5.53	121.71	111.68	20	15
5	A	433	C3S	C9-C12-C13	5.53	113.08	120.57	5	9
5	A	433	C3S	C44-C22-C20	5.53	117.86	111.66	5	8
4	A	392	PX4	C8-C7-C6	5.52	98.92	111.78	8	12
5	A	431	C3S	C44-C22-C20	5.51	117.84	111.66	1	11
4	A	357	PX4	C8-C7-C6	5.50	98.96	111.78	9	12
5	A	433	C3S	C40-C29-C26	5.50	102.50	110.61	16	16
5	A	435	C3S	C26-C29-C30	5.48	99.04	107.25	8	9
4	A	332	PX4	C8-C7-C6	5.48	99.01	111.78	15	14
4	A	401	PX4	O7-C23-C24	5.47	123.32	111.48	1	10
4	A	357	PX4	C7-O7-C23	5.47	130.88	117.80	10	7
4	A	398	PX4	O5-C8-C7	5.46	124.14	108.40	16	10
4	A	401	PX4	P1-O3-C1	5.46	95.27	121.26	16	14
4	A	342	PX4	C8-C7-C6	5.45	99.07	111.78	15	11
4	A	309	PX4	C8-C7-C6	5.45	99.08	111.78	13	12
4	A	416	PX4	O7-C23-C24	5.45	123.27	111.48	6	13
5	A	432	C3S	C1-C4-C7	5.45	119.22	110.33	20	5
4	A	306	PX4	C7-O7-C23	5.45	130.83	117.80	12	13
4	A	320	PX4	O5-C8-C7	5.44	124.09	108.40	6	15
4	A	328	PX4	C8-C7-C6	5.43	99.12	111.78	3	12
5	A	436	C3S	C7-C9-C12	5.43	119.47	111.45	1	10
4	A	372	PX4	O7-C23-C24	5.42	123.21	111.48	4	12
4	A	329	PX4	O7-C23-C24	5.42	123.20	111.48	19	10
4	A	387	PX4	C7-O7-C23	5.42	130.76	117.80	12	4
5	A	432	C3S	C29-C30-C18	5.42	122.10	114.41	19	3
5	A	434	C3S	C7-C9-C12	5.41	119.45	111.45	14	4
4	A	312	PX4	O7-C23-C24	5.41	123.18	111.48	10	12
4	A	399	PX4	C8-C7-C6	5.41	99.17	111.78	1	14
4	A	309	PX4	O7-C23-O8	5.40	111.07	123.70	12	9
4	A	327	PX4	C8-C7-C6	5.40	99.18	111.78	15	11
4	A	351	PX4	O7-C23-C24	5.41	123.17	111.48	11	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	436	C3S	C15-C18-C20	5.40	115.96	109.72	6	6
4	A	416	PX4	O7-C23-O8	5.40	111.08	123.70	11	9
5	A	432	C3S	O3-S1-O6	5.40	93.97	106.37	20	6
4	A	386	PX4	C8-C7-C6	5.39	99.21	111.78	8	12
4	A	384	PX4	P1-O3-C1	5.39	95.60	121.26	5	16
4	A	306	PX4	O7-C23-C24	5.39	123.13	111.48	14	10
4	A	338	PX4	O5-C8-C7	5.38	123.90	108.40	15	9
4	A	366	PX4	O7-C23-C24	5.38	123.11	111.48	7	9
5	A	431	C3S	C1-C22-C12	5.38	118.02	108.74	3	6
4	A	334	PX4	C8-C7-C6	5.37	99.25	111.78	18	12
4	A	308	PX4	C7-O7-C23	5.37	130.66	117.80	20	7
4	A	306	PX4	O7-C7-C6	5.37	127.61	108.34	18	9
4	A	362	PX4	O5-C8-C7	5.37	123.87	108.40	1	7
4	A	379	PX4	C8-C7-C6	5.37	99.27	111.78	12	10
5	A	435	C3S	O6-C7-C4	5.36	99.68	107.61	13	8
4	A	352	PX4	C8-C7-C6	5.36	99.30	111.78	4	12
4	A	396	PX4	C8-C7-C6	5.35	99.30	111.78	10	13
4	A	316	PX4	O7-C23-C24	5.35	123.05	111.48	12	9
5	A	432	C3S	C26-C29-C38	5.35	108.72	116.60	13	7
4	A	314	PX4	C8-C7-C6	5.34	99.33	111.78	1	13
4	A	326	PX4	C7-O7-C23	5.33	130.56	117.80	2	5
4	A	417	PX4	O5-C8-C7	5.33	123.75	108.40	7	8
4	A	420	PX4	C8-C7-C6	5.33	99.37	111.78	14	12
4	A	364	PX4	O7-C23-C24	5.32	123.00	111.48	14	12
5	A	435	C3S	C35-C38-C48	5.32	120.23	112.18	20	10
4	A	332	PX4	O7-C7-C8	5.32	127.43	108.34	20	6
4	A	395	PX4	O3-P1-O2	5.32	87.86	108.94	2	3
4	A	374	PX4	C4-N1-C3	5.32	95.01	108.98	1	2
4	A	321	PX4	C7-O7-C23	5.31	130.50	117.80	1	6
4	A	425	PX4	C8-C7-C6	5.31	99.41	111.78	3	12
4	A	359	PX4	C8-C7-C6	5.30	99.44	111.78	15	14
4	A	349	PX4	O5-C9-O6	5.29	110.39	123.63	15	5
4	A	378	PX4	O3-P1-O2	5.29	87.96	108.94	7	7
4	A	393	PX4	O5-C8-C7	5.29	123.65	108.40	17	11
4	A	406	PX4	O5-C8-C7	5.29	123.65	108.40	2	9
4	A	344	PX4	C8-C7-C6	5.28	99.47	111.78	15	10
4	A	327	PX4	C7-O7-C23	5.28	105.16	117.80	5	7
4	A	409	PX4	C8-C7-C6	5.27	99.50	111.78	4	16
4	A	396	PX4	O5-C8-C7	5.27	123.58	108.40	3	13
4	A	428	PX4	C5-N1-C3	5.27	95.14	108.98	8	8
5	A	434	C3S	C20-C22-C12	5.27	117.36	109.65	7	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	392	PX4	O5-C8-C7	5.27	123.58	108.40	6	10
5	A	433	C3S	C50-C48-C38	5.26	104.98	112.88	12	8
4	A	348	PX4	O7-C23-C24	5.26	122.86	111.48	2	13
4	A	341	PX4	O7-C23-C24	5.26	122.85	111.48	10	10
4	A	369	PX4	O7-C23-C24	5.25	122.85	111.48	6	10
4	A	390	PX4	O5-C8-C7	5.25	123.54	108.40	10	15
4	A	317	PX4	P1-O4-C6	5.25	91.27	121.35	8	13
4	A	334	PX4	O5-C8-C7	5.25	123.53	108.40	15	8
4	A	383	PX4	C8-C7-C6	5.25	99.54	111.78	18	8
4	A	413	PX4	C5-N1-C3	5.25	95.19	108.98	9	7
4	A	344	PX4	O5-C8-C7	5.24	123.51	108.40	1	9
4	A	356	PX4	C8-C7-C6	5.24	99.56	111.78	13	12
4	A	317	PX4	O5-C8-C7	5.24	123.50	108.40	2	12
4	A	335	PX4	C8-C7-C6	5.23	99.59	111.78	8	11
4	A	421	PX4	O5-C9-O6	5.23	110.54	123.63	1	7
5	A	432	C3S	C4-C7-C9	5.23	103.70	110.97	16	12
4	A	309	PX4	C5-N1-C4	5.23	95.24	108.98	12	5
4	A	422	PX4	C8-C7-C6	5.23	99.59	111.78	11	10
4	A	379	PX4	O7-C7-C8	5.23	127.10	108.34	10	10
5	A	431	C3S	C20-C18-C30	5.23	115.91	109.09	16	10
4	A	358	PX4	C8-C7-C6	5.23	99.60	111.78	12	15
4	A	397	PX4	C7-O7-C23	5.22	130.29	117.80	10	7
5	A	436	C3S	C23-C26-C29	5.22	121.54	112.74	7	7
4	A	419	PX4	O7-C23-C24	5.21	122.75	111.48	14	12
4	A	311	PX4	O7-C7-C6	5.21	127.02	108.34	12	6
4	A	380	PX4	C5-N1-C4	5.21	95.30	108.98	20	5
4	A	354	PX4	O7-C23-O8	5.20	111.55	123.70	1	7
5	A	431	C3S	C1-C4-C7	5.20	118.81	110.33	3	6
4	A	408	PX4	O5-C8-C7	5.20	123.38	108.40	7	9
4	A	311	PX4	O7-C23-C24	5.18	122.69	111.48	14	16
4	A	382	PX4	C5-N1-C4	5.18	95.37	108.98	20	5
4	A	329	PX4	C8-C7-C6	5.17	99.74	111.78	12	15
4	A	340	PX4	C1-C2-N1	5.17	132.40	115.82	13	5
4	A	377	PX4	C8-C7-C6	5.16	99.76	111.78	7	8
4	A	422	PX4	O5-C8-C7	5.16	123.26	108.40	4	7
4	A	312	PX4	O5-C8-C7	5.15	123.25	108.40	5	7
5	A	434	C3S	C4-C1-C22	5.15	123.76	112.78	7	12
4	A	339	PX4	P1-O3-C1	5.15	96.76	121.26	18	14
4	A	428	PX4	C7-O7-C23	5.14	130.11	117.80	7	6
4	A	420	PX4	O7-C23-C24	5.14	122.60	111.48	19	10
4	A	402	PX4	C7-O7-C23	5.14	130.09	117.80	13	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	375	PX4	O7-C23-C24	5.14	122.59	111.48	18	10
5	A	434	C3S	C15-C13-C12	5.13	116.35	125.02	14	8
4	A	331	PX4	O7-C23-C24	5.13	122.58	111.48	13	15
4	A	367	PX4	P1-O3-C1	5.13	96.83	121.26	6	14
4	A	351	PX4	C8-C7-C6	5.13	99.83	111.78	13	14
4	A	370	PX4	C8-C7-C6	5.12	99.84	111.78	16	14
4	A	335	PX4	C5-N1-C3	5.12	95.53	108.98	1	5
4	A	371	PX4	O5-C8-C7	5.12	123.15	108.40	10	13
4	A	335	PX4	O7-C23-O8	5.11	111.75	123.70	12	8
4	A	342	PX4	C1-C2-N1	5.11	132.23	115.82	16	8
4	A	355	PX4	C7-O7-C23	5.11	130.04	117.80	17	15
5	A	433	C3S	C4-C7-C9	5.12	118.08	110.97	14	6
4	A	419	PX4	O5-C8-C7	5.11	123.13	108.40	20	7
4	A	327	PX4	O7-C23-O8	5.11	111.76	123.70	9	7
4	A	361	PX4	O7-C23-C24	5.11	122.53	111.48	8	11
4	A	339	PX4	O7-C23-C24	5.10	122.52	111.48	10	10
4	A	360	PX4	O5-C8-C7	5.10	123.10	108.40	4	13
5	A	436	C3S	C32-C30-C29	5.10	97.84	103.84	5	8
4	A	320	PX4	C8-C7-C6	5.09	99.91	111.78	7	14
5	A	432	C3S	C15-C18-C20	5.09	103.83	109.72	18	12
4	A	419	PX4	O1-P1-O3	5.09	84.50	107.57	18	1
4	A	344	PX4	O7-C7-C8	5.09	126.59	108.34	11	7
4	A	345	PX4	P1-O3-C1	5.08	97.09	121.26	11	17
4	A	350	PX4	C8-C7-C6	5.08	99.94	111.78	8	13
4	A	419	PX4	O3-P1-O2	5.08	88.81	108.94	1	8
5	A	436	C3S	C35-C38-C29	5.08	97.87	103.84	16	13
4	A	404	PX4	C8-C7-C6	5.07	99.96	111.78	8	11
4	A	305	PX4	C5-N1-C4	5.07	95.66	108.98	2	4
4	A	412	PX4	O7-C23-C24	5.07	122.45	111.48	1	9
4	A	340	PX4	C8-C7-C6	5.07	99.97	111.78	9	12
4	A	385	PX4	O7-C23-O8	5.06	111.87	123.70	20	10
4	A	417	PX4	O7-C23-C24	5.06	122.44	111.48	16	11
4	A	340	PX4	O5-C8-C7	5.06	122.99	108.40	9	17
4	A	325	PX4	O5-C8-C7	5.05	122.96	108.40	20	12
4	A	379	PX4	C7-O7-C23	5.05	129.89	117.80	7	8
4	A	372	PX4	O5-C8-C7	5.05	122.95	108.40	4	12
4	A	384	PX4	C8-C7-C6	5.05	100.02	111.78	3	12
4	A	332	PX4	P1-O3-C1	5.04	97.25	121.26	4	15
4	A	332	PX4	O5-C8-C7	5.04	122.94	108.40	3	12
4	A	380	PX4	C8-C7-C6	5.04	100.02	111.78	11	9
4	A	318	PX4	O5-C8-C7	5.04	122.93	108.40	19	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	364	PX4	O5-C9-O6	5.04	111.03	123.63	19	5
4	A	407	PX4	P1-O3-C1	5.04	97.29	121.26	10	15
4	A	411	PX4	O5-C8-C7	5.03	122.88	108.40	3	10
4	A	427	PX4	C8-C7-C6	5.02	100.07	111.78	10	9
5	A	435	C3S	C23-C20-C18	5.02	104.77	111.78	3	8
4	A	353	PX4	O5-C8-C7	5.01	122.85	108.40	16	14
4	A	310	PX4	C8-C7-C6	5.01	100.11	111.78	7	15
4	A	342	PX4	O5-C9-O6	5.01	111.10	123.63	9	8
4	A	366	PX4	C8-C7-C6	5.01	100.11	111.78	7	12
4	A	372	PX4	O5-C9-O6	5.01	111.10	123.63	11	5
4	A	369	PX4	P1-O3-C1	5.00	97.45	121.26	17	13
4	A	379	PX4	O5-C8-C7	5.00	122.81	108.40	6	12
5	A	431	C3S	C35-C38-C48	5.00	104.62	112.18	4	11
4	A	330	PX4	O5-C8-C7	4.99	122.79	108.40	18	15
4	A	316	PX4	C7-O7-C23	4.99	129.75	117.80	17	8
4	A	355	PX4	O5-C9-C10	4.99	127.06	111.83	19	4
4	A	307	PX4	O5-C8-C7	4.99	122.78	108.40	4	11
4	A	362	PX4	C8-C7-C6	4.99	100.15	111.78	14	13
4	A	387	PX4	C8-C7-C6	4.98	100.16	111.78	15	9
4	A	357	PX4	O7-C23-O8	4.98	112.06	123.70	9	7
4	A	397	PX4	C8-C7-C6	4.98	100.18	111.78	20	11
4	A	357	PX4	O7-C23-C24	4.98	122.25	111.48	17	8
4	A	373	PX4	C8-C7-C6	4.97	100.19	111.78	14	13
4	A	423	PX4	C8-C7-C6	4.97	100.20	111.78	9	15
5	A	434	C3S	C18-C15-C13	4.96	105.89	112.76	14	5
4	A	327	PX4	O5-C8-C7	4.96	122.69	108.40	11	12
4	A	415	PX4	C7-O7-C23	4.96	129.66	117.80	13	6
5	A	432	C3S	C9-C12-C13	4.95	113.86	120.57	12	10
5	A	435	C3S	C50-C48-C38	4.95	120.32	112.88	10	10
4	A	319	PX4	O7-C23-C24	4.95	122.19	111.48	4	13
5	A	431	C3S	C9-C12-C13	4.95	113.86	120.57	2	12
4	A	343	PX4	C8-C7-C6	4.95	100.25	111.78	16	15
4	A	412	PX4	P1-O3-C1	4.95	97.71	121.26	5	15
4	A	375	PX4	P1-O3-C1	4.94	97.72	121.26	12	15
4	A	398	PX4	C8-C7-C6	4.94	100.26	111.78	2	12
4	A	424	PX4	O3-P1-O2	4.94	89.34	108.94	18	7
4	A	381	PX4	C8-C7-C6	4.94	100.26	111.78	9	16
4	A	318	PX4	C8-C7-C6	4.94	100.27	111.78	17	16
4	A	321	PX4	P1-O3-C1	4.94	97.76	121.26	7	15
4	A	325	PX4	C8-C7-C6	4.94	100.27	111.78	10	13
4	A	341	PX4	C8-C7-C6	4.94	100.27	111.78	14	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	422	PX4	O7-C23-O8	4.94	112.16	123.70	1	7
4	A	361	PX4	O5-C9-O6	4.93	111.28	123.63	15	6
4	A	389	PX4	O5-C8-C7	4.94	122.62	108.40	19	10
5	A	431	C3S	C40-C29-C30	4.93	120.63	111.68	15	17
5	A	432	C3S	C18-C15-C13	4.93	105.93	112.76	2	7
5	A	434	C3S	C35-C38-C48	4.93	104.71	112.18	15	6
4	A	328	PX4	O7-C7-C8	4.93	126.02	108.34	19	9
4	A	393	PX4	C7-O7-C23	4.93	129.59	117.80	2	8
5	A	431	C3S	C4-C7-C9	4.93	117.82	110.97	1	9
5	A	435	C3S	C23-C26-C29	4.92	121.05	112.74	10	9
4	A	383	PX4	O7-C23-C24	4.92	122.13	111.48	10	11
4	A	340	PX4	P1-O3-C1	4.92	97.84	121.26	13	16
5	A	432	C3S	C1-C22-C20	4.92	102.23	108.74	8	8
4	A	368	PX4	O7-C23-C24	4.92	122.12	111.48	4	11
4	A	365	PX4	P1-O3-C1	4.91	97.86	121.26	8	14
4	A	401	PX4	C5-N1-C4	4.92	96.06	108.98	18	6
4	A	430	PX4	O7-C23-C24	4.91	122.11	111.48	18	10
4	A	310	PX4	O7-C23-C24	4.91	122.10	111.48	7	11
4	A	308	PX4	O7-C23-C24	4.91	122.09	111.48	14	9
4	A	352	PX4	O5-C8-C7	4.91	122.54	108.40	18	14
4	A	412	PX4	O5-C8-C7	4.90	122.53	108.40	17	12
5	A	433	C3S	C50-C48-C54	4.90	117.93	110.34	3	13
4	A	334	PX4	C4-N1-C3	4.90	96.10	108.98	15	5
4	A	430	PX4	P1-O3-C1	4.90	97.93	121.26	4	14
4	A	319	PX4	C8-C7-C6	4.90	100.36	111.78	13	12
4	A	346	PX4	O5-C9-C10	4.90	126.76	111.83	19	9
4	A	386	PX4	O7-C23-C24	4.89	122.07	111.48	2	10
4	A	416	PX4	C8-C7-C6	4.89	100.38	111.78	11	13
5	A	435	C3S	C54-C48-C38	4.89	120.47	110.33	16	10
4	A	319	PX4	P1-O3-C1	4.88	98.02	121.26	2	12
4	A	407	PX4	O5-C8-C7	4.88	122.47	108.40	18	9
5	A	432	C3S	C7-C9-C12	4.88	118.66	111.45	14	10
4	A	388	PX4	C26-C25-C24	4.86	95.26	113.13	10	5
4	A	427	PX4	C7-O7-C23	4.86	129.43	117.80	3	7
4	A	316	PX4	P1-O3-C1	4.86	98.13	121.26	6	16
4	A	356	PX4	O5-C8-C7	4.86	122.40	108.40	20	15
4	A	398	PX4	O7-C23-O8	4.86	112.35	123.70	20	7
5	A	435	C3S	C32-C30-C29	4.86	98.13	103.84	8	6
4	A	407	PX4	O7-C23-C24	4.85	121.98	111.48	2	11
4	A	377	PX4	P1-O3-C1	4.85	98.16	121.26	2	14
4	A	368	PX4	C1-C2-N1	4.85	131.39	115.82	2	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	410	PX4	C8-C7-C6	4.85	100.48	111.78	4	9
4	A	360	PX4	O7-C23-C24	4.85	121.96	111.48	20	12
4	A	429	PX4	O7-C23-O8	4.84	112.39	123.70	13	8
4	A	333	PX4	O7-C23-C24	4.84	121.95	111.48	12	8
4	A	409	PX4	C5-N1-C3	4.84	96.27	108.98	20	3
4	A	408	PX4	O7-C23-C24	4.84	121.94	111.48	17	6
4	A	415	PX4	O3-P1-O2	4.84	89.77	108.94	13	8
4	A	349	PX4	O5-C8-C7	4.83	122.32	108.40	11	9
4	A	329	PX4	O3-P1-O2	4.83	89.81	108.94	18	3
4	A	418	PX4	C8-C7-C6	4.82	100.54	111.78	18	13
4	A	348	PX4	O3-P1-O2	4.82	89.84	108.94	13	4
5	A	436	C3S	C23-C20-C18	4.82	105.06	111.78	19	8
5	A	436	C3S	C1-C22-C20	4.81	115.11	108.74	9	7
4	A	389	PX4	P1-O3-C1	4.81	98.36	121.26	7	15
4	A	395	PX4	C5-N1-C4	4.81	96.34	108.98	20	5
5	A	431	C3S	C20-C22-C12	4.81	116.70	109.65	13	8
4	A	326	PX4	O7-C23-C24	4.81	121.88	111.48	19	7
4	A	341	PX4	C1-C2-N1	4.81	131.25	115.82	10	6
4	A	419	PX4	C7-O7-C23	4.81	129.30	117.80	9	11
4	A	321	PX4	O7-C23-C24	4.80	121.87	111.48	20	12
4	A	332	PX4	O7-C23-C24	4.80	121.87	111.48	7	6
4	A	356	PX4	O1-P1-O3	4.80	85.80	107.57	17	2
4	A	322	PX4	C8-C7-C6	4.80	100.59	111.78	10	13
4	A	366	PX4	O7-C23-O8	4.80	112.48	123.70	14	8
4	A	354	PX4	O7-C23-C24	4.80	121.86	111.48	12	12
4	A	312	PX4	P1-O4-C6	4.80	93.87	121.35	1	12
4	A	375	PX4	O5-C8-C7	4.80	122.22	108.40	4	9
4	A	334	PX4	O7-C23-O8	4.79	112.50	123.70	18	7
4	A	348	PX4	C8-C7-C6	4.79	100.61	111.78	15	9
4	A	357	PX4	O5-C8-C7	4.79	122.19	108.40	2	13
5	A	432	C3S	C50-C48-C38	4.78	105.70	112.88	15	7
4	A	313	PX4	O5-C9-O6	4.78	111.67	123.63	20	6
4	A	342	PX4	O5-C9-C10	4.78	126.40	111.83	9	8
4	A	373	PX4	O5-C8-C7	4.78	122.17	108.40	19	9
4	A	331	PX4	O5-C9-O6	4.78	111.68	123.63	12	6
4	A	369	PX4	O5-C8-C7	4.77	122.15	108.40	18	9
4	A	429	PX4	C3-N1-C2	4.77	128.87	109.91	12	3
4	A	319	PX4	O5-C8-C7	4.77	122.14	108.40	8	11
4	A	381	PX4	O7-C7-C8	4.77	125.45	108.34	6	13
4	A	386	PX4	C7-O7-C23	4.76	106.39	117.80	3	8
4	A	321	PX4	C1-C2-N1	4.76	131.11	115.82	14	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	337	PX4	O5-C8-C7	4.76	122.12	108.40	3	10
4	A	363	PX4	O7-C23-O8	4.76	112.59	123.70	16	8
4	A	369	PX4	C8-C7-C6	4.75	100.70	111.78	3	9
4	A	324	PX4	P1-O3-C1	4.75	98.64	121.26	6	12
4	A	367	PX4	O7-C7-C8	4.75	125.39	108.34	18	11
4	A	367	PX4	O7-C23-O8	4.74	112.62	123.70	18	6
4	A	305	PX4	C7-O7-C23	4.74	129.14	117.80	6	5
4	A	399	PX4	O7-C23-C24	4.74	121.73	111.48	7	12
4	A	305	PX4	O7-C23-C24	4.74	121.73	111.48	10	10
5	A	434	C3S	C50-C48-C38	4.74	105.78	112.88	10	7
4	A	356	PX4	P1-O3-C1	4.74	98.72	121.26	17	17
4	A	393	PX4	C4-N1-C3	4.73	96.54	108.98	19	3
4	A	332	PX4	C5-N1-C3	4.73	96.55	108.98	8	7
4	A	410	PX4	O5-C9-O6	4.73	111.80	123.63	12	7
4	A	328	PX4	C5-N1-C4	4.73	96.56	108.98	13	4
4	A	425	PX4	O5-C9-C10	4.73	126.25	111.83	20	7
4	A	338	PX4	O7-C23-C24	4.72	121.69	111.48	4	9
4	A	384	PX4	C5-N1-C3	4.72	96.58	108.98	10	5
4	A	322	PX4	O7-C23-O8	4.72	112.67	123.70	19	10
4	A	341	PX4	C5-N1-C3	4.72	96.58	108.98	13	4
4	A	336	PX4	O7-C7-C8	4.71	125.26	108.34	9	11
4	A	362	PX4	C7-O7-C23	4.71	129.08	117.80	15	1
4	A	395	PX4	O7-C23-C24	4.71	121.68	111.48	20	10
4	A	421	PX4	O3-P1-O2	4.71	90.25	108.94	14	7
4	A	365	PX4	O7-C23-C24	4.71	121.67	111.48	18	10
4	A	369	PX4	O7-C23-O8	4.71	112.70	123.70	1	5
4	A	330	PX4	P1-O3-C1	4.71	98.86	121.26	15	17
5	A	436	C3S	C40-C29-C30	4.71	120.21	111.68	4	13
4	A	315	PX4	C8-C7-C6	4.70	100.82	111.78	19	10
4	A	404	PX4	O5-C8-C7	4.70	121.96	108.40	9	5
4	A	370	PX4	O7-C23-O8	4.70	112.71	123.70	17	6
4	A	389	PX4	C7-O7-C23	4.70	129.05	117.80	15	6
4	A	385	PX4	C8-C7-C6	4.70	100.83	111.78	9	12
5	A	435	C3S	C15-C18-C20	4.69	104.30	109.72	6	5
4	A	346	PX4	O7-C23-C24	4.69	121.63	111.48	4	9
4	A	402	PX4	O5-C8-C7	4.69	121.92	108.40	9	11
4	A	317	PX4	C4-N1-C3	4.69	96.66	108.98	9	4
4	A	414	PX4	C8-C7-C6	4.69	100.85	111.78	20	15
4	A	317	PX4	O7-C23-C24	4.69	121.62	111.48	16	7
4	A	358	PX4	O5-C8-C7	4.69	121.91	108.40	4	10
4	A	367	PX4	O5-C8-C7	4.69	121.91	108.40	13	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	309	PX4	O7-C7-C8	4.68	125.15	108.34	12	13
5	A	436	C3S	O3-S1-O6	4.68	95.61	106.37	16	12
4	A	376	PX4	C4-N1-C3	4.68	121.28	108.98	6	8
4	A	415	PX4	C5-N1-C3	4.68	96.68	108.98	13	8
4	A	357	PX4	C5-N1-C4	4.68	96.69	108.98	12	4
4	A	364	PX4	C8-C7-C6	4.68	100.88	111.78	14	15
4	A	388	PX4	C1-C2-N1	4.68	130.84	115.82	19	10
4	A	314	PX4	P1-O3-C1	4.68	99.00	121.26	18	12
4	A	379	PX4	O7-C23-O8	4.68	112.77	123.70	20	5
4	A	337	PX4	P1-O3-C1	4.67	99.01	121.26	5	15
4	A	358	PX4	O7-C23-O8	4.67	112.78	123.70	8	6
4	A	364	PX4	P1-O3-C1	4.68	99.01	121.26	12	13
4	A	419	PX4	O5-C9-O6	4.67	111.94	123.63	7	8
5	A	436	C3S	C22-C12-C13	4.67	116.11	122.93	17	5
5	A	436	C3S	C1-C4-C7	4.67	117.95	110.33	18	2
4	A	359	PX4	O7-C23-O8	4.67	112.79	123.70	8	7
5	A	431	C3S	C32-C30-C29	4.67	98.35	103.84	5	6
4	A	311	PX4	P1-O3-C1	4.67	99.05	121.26	1	15
4	A	336	PX4	P1-O3-C1	4.66	99.05	121.26	7	18
4	A	379	PX4	O5-C9-O6	4.67	111.96	123.63	12	7
4	A	358	PX4	P1-O3-C1	4.66	99.08	121.26	16	15
4	A	353	PX4	O7-C23-O8	4.66	112.82	123.70	17	10
4	A	405	PX4	P1-O3-C1	4.65	99.11	121.26	17	17
4	A	394	PX4	C5-N1-C4	4.65	96.76	108.98	14	8
4	A	395	PX4	C4-N1-C3	4.65	96.77	108.98	5	4
4	A	422	PX4	P1-O3-C1	4.65	99.14	121.26	8	16
4	A	365	PX4	C5-N1-C4	4.64	96.78	108.98	10	3
4	A	326	PX4	O5-C8-C7	4.64	121.77	108.40	4	7
4	A	329	PX4	O1-P1-O4	4.64	128.60	107.57	10	2
4	A	345	PX4	C7-O7-C23	4.64	128.90	117.80	15	6
4	A	349	PX4	O7-C7-C8	4.64	124.99	108.34	12	6
4	A	426	PX4	C8-C7-C6	4.64	100.97	111.78	4	11
4	A	340	PX4	O7-C23-C24	4.64	121.51	111.48	7	9
4	A	347	PX4	O7-C23-C24	4.64	121.51	111.48	15	7
4	A	356	PX4	O7-C23-C24	4.64	121.51	111.48	10	11
4	A	382	PX4	O7-C23-C24	4.64	121.51	111.48	7	8
4	A	402	PX4	P1-O3-C1	4.63	99.20	121.26	10	14
4	A	348	PX4	O7-C7-C8	4.63	124.96	108.34	20	6
4	A	372	PX4	P1-O3-C1	4.63	99.23	121.26	8	12
4	A	382	PX4	C7-O7-C23	4.63	128.87	117.80	11	8
4	A	414	PX4	O5-C9-O6	4.63	112.06	123.63	1	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	380	PX4	P1-O3-C1	4.62	99.26	121.26	9	18
4	A	315	PX4	O5-C8-C7	4.62	121.71	108.40	7	8
4	A	333	PX4	C7-O7-C23	4.61	106.75	117.80	3	6
4	A	349	PX4	C8-C7-C6	4.61	101.03	111.78	11	11
4	A	358	PX4	C26-C25-C24	4.61	96.18	113.13	16	5
4	A	359	PX4	O5-C8-C7	4.61	121.69	108.40	17	12
4	A	360	PX4	O5-C9-O6	4.61	112.09	123.63	12	5
4	A	374	PX4	O7-C23-O8	4.61	112.92	123.70	11	8
4	A	381	PX4	O5-C8-C7	4.61	121.69	108.40	14	13
4	A	339	PX4	O5-C8-C7	4.61	121.69	108.40	9	11
4	A	313	PX4	P1-O3-C1	4.61	99.33	121.26	9	14
4	A	341	PX4	O5-C8-C7	4.61	121.68	108.40	1	12
4	A	351	PX4	P1-O3-C1	4.61	99.33	121.26	10	13
4	A	373	PX4	C4-N1-C3	4.60	96.89	108.98	14	8
4	A	427	PX4	O7-C23-O8	4.60	112.94	123.70	14	6
5	A	432	C3S	C35-C32-C30	4.60	96.14	105.14	16	13
4	A	345	PX4	O5-C8-C7	4.59	121.64	108.40	10	10
5	A	433	C3S	C30-C29-C38	4.60	94.83	100.10	4	6
4	A	397	PX4	P1-O3-C1	4.59	99.40	121.26	10	16
5	A	434	C3S	C22-C12-C13	4.59	116.23	122.93	7	11
4	A	305	PX4	O5-C8-C7	4.59	121.62	108.40	1	10
4	A	348	PX4	O1-P1-O2	4.58	133.77	112.44	2	15
5	A	431	C3S	C32-C35-C38	4.58	114.12	105.14	18	12
4	A	374	PX4	O7-C23-C24	4.58	121.40	111.48	9	12
4	A	313	PX4	O3-P1-O2	4.58	90.78	108.94	12	4
4	A	402	PX4	O7-C23-C24	4.58	121.39	111.48	17	7
5	A	435	C3S	C44-C22-C12	4.58	101.38	108.38	8	9
4	A	391	PX4	O3-P1-O2	4.58	90.78	108.94	16	5
4	A	430	PX4	O5-C8-C7	4.58	121.59	108.40	7	5
4	A	393	PX4	C5-N1-C3	4.57	96.97	108.98	18	4
5	A	436	C3S	C32-C30-C18	4.57	126.39	119.10	3	6
4	A	338	PX4	C7-O7-C23	4.57	128.74	117.80	9	11
5	A	436	C3S	C15-C18-C30	4.57	104.46	110.93	2	5
4	A	312	PX4	P1-O3-C1	4.57	99.52	121.26	5	17
4	A	375	PX4	O1-P1-O3	4.56	86.88	107.57	5	4
5	A	436	C3S	C44-C22-C1	4.56	102.48	109.43	10	3
4	A	315	PX4	P1-O3-C1	4.56	99.54	121.26	10	13
4	A	320	PX4	O7-C23-C24	4.56	121.35	111.48	6	8
4	A	393	PX4	O5-C9-O6	4.56	112.22	123.63	20	5
4	A	368	PX4	C8-C7-C6	4.56	101.16	111.78	15	10
4	A	339	PX4	C8-C7-C6	4.55	101.17	111.78	3	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	429	PX4	C8-C7-C6	4.55	101.17	111.78	13	11
4	A	341	PX4	C5-N1-C4	4.54	120.90	108.98	7	4
4	A	337	PX4	O1-P1-O2	4.54	133.55	112.44	3	11
4	A	349	PX4	C7-O7-C23	4.54	106.94	117.80	5	7
4	A	333	PX4	O7-C23-O8	4.54	113.10	123.70	15	4
4	A	350	PX4	O7-C23-C24	4.53	121.29	111.48	7	10
4	A	378	PX4	P1-O3-C1	4.53	99.68	121.26	11	12
4	A	398	PX4	O7-C7-C8	4.53	124.61	108.34	1	13
4	A	362	PX4	O3-P1-O2	4.53	90.98	108.94	16	5
4	A	418	PX4	C7-O7-C23	4.53	106.96	117.80	3	3
5	A	433	C3S	C15-C13-C12	4.53	117.38	125.02	5	4
4	A	364	PX4	O5-C8-C7	4.52	121.44	108.40	1	11
5	A	431	C3S	C50-C48-C54	4.52	103.34	110.34	19	15
4	A	375	PX4	C7-O7-C23	4.52	128.61	117.80	6	4
4	A	339	PX4	P1-O4-C6	4.52	95.46	121.35	5	10
4	A	372	PX4	O7-C23-O8	4.52	113.14	123.70	17	9
4	A	370	PX4	P1-O4-C6	4.52	95.47	121.35	14	14
4	A	419	PX4	O7-C7-C6	4.52	124.55	108.34	2	7
4	A	408	PX4	P1-O3-C1	4.51	99.79	121.26	6	17
4	A	408	PX4	O3-P1-O2	4.51	91.07	108.94	15	7
4	A	331	PX4	O5-C8-C7	4.51	121.39	108.40	8	11
4	A	354	PX4	C7-O7-C23	4.50	128.58	117.80	9	9
4	A	322	PX4	O5-C8-C7	4.50	121.38	108.40	18	16
4	A	363	PX4	C8-C7-C6	4.50	101.29	111.78	12	10
4	A	329	PX4	O7-C23-O8	4.50	113.19	123.70	8	10
4	A	429	PX4	O7-C7-C8	4.50	124.48	108.34	4	5
4	A	363	PX4	O7-C23-C24	4.50	121.21	111.48	12	11
4	A	401	PX4	O1-P1-O3	4.50	87.19	107.57	15	3
4	A	410	PX4	O7-C23-C24	4.49	121.20	111.48	10	7
4	A	313	PX4	C8-C7-C6	4.49	101.31	111.78	11	12
4	A	320	PX4	O3-P1-O2	4.49	91.13	108.94	3	3
4	A	396	PX4	C5-N1-C3	4.49	97.18	108.98	14	6
4	A	318	PX4	O7-C23-C24	4.48	121.18	111.48	1	8
4	A	338	PX4	C8-C7-C6	4.48	101.34	111.78	3	9
4	A	384	PX4	O5-C8-C7	4.48	121.32	108.40	2	7
4	A	418	PX4	O7-C7-C8	4.48	124.42	108.34	13	11
4	A	422	PX4	O7-C23-C24	4.48	121.18	111.48	10	10
4	A	329	PX4	C7-O7-C23	4.48	107.08	117.80	5	6
4	A	386	PX4	O3-P1-O2	4.47	91.20	108.94	11	6
4	A	338	PX4	O7-C7-C6	4.47	124.39	108.34	13	10
4	A	368	PX4	C7-O7-C23	4.47	128.50	117.80	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	432	C3S	C20-C18-C30	4.47	114.93	109.09	16	8
4	A	366	PX4	C5-N1-C4	4.47	97.23	108.98	8	4
4	A	405	PX4	O7-C23-O8	4.47	113.25	123.70	3	9
4	A	359	PX4	O1-P1-O2	4.46	133.22	112.44	5	12
4	A	315	PX4	O7-C23-C24	4.46	121.13	111.48	5	11
4	A	385	PX4	C5-N1-C3	4.46	120.69	108.98	14	6
4	A	322	PX4	O5-C9-C10	4.46	125.43	111.83	13	6
4	A	379	PX4	O7-C23-C24	4.46	121.13	111.48	3	6
4	A	306	PX4	P1-O3-C1	4.46	100.05	121.26	8	17
4	A	328	PX4	P1-O3-C1	4.46	100.05	121.26	2	15
4	A	379	PX4	P1-O4-C6	4.45	95.83	121.35	9	12
5	A	434	C3S	C9-C12-C13	4.45	114.53	120.57	4	15
4	A	351	PX4	C25-C24-C23	4.45	97.39	113.69	12	2
4	A	385	PX4	C5-N1-C4	4.45	97.29	108.98	15	6
4	A	421	PX4	O7-C23-C24	4.45	121.11	111.48	17	14
4	A	399	PX4	O7-C7-C8	4.45	124.31	108.34	1	9
4	A	403	PX4	O5-C8-C7	4.45	121.22	108.40	9	13
4	A	306	PX4	O5-C8-C7	4.44	121.21	108.40	5	13
4	A	398	PX4	P1-O3-C1	4.44	100.11	121.26	16	15
4	A	333	PX4	O5-C8-C7	4.44	121.19	108.40	13	7
4	A	428	PX4	O5-C8-C7	4.44	121.19	108.40	20	9
5	A	431	C3S	C54-C48-C38	4.44	119.53	110.33	20	6
4	A	347	PX4	C8-C7-C6	4.43	101.45	111.78	6	16
4	A	323	PX4	O3-P1-O2	4.43	91.38	108.94	14	9
4	A	359	PX4	O7-C23-C24	4.43	121.06	111.48	1	7
4	A	377	PX4	C7-O7-C23	4.43	128.40	117.80	5	11
4	A	413	PX4	O7-C23-O8	4.43	113.35	123.70	14	4
4	A	388	PX4	P1-O3-C1	4.42	100.20	121.26	11	15
4	A	348	PX4	P1-O3-C1	4.42	100.21	121.26	19	15
4	A	359	PX4	P1-O3-C1	4.42	100.21	121.26	12	14
4	A	398	PX4	P1-O4-C6	4.42	96.00	121.35	16	11
4	A	405	PX4	O7-C23-C24	4.42	121.05	111.48	4	11
4	A	323	PX4	C8-C7-C6	4.42	101.48	111.78	13	15
4	A	415	PX4	C8-C7-C6	4.42	101.48	111.78	17	13
4	A	419	PX4	O7-C23-O8	4.42	113.38	123.70	14	7
4	A	429	PX4	P1-O3-C1	4.42	100.24	121.26	7	16
4	A	333	PX4	P1-O3-C1	4.41	100.25	121.26	19	11
4	A	322	PX4	C7-O7-C23	4.41	128.36	117.80	14	8
4	A	361	PX4	O5-C8-C7	4.41	121.12	108.40	14	11
4	A	425	PX4	O7-C23-C24	4.41	121.03	111.48	11	14
4	A	430	PX4	O7-C23-O8	4.41	113.39	123.70	16	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	361	PX4	P1-O3-C1	4.41	100.29	121.26	16	17
5	A	435	C3S	C44-C22-C1	4.41	116.13	109.43	5	8
4	A	331	PX4	O5-C9-C10	4.40	125.26	111.83	12	7
4	A	395	PX4	C8-C7-C6	4.40	101.52	111.78	2	12
4	A	368	PX4	C5-N1-C4	4.40	120.54	108.98	7	3
4	A	404	PX4	P1-O3-C1	4.40	100.31	121.26	1	16
5	A	434	C3S	C30-C29-C38	4.40	105.15	100.10	18	4
4	A	391	PX4	C4-N1-C3	4.40	97.42	108.98	2	8
5	A	433	C3S	C18-C15-C13	4.40	118.86	112.76	13	6
5	A	432	C3S	C30-C29-C38	4.39	105.14	100.10	14	6
4	A	355	PX4	O5-C8-C7	4.39	121.06	108.40	1	9
5	A	433	C3S	C22-C20-C18	4.39	119.13	112.71	4	7
4	A	425	PX4	O5-C8-C7	4.39	121.04	108.40	3	9
4	A	404	PX4	O7-C7-C6	4.38	124.07	108.34	11	5
4	A	311	PX4	O5-C9-C10	4.38	125.19	111.83	7	7
4	A	315	PX4	O1-P1-O2	4.38	132.81	112.44	20	12
5	A	435	C3S	C35-C32-C30	4.38	96.58	105.14	17	13
4	A	305	PX4	P1-O3-C1	4.38	100.43	121.26	11	13
4	A	366	PX4	O5-C8-C7	4.37	121.01	108.40	4	8
4	A	371	PX4	C4-N1-C3	4.38	97.48	108.98	7	4
4	A	409	PX4	P1-O3-C1	4.37	100.44	121.26	15	13
4	A	380	PX4	O5-C8-C7	4.37	121.00	108.40	15	13
4	A	403	PX4	P1-O3-C1	4.37	100.45	121.26	4	15
5	A	434	C3S	C26-C29-C38	4.37	110.16	116.60	11	5
4	A	323	PX4	P1-O3-C1	4.37	100.46	121.26	13	18
4	A	357	PX4	O1-P1-O2	4.37	132.77	112.44	12	7
4	A	406	PX4	O7-C23-C24	4.37	120.93	111.48	5	12
4	A	421	PX4	O1-P1-O2	4.37	132.76	112.44	8	10
5	A	436	C3S	C26-C29-C30	4.37	100.71	107.25	7	5
4	A	323	PX4	O7-C23-C24	4.36	120.92	111.48	8	9
4	A	424	PX4	O7-C23-C24	4.36	120.92	111.48	6	8
4	A	420	PX4	O5-C8-C7	4.36	120.97	108.40	6	14
4	A	400	PX4	O5-C8-C7	4.36	120.97	108.40	8	10
4	A	390	PX4	C8-C7-C6	4.36	101.62	111.78	9	9
4	A	394	PX4	O7-C23-C24	4.36	120.92	111.48	7	9
4	A	382	PX4	C5-N1-C3	4.36	97.53	108.98	4	4
5	A	431	C3S	C32-C30-C18	4.36	112.15	119.10	5	9
5	A	433	C3S	C23-C20-C22	4.36	118.46	113.08	4	9
4	A	334	PX4	C5-N1-C4	4.35	97.55	108.98	12	4
4	A	388	PX4	O5-C8-C7	4.35	120.94	108.40	16	11
4	A	427	PX4	P1-O3-C1	4.35	100.55	121.26	7	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	O7-C7-C8	4.35	123.94	108.34	7	9
4	A	411	PX4	O1-P1-O2	4.35	132.67	112.44	13	13
4	A	378	PX4	O5-C9-O6	4.35	112.76	123.63	12	5
5	A	436	C3S	C4-C7-C9	4.35	104.93	110.97	2	9
4	A	316	PX4	C8-C7-C6	4.34	101.66	111.78	18	15
5	A	431	C3S	C15-C18-C30	4.34	104.78	110.93	10	6
4	A	350	PX4	P1-O3-C1	4.34	100.60	121.26	9	13
4	A	387	PX4	C5-N1-C4	4.34	120.38	108.98	16	2
5	A	431	C3S	C26-C29-C30	4.34	100.75	107.25	8	10
4	A	361	PX4	O5-C9-C10	4.33	125.04	111.83	8	5
4	A	341	PX4	P1-O3-C1	4.33	100.65	121.26	10	15
4	A	356	PX4	P1-O4-C6	4.33	96.54	121.35	19	11
4	A	381	PX4	O7-C23-O8	4.33	113.59	123.70	18	9
4	A	319	PX4	C25-C24-C23	4.33	97.84	113.69	17	2
4	A	330	PX4	O7-C23-C24	4.33	120.84	111.48	11	8
4	A	382	PX4	P1-O3-C1	4.33	100.66	121.26	6	14
4	A	406	PX4	O7-C7-C8	4.33	123.87	108.34	9	9
4	A	399	PX4	C1-C2-N1	4.33	129.71	115.82	20	4
4	A	308	PX4	O7-C23-O8	4.32	113.59	123.70	2	6
4	A	343	PX4	C5-N1-C3	4.32	97.62	108.98	2	3
4	A	383	PX4	O7-C23-O8	4.32	113.60	123.70	9	5
4	A	400	PX4	C4-N1-C3	4.32	97.63	108.98	1	8
5	A	434	C3S	C26-C29-C30	4.32	100.78	107.25	8	9
4	A	353	PX4	O1-P1-O2	4.32	132.54	112.44	18	13
4	A	377	PX4	P1-O4-C6	4.32	96.61	121.35	2	14
4	A	349	PX4	P1-O4-C6	4.32	96.61	121.35	7	19
4	A	412	PX4	C5-N1-C3	4.32	97.64	108.98	8	6
4	A	353	PX4	O3-P1-O2	4.31	91.84	108.94	13	4
4	A	320	PX4	O7-C23-O8	4.31	113.63	123.70	18	7
4	A	322	PX4	P1-O3-C1	4.31	100.75	121.26	12	16
4	A	373	PX4	O7-C23-O8	4.31	113.63	123.70	4	7
4	A	415	PX4	O7-C23-C24	4.31	120.81	111.48	14	10
5	A	434	C3S	O3-S1-O6	4.31	96.47	106.37	10	6
4	A	418	PX4	C5-N1-C3	4.31	97.66	108.98	16	6
5	A	431	C3S	C22-C12-C13	4.30	116.64	122.93	10	6
5	A	432	C3S	O3-S1-O2	4.31	123.62	108.56	14	18
5	A	435	C3S	O3-S1-O2	4.31	123.62	108.56	7	19
4	A	309	PX4	C5-N1-C3	4.30	97.67	108.98	11	4
4	A	358	PX4	P1-O4-C6	4.30	96.69	121.35	7	13
4	A	395	PX4	P1-O3-C1	4.30	100.77	121.26	16	14
4	A	334	PX4	C7-O7-C23	4.30	128.09	117.80	15	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	425	PX4	P1-O3-C1	4.30	100.78	121.26	6	15
5	A	433	C3S	C32-C30-C29	4.30	98.78	103.84	10	8
4	A	373	PX4	P1-O4-C6	4.30	96.71	121.35	12	12
4	A	307	PX4	O7-C23-O8	4.30	113.66	123.70	11	9
4	A	332	PX4	O3-P1-O2	4.30	91.90	108.94	5	5
4	A	402	PX4	O5-C9-C10	4.30	124.94	111.83	19	6
4	A	308	PX4	O5-C8-C7	4.30	120.78	108.40	2	12
4	A	383	PX4	P1-O3-C1	4.30	100.81	121.26	11	11
4	A	343	PX4	O7-C7-C6	4.29	123.75	108.34	2	9
4	A	399	PX4	C5-N1-C4	4.29	97.69	108.98	10	6
5	A	434	C3S	C29-C30-C18	4.29	120.51	114.41	4	9
4	A	307	PX4	O7-C23-C24	4.29	120.77	111.48	16	9
4	A	385	PX4	O7-C23-C24	4.29	120.77	111.48	13	10
4	A	396	PX4	O7-C23-C24	4.29	120.77	111.48	7	10
4	A	323	PX4	O5-C9-C10	4.29	124.92	111.83	1	3
4	A	324	PX4	O7-C7-C8	4.29	123.73	108.34	2	13
4	A	352	PX4	O5-C9-O6	4.29	112.90	123.63	2	8
4	A	392	PX4	O7-C23-C24	4.29	120.76	111.48	7	9
4	A	342	PX4	P1-O3-C1	4.29	100.85	121.26	7	11
5	A	436	C3S	C32-C35-C38	4.29	113.53	105.14	18	10
4	A	350	PX4	O5-C8-C7	4.28	120.75	108.40	19	13
4	A	384	PX4	O7-C23-C24	4.28	120.75	111.48	6	10
4	A	423	PX4	O7-C23-C24	4.28	120.74	111.48	5	10
4	A	400	PX4	P1-O3-C1	4.28	100.90	121.26	16	13
4	A	403	PX4	O7-C23-C24	4.27	120.73	111.48	6	10
5	A	434	C3S	C22-C20-C18	4.28	118.96	112.71	5	4
4	A	325	PX4	C5-N1-C4	4.27	97.75	108.98	8	5
4	A	357	PX4	P1-O4-C6	4.27	96.86	121.35	13	14
4	A	364	PX4	P1-O4-C6	4.27	96.88	121.35	10	14
4	A	428	PX4	C12-C11-C10	4.27	97.43	113.13	8	6
5	A	433	C3S	C44-C22-C1	4.27	102.93	109.43	8	4
4	A	387	PX4	C3-N1-C2	4.27	92.94	109.91	15	5
4	A	367	PX4	C7-O7-C23	4.26	107.59	117.80	16	5
5	A	431	C3S	C35-C32-C30	4.26	96.80	105.14	18	9
4	A	358	PX4	O7-C23-C24	4.26	120.70	111.48	16	7
4	A	362	PX4	P1-O3-C1	4.26	100.98	121.26	15	15
5	A	433	C3S	C32-C30-C18	4.26	125.90	119.10	13	9
4	A	397	PX4	C1-C2-N1	4.26	129.49	115.82	18	6
5	A	433	C3S	O3-S1-O2	4.26	123.46	108.56	1	17
4	A	389	PX4	O7-C23-C24	4.26	120.69	111.48	9	8
4	A	409	PX4	O5-C8-C7	4.26	120.67	108.40	5	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	409	PX4	O3-P1-O2	4.26	92.07	108.94	3	2
4	A	409	PX4	C7-O7-C23	4.25	127.98	117.80	2	10
4	A	411	PX4	O7-C23-O8	4.25	113.77	123.70	5	8
5	A	433	C3S	C40-C29-C38	4.25	119.38	111.68	4	6
4	A	319	PX4	C5-N1-C3	4.25	97.82	108.98	9	4
4	A	343	PX4	C4-N1-C3	4.25	120.14	108.98	17	6
4	A	307	PX4	P1-O3-C1	4.24	101.05	121.26	17	14
4	A	390	PX4	C25-C24-C23	4.25	98.14	113.69	11	2
5	A	434	C3S	C54-C48-C38	4.25	119.13	110.33	5	11
4	A	367	PX4	C8-C7-C6	4.24	101.89	111.78	8	6
4	A	376	PX4	P1-O3-C1	4.24	101.07	121.26	2	15
4	A	323	PX4	P1-O4-C6	4.24	97.05	121.35	20	14
4	A	343	PX4	P1-O4-C6	4.24	97.05	121.35	1	12
4	A	375	PX4	C4-N1-C3	4.24	120.11	108.98	20	5
4	A	413	PX4	O1-P1-O2	4.24	132.17	112.44	14	10
4	A	362	PX4	O7-C23-C24	4.24	120.65	111.48	4	13
4	A	372	PX4	C5-N1-C4	4.24	97.84	108.98	4	6
4	A	395	PX4	O7-C7-C6	4.24	123.55	108.34	8	8
4	A	394	PX4	P1-O3-C1	4.24	101.10	121.26	19	12
4	A	423	PX4	C4-N1-C3	4.24	97.85	108.98	9	3
5	A	436	C3S	C15-C13-C12	4.24	117.87	125.02	3	8
4	A	311	PX4	O7-C23-O8	4.23	113.81	123.70	14	6
4	A	336	PX4	O4-P1-O2	4.23	125.70	108.94	10	4
4	A	391	PX4	C7-O7-C23	4.23	127.92	117.80	14	7
4	A	383	PX4	O1-P1-O2	4.23	132.11	112.44	7	8
4	A	416	PX4	P1-O3-C1	4.23	101.14	121.26	18	16
4	A	326	PX4	O4-P1-O2	4.23	125.69	108.94	17	3
4	A	323	PX4	O5-C8-C7	4.22	120.57	108.40	2	12
4	A	322	PX4	O7-C23-C24	4.22	120.62	111.48	10	11
4	A	346	PX4	C8-C7-C6	4.22	101.94	111.78	6	10
4	A	402	PX4	C32-C31-C30	4.22	93.03	114.37	11	2
4	A	422	PX4	C5-N1-C3	4.22	120.07	108.98	2	5
4	A	331	PX4	P1-O3-C1	4.22	101.17	121.26	8	14
4	A	329	PX4	O7-C7-C8	4.22	123.47	108.34	20	7
4	A	375	PX4	O7-C23-O8	4.22	113.85	123.70	8	6
4	A	387	PX4	O7-C7-C8	4.22	123.47	108.34	18	8
4	A	420	PX4	C7-O7-C23	4.22	107.70	117.80	11	6
5	A	434	C3S	C23-C20-C18	4.22	105.89	111.78	18	7
4	A	430	PX4	C8-C7-C6	4.22	101.96	111.78	11	13
5	A	434	C3S	C32-C30-C18	4.22	125.83	119.10	17	5
4	A	325	PX4	O7-C7-C6	4.21	123.46	108.34	10	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	327	PX4	P1-O3-C1	4.22	101.19	121.26	3	16
4	A	412	PX4	C7-O7-C23	4.22	127.88	117.80	14	5
4	A	407	PX4	O5-C9-O6	4.21	113.09	123.63	16	6
4	A	387	PX4	P1-O3-C1	4.21	101.21	121.26	15	18
4	A	390	PX4	C7-O7-C23	4.21	107.72	117.80	6	4
4	A	399	PX4	O7-C7-C6	4.21	123.45	108.34	12	7
4	A	314	PX4	O7-C7-C8	4.21	123.44	108.34	20	8
4	A	409	PX4	O7-C23-O8	4.21	113.86	123.70	15	9
4	A	370	PX4	C5-N1-C4	4.21	97.92	108.98	4	3
4	A	384	PX4	C7-O7-C23	4.21	127.87	117.80	3	10
4	A	427	PX4	P1-O4-C6	4.21	97.24	121.35	16	12
4	A	313	PX4	C5-N1-C4	4.21	97.93	108.98	13	6
4	A	338	PX4	C12-C11-C10	4.20	97.68	113.13	17	7
4	A	325	PX4	O7-C7-C8	4.20	123.42	108.34	1	5
5	A	436	C3S	C35-C32-C30	4.20	96.92	105.14	6	9
4	A	364	PX4	C33-C32-C31	4.20	93.14	114.37	7	2
4	A	379	PX4	O3-P1-O2	4.20	92.29	108.94	18	9
4	A	425	PX4	P1-O4-C6	4.20	97.29	121.35	19	11
4	A	426	PX4	P1-O3-C1	4.20	101.27	121.26	6	13
4	A	420	PX4	P1-O3-C1	4.20	101.28	121.26	18	11
5	A	431	C3S	C4-C1-C22	4.20	121.72	112.78	18	6
4	A	345	PX4	C34-C33-C32	4.20	93.16	114.37	13	3
4	A	347	PX4	O1-P1-O2	4.19	131.95	112.44	13	14
4	A	383	PX4	O3-P1-O2	4.19	92.33	108.94	10	4
4	A	387	PX4	C5-N1-C3	4.19	97.98	108.98	19	7
4	A	428	PX4	P1-O4-C6	4.19	97.35	121.35	18	11
4	A	333	PX4	O7-C7-C8	4.19	123.36	108.34	14	10
4	A	366	PX4	C5-N1-C3	4.18	119.97	108.98	13	4
4	A	372	PX4	C7-O7-C23	4.18	127.81	117.80	8	7
4	A	429	PX4	O5-C8-C7	4.18	120.46	108.40	7	10
4	A	421	PX4	O7-C23-O8	4.18	113.93	123.70	8	6
4	A	401	PX4	O5-C9-O6	4.18	113.17	123.63	16	6
4	A	416	PX4	P1-O4-C6	4.18	97.40	121.35	12	13
5	A	436	C3S	C30-C29-C38	4.18	104.89	100.10	15	6
4	A	328	PX4	C17-C16-C15	4.18	93.26	114.37	12	2
4	A	408	PX4	O7-C23-O8	4.18	113.94	123.70	10	7
4	A	321	PX4	P1-O4-C6	4.17	97.44	121.35	13	12
4	A	391	PX4	P1-O3-C1	4.17	101.39	121.26	9	16
4	A	404	PX4	C11-C10-C9	4.17	98.40	113.69	20	2
4	A	361	PX4	C1-C2-N1	4.17	129.21	115.82	5	6
4	A	420	PX4	O7-C7-C8	4.17	123.31	108.34	5	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	371	PX4	O3-P1-O2	4.17	92.42	108.94	20	3
5	A	436	C3S	C54-C48-C38	4.17	118.97	110.33	12	2
4	A	310	PX4	O7-C23-O8	4.16	113.97	123.70	20	6
4	A	321	PX4	O5-C9-C10	4.16	124.53	111.83	19	5
4	A	402	PX4	O5-C9-O6	4.16	113.21	123.63	8	4
4	A	421	PX4	P1-O3-C1	4.16	101.44	121.26	16	12
4	A	422	PX4	C12-C11-C10	4.16	97.83	113.13	6	4
4	A	429	PX4	O5-C9-C10	4.16	124.53	111.83	20	10
4	A	390	PX4	C12-C11-C10	4.16	97.84	113.13	18	5
4	A	392	PX4	P1-O3-C1	4.16	101.45	121.26	10	11
4	A	424	PX4	C8-C7-C6	4.16	102.08	111.78	8	10
4	A	320	PX4	P1-O3-C1	4.16	101.46	121.26	8	16
4	A	325	PX4	O7-C23-O8	4.16	113.98	123.70	20	8
4	A	347	PX4	P1-O3-C1	4.16	101.46	121.26	7	19
4	A	413	PX4	P1-O3-C1	4.16	101.46	121.26	5	14
4	A	342	PX4	C12-C11-C10	4.16	97.85	113.13	5	2
4	A	396	PX4	O3-P1-O2	4.16	92.45	108.94	8	4
4	A	340	PX4	C26-C25-C24	4.16	97.86	113.13	5	3
4	A	358	PX4	C4-N1-C3	4.15	98.06	108.98	8	4
4	A	389	PX4	C5-N1-C3	4.15	98.07	108.98	17	5
4	A	408	PX4	O5-C9-C10	4.15	124.50	111.83	17	7
4	A	305	PX4	O3-P1-O2	4.15	92.48	108.94	14	6
4	A	337	PX4	O7-C7-C8	4.15	123.24	108.34	11	9
5	A	431	C3S	C30-C29-C38	4.15	104.86	100.10	16	4
4	A	321	PX4	C5-N1-C4	4.15	98.08	108.98	3	4
4	A	337	PX4	C7-O7-C23	4.15	107.87	117.80	2	4
5	A	431	C3S	C18-C15-C13	4.15	118.51	112.76	18	7
4	A	353	PX4	P1-O3-C1	4.14	101.54	121.26	12	15
4	A	308	PX4	P1-O3-C1	4.14	101.55	121.26	14	15
4	A	309	PX4	O1-P1-O4	4.14	126.34	107.57	2	2
4	A	412	PX4	C4-N1-C3	4.14	119.85	108.98	10	8
4	A	425	PX4	O7-C23-O8	4.14	114.03	123.70	19	10
4	A	402	PX4	O7-C7-C6	4.14	123.19	108.34	10	6
4	A	357	PX4	O5-C9-O6	4.14	113.28	123.63	10	8
4	A	427	PX4	C4-N1-C3	4.14	98.10	108.98	3	4
4	A	313	PX4	O5-C8-C7	4.14	120.32	108.40	16	9
4	A	430	PX4	P1-O4-C6	4.14	97.64	121.35	12	11
4	A	428	PX4	C8-O5-C9	4.14	102.00	117.12	3	3
5	A	435	C3S	C23-C20-C22	4.14	118.19	113.08	2	10
4	A	322	PX4	O1-P1-O2	4.13	131.68	112.44	7	10
4	A	365	PX4	O7-C23-O8	4.14	114.04	123.70	15	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	O7-C23-O8	4.13	114.04	123.70	16	4
4	A	382	PX4	C4-N1-C3	4.13	98.12	108.98	10	8
4	A	398	PX4	O1-P1-O4	4.13	126.30	107.57	6	3
4	A	399	PX4	P1-O3-C1	4.13	101.59	121.26	20	16
4	A	315	PX4	O3-P1-O2	4.13	92.57	108.94	15	5
4	A	320	PX4	O7-C7-C6	4.13	123.16	108.34	13	12
5	A	433	C3S	C15-C18-C30	4.13	116.78	110.93	6	9
4	A	338	PX4	P1-O4-C6	4.13	97.69	121.35	16	12
4	A	342	PX4	C5-N1-C3	4.13	98.13	108.98	7	5
4	A	363	PX4	O5-C8-C7	4.13	120.30	108.40	3	12
4	A	395	PX4	C25-C24-C23	4.13	98.58	113.69	20	4
4	A	332	PX4	P1-O4-C6	4.12	97.72	121.35	19	10
4	A	378	PX4	O5-C9-C10	4.12	124.40	111.83	13	9
4	A	394	PX4	O7-C23-O8	4.12	114.07	123.70	7	9
4	A	384	PX4	O4-P1-O2	4.12	125.26	108.94	19	2
4	A	377	PX4	C5-N1-C4	4.12	98.16	108.98	15	5
5	A	436	C3S	C18-C15-C13	4.12	118.47	112.76	13	4
4	A	319	PX4	C5-N1-C4	4.11	98.17	108.98	19	8
4	A	351	PX4	O7-C7-C8	4.12	123.11	108.34	12	10
4	A	366	PX4	P1-O3-C1	4.12	101.67	121.26	5	16
4	A	346	PX4	C5-N1-C3	4.11	98.17	108.98	10	6
4	A	418	PX4	P1-O4-C6	4.11	97.79	121.35	2	9
4	A	428	PX4	C4-N1-C3	4.11	98.18	108.98	17	1
4	A	387	PX4	C4-N1-C3	4.11	98.18	108.98	16	9
4	A	329	PX4	O5-C8-C7	4.11	120.24	108.40	17	9
5	A	435	C3S	C20-C22-C12	4.11	115.67	109.65	7	7
4	A	379	PX4	O1-P1-O4	4.11	126.18	107.57	6	6
4	A	415	PX4	C11-C10-C9	4.11	98.65	113.69	10	2
4	A	346	PX4	P1-O3-C1	4.10	101.73	121.26	14	17
4	A	354	PX4	C5-N1-C3	4.10	98.21	108.98	6	3
4	A	306	PX4	O5-C9-O6	4.10	113.38	123.63	14	10
4	A	307	PX4	P1-O4-C6	4.10	97.87	121.35	1	12
4	A	336	PX4	C4-N1-C3	4.10	98.21	108.98	2	4
4	A	390	PX4	P1-O3-C1	4.10	101.75	121.26	17	12
5	A	432	C3S	C15-C18-C30	4.10	116.74	110.93	17	6
4	A	315	PX4	C5-N1-C4	4.10	98.21	108.98	16	4
4	A	411	PX4	P1-O3-C1	4.10	101.76	121.26	1	15
4	A	365	PX4	C25-C24-C23	4.10	98.69	113.69	6	4
4	A	368	PX4	P1-O4-C6	4.09	97.89	121.35	10	13
4	A	318	PX4	C5-N1-C3	4.09	119.73	108.98	3	5
4	A	425	PX4	O5-C9-O6	4.09	113.39	123.63	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	324	PX4	O7-C23-C24	4.09	120.33	111.48	13	5
4	A	402	PX4	C5-N1-C4	4.09	98.23	108.98	5	6
5	A	435	C3S	C18-C15-C13	4.09	118.43	112.76	7	9
4	A	348	PX4	O5-C9-O6	4.09	113.40	123.63	14	7
4	A	395	PX4	C7-O7-C23	4.09	108.01	117.80	18	5
4	A	372	PX4	O1-P1-O4	4.09	126.10	107.57	7	6
4	A	307	PX4	O4-P1-O2	4.09	125.14	108.94	13	3
4	A	424	PX4	P1-O3-C1	4.09	101.80	121.26	8	17
4	A	326	PX4	O7-C7-C8	4.09	123.00	108.34	3	9
5	A	431	C3S	C26-C29-C38	4.09	110.58	116.60	8	7
4	A	315	PX4	O7-C23-O8	4.08	114.16	123.70	5	9
4	A	320	PX4	O5-C9-O6	4.08	113.42	123.63	17	9
4	A	315	PX4	C1-C2-N1	4.08	128.92	115.82	5	10
4	A	347	PX4	O7-C7-C6	4.08	122.99	108.34	6	9
4	A	396	PX4	C7-O7-C23	4.08	127.57	117.80	9	3
5	A	434	C3S	C44-C22-C1	4.08	103.22	109.43	13	8
4	A	305	PX4	O1-P1-O2	4.08	131.42	112.44	9	9
4	A	326	PX4	O7-C23-O8	4.08	114.17	123.70	14	8
4	A	365	PX4	P1-O4-C6	4.08	97.98	121.35	19	14
4	A	409	PX4	O7-C7-C8	4.08	122.98	108.34	17	11
4	A	415	PX4	O5-C8-C7	4.08	120.15	108.40	5	10
4	A	376	PX4	C5-N1-C3	4.08	98.27	108.98	14	6
4	A	411	PX4	O7-C7-C8	4.08	122.97	108.34	20	5
4	A	421	PX4	C1-C2-N1	4.08	128.91	115.82	6	7
5	A	434	C3S	C15-C18-C20	4.08	114.43	109.72	2	7
4	A	417	PX4	C1-C2-N1	4.08	128.91	115.82	12	9
4	A	358	PX4	C7-O7-C23	4.07	127.55	117.80	8	7
4	A	392	PX4	C1-C2-N1	4.08	128.90	115.82	14	3
4	A	407	PX4	P1-O4-C6	4.07	98.00	121.35	11	14
5	A	432	C3S	C35-C38-C29	4.07	99.05	103.84	13	10
5	A	432	C3S	C32-C30-C29	4.07	99.05	103.84	2	9
4	A	357	PX4	O7-C7-C8	4.07	122.95	108.34	14	10
4	A	344	PX4	P1-O3-C1	4.07	101.89	121.26	12	14
4	A	356	PX4	O1-P1-O2	4.07	131.38	112.44	17	9
4	A	399	PX4	O5-C8-C7	4.07	120.13	108.40	13	10
4	A	420	PX4	O1-P1-O4	4.07	126.01	107.57	14	6
4	A	421	PX4	C5-N1-C3	4.07	98.29	108.98	10	5
4	A	421	PX4	O7-C7-C6	4.07	122.94	108.34	11	6
4	A	308	PX4	P1-O4-C6	4.07	98.04	121.35	4	11
4	A	409	PX4	O5-C9-O6	4.07	113.45	123.63	11	6
4	A	318	PX4	O7-C23-O8	4.07	114.20	123.70	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	O7-C7-C6	4.07	122.93	108.34	15	7
5	A	436	C3S	O3-S1-O2	4.07	122.78	108.56	10	18
4	A	341	PX4	C7-O7-C23	4.06	127.52	117.80	14	3
4	A	394	PX4	O1-P1-O2	4.06	131.35	112.44	3	13
4	A	405	PX4	C5-N1-C3	4.06	119.64	108.98	10	5
4	A	361	PX4	P1-O4-C6	4.06	98.08	121.35	14	12
4	A	413	PX4	O5-C8-C7	4.06	120.10	108.40	20	10
4	A	352	PX4	O3-P1-O2	4.06	92.85	108.94	12	3
4	A	336	PX4	O1-P1-O2	4.06	131.32	112.44	11	11
4	A	397	PX4	O7-C23-C24	4.06	120.26	111.48	2	12
4	A	414	PX4	O3-P1-O2	4.06	92.86	108.94	17	3
4	A	419	PX4	C1-C2-N1	4.06	128.84	115.82	10	11
4	A	325	PX4	O5-C9-O6	4.05	113.49	123.63	9	7
4	A	348	PX4	O5-C8-C7	4.05	120.08	108.40	12	10
4	A	371	PX4	O7-C7-C8	4.05	122.88	108.34	7	5
4	A	387	PX4	C25-C24-C23	4.05	98.85	113.69	14	5
4	A	393	PX4	P1-O4-C6	4.05	98.15	121.35	20	13
4	A	408	PX4	O1-P1-O2	4.05	131.28	112.44	11	13
4	A	418	PX4	P1-O3-C1	4.05	101.99	121.26	14	16
4	A	429	PX4	O1-P1-O2	4.05	131.28	112.44	12	9
5	A	435	C3S	C1-C22-C20	4.05	103.38	108.74	12	9
4	A	335	PX4	O5-C8-C7	4.05	120.06	108.40	17	9
4	A	374	PX4	C8-C7-C6	4.05	102.35	111.78	15	7
4	A	416	PX4	C5-N1-C4	4.05	98.34	108.98	2	4
4	A	429	PX4	O7-C23-C24	4.05	120.24	111.48	5	8
4	A	345	PX4	P1-O4-C6	4.04	98.17	121.35	3	9
4	A	368	PX4	P1-O3-C1	4.04	102.01	121.26	12	13
4	A	380	PX4	O7-C23-C24	4.04	120.23	111.48	12	7
4	A	392	PX4	O7-C7-C8	4.04	122.85	108.34	14	7
4	A	328	PX4	O5-C9-O6	4.04	113.52	123.63	4	6
4	A	354	PX4	O7-C7-C8	4.04	122.84	108.34	17	8
4	A	389	PX4	C4-N1-C3	4.04	98.37	108.98	8	7
4	A	368	PX4	O7-C7-C8	4.04	122.83	108.34	6	10
4	A	378	PX4	O7-C23-C24	4.04	120.22	111.48	17	8
4	A	385	PX4	O7-C7-C8	4.04	122.83	108.34	8	7
4	A	420	PX4	O1-P1-O2	4.04	131.23	112.44	15	11
4	A	418	PX4	O7-C23-O8	4.03	114.27	123.70	1	10
4	A	424	PX4	P1-O4-C6	4.03	98.25	121.35	9	10
5	A	436	C3S	C26-C29-C38	4.03	110.66	116.60	20	5
4	A	370	PX4	P1-O3-C1	4.03	102.08	121.26	3	16
4	A	314	PX4	O7-C23-C24	4.03	120.19	111.48	1	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	334	PX4	C25-C24-C23	4.03	98.94	113.69	16	3
4	A	377	PX4	O7-C23-O8	4.03	114.29	123.70	15	11
4	A	380	PX4	O7-C7-C8	4.03	122.79	108.34	10	12
4	A	334	PX4	O7-C23-C24	4.02	120.19	111.48	11	11
4	A	344	PX4	C7-O7-C23	4.02	127.42	117.80	4	5
4	A	317	PX4	P1-O3-C1	4.02	102.12	121.26	15	11
4	A	404	PX4	C5-N1-C3	4.02	98.42	108.98	15	5
4	A	428	PX4	O7-C23-C24	4.02	120.18	111.48	16	8
4	A	334	PX4	O5-C9-O6	4.02	113.58	123.63	7	6
4	A	381	PX4	O7-C7-C6	4.02	122.76	108.34	7	7
4	A	416	PX4	C12-C11-C10	4.02	98.36	113.13	12	3
4	A	427	PX4	C1-C2-N1	4.02	128.72	115.82	19	5
4	A	310	PX4	O5-C8-C7	4.02	119.98	108.40	5	8
4	A	344	PX4	O7-C23-C24	4.02	120.17	111.48	4	8
4	A	393	PX4	O3-P1-O2	4.02	93.02	108.94	17	5
4	A	428	PX4	C8-C7-C6	4.01	102.42	111.78	20	10
4	A	313	PX4	O4-P1-O2	4.01	124.84	108.94	6	5
4	A	324	PX4	O3-P1-O2	4.01	93.03	108.94	11	5
4	A	332	PX4	C7-O7-C23	4.01	108.19	117.80	9	3
4	A	349	PX4	P1-O3-C1	4.01	102.17	121.26	17	12
4	A	396	PX4	O7-C23-O8	4.01	114.33	123.70	9	5
4	A	408	PX4	O7-C7-C8	4.01	122.73	108.34	14	9
4	A	426	PX4	C1-C2-N1	4.01	128.69	115.82	15	6
4	A	390	PX4	P1-O4-C6	4.01	98.38	121.35	18	14
4	A	364	PX4	O1-P1-O2	4.01	131.08	112.44	17	11
4	A	351	PX4	O5-C8-C7	4.00	119.94	108.40	4	12
4	A	410	PX4	O3-P1-O2	4.00	93.06	108.94	7	2
4	A	368	PX4	O7-C7-C6	4.00	122.70	108.34	4	8
4	A	323	PX4	C12-C11-C10	4.00	98.43	113.13	12	5
4	A	329	PX4	C4-N1-C3	4.00	98.46	108.98	8	6
4	A	354	PX4	P1-O4-C6	4.00	98.42	121.35	9	10
4	A	355	PX4	O7-C7-C6	4.00	122.70	108.34	12	8
4	A	315	PX4	O1-P1-O4	4.00	125.70	107.57	7	3
4	A	333	PX4	O7-C7-C6	4.00	122.70	108.34	17	6
4	A	399	PX4	O4-P1-O2	4.00	124.79	108.94	4	6
4	A	355	PX4	C8-C7-C6	4.00	102.46	111.78	7	8
4	A	357	PX4	P1-O3-C1	4.00	102.22	121.26	1	15
4	A	359	PX4	P1-O4-C6	4.00	98.43	121.35	16	12
4	A	383	PX4	O5-C9-O6	4.00	113.62	123.63	19	6
4	A	398	PX4	C5-N1-C2	4.00	94.01	109.91	5	4
4	A	318	PX4	O7-C7-C8	4.00	122.69	108.34	7	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	O7-C7-C8	4.00	122.69	108.34	6	9
4	A	372	PX4	O5-C9-C10	4.00	124.02	111.83	11	6
4	A	339	PX4	C1-C2-N1	4.00	128.65	115.82	4	2
4	A	354	PX4	O7-C7-C6	4.00	122.68	108.34	13	4
4	A	316	PX4	C1-C2-N1	3.99	128.64	115.82	19	3
4	A	325	PX4	O5-C9-C10	3.99	124.02	111.83	17	3
4	A	335	PX4	C14-C13-C12	3.99	94.18	114.37	17	1
4	A	387	PX4	O7-C23-C24	3.99	120.12	111.48	11	10
4	A	400	PX4	O5-C9-O6	3.99	113.64	123.63	13	6
4	A	412	PX4	O7-C23-O8	3.99	114.37	123.70	13	8
4	A	347	PX4	P1-O4-C6	3.99	98.49	121.35	6	17
4	A	427	PX4	O1-P1-O2	3.99	130.99	112.44	10	11
4	A	376	PX4	O7-C23-O8	3.98	114.39	123.70	13	7
4	A	388	PX4	O7-C23-O8	3.98	114.39	123.70	7	8
4	A	395	PX4	O1-P1-O2	3.98	130.97	112.44	6	12
4	A	428	PX4	O5-C9-O6	3.98	113.66	123.63	12	7
4	A	350	PX4	C1-C2-N1	3.98	128.60	115.82	5	5
4	A	371	PX4	O5-C9-O6	3.98	113.67	123.63	16	9
4	A	318	PX4	O5-C9-C10	3.98	123.97	111.83	14	7
4	A	352	PX4	O7-C23-O8	3.98	114.40	123.70	20	9
4	A	393	PX4	O7-C7-C8	3.98	122.62	108.34	16	6
5	A	433	C3S	C7-C9-C12	3.98	117.33	111.45	12	11
4	A	309	PX4	C7-O7-C23	3.97	127.31	117.80	6	6
4	A	360	PX4	C7-O7-C23	3.97	108.28	117.80	1	6
4	A	378	PX4	O1-P1-O2	3.97	130.93	112.44	1	14
4	A	391	PX4	O7-C7-C6	3.97	122.60	108.34	11	13
4	A	421	PX4	P1-O4-C6	3.97	98.58	121.35	9	17
4	A	424	PX4	O1-P1-O4	3.97	89.56	107.57	2	3
4	A	425	PX4	O3-C1-C2	3.97	128.77	109.65	4	2
4	A	428	PX4	P1-O3-C1	3.97	102.35	121.26	10	17
4	A	429	PX4	C5-N1-C3	3.97	98.54	108.98	11	3
4	A	380	PX4	P1-O4-C6	3.97	98.59	121.35	5	11
4	A	328	PX4	C7-O7-C23	3.97	127.30	117.80	12	11
4	A	306	PX4	P1-O4-C6	3.97	98.61	121.35	19	15
4	A	363	PX4	P1-O3-C1	3.97	102.36	121.26	2	16
4	A	366	PX4	P1-O4-C6	3.97	98.60	121.35	2	14
4	A	375	PX4	O7-C7-C8	3.97	122.58	108.34	2	8
4	A	346	PX4	O3-P1-O2	3.97	93.21	108.94	19	2
4	A	399	PX4	C11-C10-C9	3.97	99.16	113.69	10	1
5	A	433	C3S	C26-C29-C38	3.97	110.76	116.60	19	8
4	A	333	PX4	P1-O4-C6	3.97	98.63	121.35	12	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	O5-C9-O6	3.97	113.71	123.63	15	4
4	A	403	PX4	C5-N1-C4	3.97	119.39	108.98	12	2
4	A	306	PX4	O5-C9-C10	3.96	123.92	111.83	14	5
4	A	337	PX4	O3-P1-O2	3.96	93.23	108.94	18	2
4	A	399	PX4	O3-P1-O2	3.96	93.23	108.94	5	6
4	A	419	PX4	O1-P1-O2	3.96	130.88	112.44	5	11
4	A	355	PX4	O7-C7-C8	3.96	122.55	108.34	2	13
4	A	388	PX4	C7-O7-C23	3.96	127.28	117.80	18	6
4	A	386	PX4	O5-C8-C7	3.96	119.81	108.40	7	9
5	A	432	C3S	C32-C30-C18	3.96	125.42	119.10	6	3
4	A	326	PX4	P1-O3-C1	3.96	102.43	121.26	5	17
4	A	359	PX4	C5-N1-C4	3.96	98.58	108.98	16	5
4	A	403	PX4	O5-C9-C10	3.96	123.90	111.83	19	6
4	A	393	PX4	P1-O3-C1	3.95	102.44	121.26	1	15
4	A	400	PX4	C7-O7-C23	3.95	127.26	117.80	14	5
4	A	305	PX4	O5-C9-C10	3.95	123.89	111.83	8	4
4	A	306	PX4	C26-C25-C24	3.95	98.61	113.13	5	2
4	A	416	PX4	O5-C9-O6	3.95	113.74	123.63	16	7
5	A	434	C3S	C1-C4-C7	3.95	116.77	110.33	9	8
5	A	435	C3S	C32-C35-C38	3.95	112.87	105.14	16	12
4	A	409	PX4	C5-N1-C4	3.95	98.61	108.98	2	9
4	A	403	PX4	O7-C7-C6	3.94	122.49	108.34	15	13
4	A	406	PX4	C25-C24-C23	3.94	99.26	113.69	14	1
4	A	417	PX4	C5-N1-C3	3.94	98.63	108.98	11	6
4	A	424	PX4	C12-C11-C10	3.94	98.65	113.13	14	2
4	A	319	PX4	O4-P1-O2	3.94	124.54	108.94	5	4
4	A	314	PX4	O3-P1-O2	3.94	93.33	108.94	9	5
4	A	355	PX4	O5-C9-O6	3.94	113.78	123.63	18	5
4	A	360	PX4	P1-O4-C6	3.94	98.79	121.35	9	13
4	A	362	PX4	C19-C18-C17	3.94	94.48	114.37	1	3
4	A	334	PX4	P1-O3-C1	3.93	102.54	121.26	8	15
4	A	386	PX4	C4-N1-C3	3.93	98.64	108.98	4	9
4	A	339	PX4	O1-P1-O2	3.93	130.73	112.44	11	10
4	A	356	PX4	O7-C23-O8	3.93	114.52	123.70	3	11
4	A	325	PX4	C11-C10-C9	3.93	99.30	113.69	10	2
4	A	329	PX4	O5-C9-O6	3.93	113.80	123.63	17	3
4	A	336	PX4	C7-O7-C23	3.93	127.20	117.80	6	3
4	A	416	PX4	O1-P1-O4	3.93	125.38	107.57	16	4
4	A	405	PX4	O1-P1-O2	3.93	130.72	112.44	1	11
4	A	314	PX4	C4-N1-C3	3.93	98.66	108.98	12	5
4	A	379	PX4	O1-P1-O2	3.92	130.70	112.44	17	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	380	PX4	C8-O5-C9	3.92	102.78	117.12	11	3
4	A	309	PX4	P1-O3-C1	3.92	102.59	121.26	13	13
4	A	397	PX4	O5-C9-O6	3.92	113.82	123.63	3	7
4	A	366	PX4	O5-C9-C10	3.92	123.78	111.83	1	6
4	A	316	PX4	O7-C7-C8	3.92	122.40	108.34	20	8
4	A	373	PX4	O7-C23-C24	3.92	119.95	111.48	20	10
4	A	373	PX4	O7-C7-C8	3.92	122.40	108.34	16	8
4	A	405	PX4	C7-O7-C23	3.92	127.17	117.80	1	7
4	A	415	PX4	P1-O3-C1	3.92	102.61	121.26	4	16
4	A	311	PX4	O1-P1-O3	3.92	89.82	107.57	11	4
4	A	356	PX4	O7-C7-C8	3.91	122.39	108.34	12	14
5	A	431	C3S	C15-C13-C12	3.91	118.41	125.02	8	6
4	A	316	PX4	O5-C9-C10	3.91	123.76	111.83	1	2
4	A	414	PX4	C7-O7-C23	3.91	127.15	117.80	12	6
4	A	353	PX4	O7-C7-C8	3.91	122.36	108.34	16	7
4	A	416	PX4	C4-N1-C3	3.91	119.24	108.98	18	5
5	A	433	C3S	C29-C30-C18	3.91	119.96	114.41	11	4
4	A	349	PX4	O5-C9-C10	3.90	123.74	111.83	15	5
4	A	351	PX4	C4-N1-C3	3.90	98.72	108.98	19	5
4	A	374	PX4	C1-C2-N1	3.90	128.35	115.82	13	5
4	A	365	PX4	O5-C9-C10	3.90	123.73	111.83	14	5
5	A	431	C3S	C23-C26-C29	3.90	119.33	112.74	17	6
4	A	384	PX4	C12-C11-C10	3.90	98.79	113.13	12	5
4	A	416	PX4	O7-C7-C8	3.90	122.34	108.34	3	7
5	A	434	C3S	C1-C22-C20	3.90	103.57	108.74	1	6
4	A	307	PX4	O7-C7-C8	3.90	122.34	108.34	20	10
4	A	333	PX4	C4-N1-C3	3.90	98.73	108.98	19	6
4	A	353	PX4	C4-N1-C3	3.90	98.73	108.98	11	4
4	A	367	PX4	P1-O4-C6	3.90	99.01	121.35	10	13
4	A	385	PX4	O1-P1-O2	3.90	130.58	112.44	19	14
4	A	423	PX4	P1-O3-C1	3.90	102.70	121.26	16	16
4	A	312	PX4	O7-C23-O8	3.90	114.60	123.70	18	6
4	A	373	PX4	P1-O3-C1	3.89	102.72	121.26	19	13
4	A	308	PX4	C5-N1-C3	3.89	98.75	108.98	17	1
4	A	377	PX4	C1-C2-N1	3.89	128.31	115.82	13	6
5	A	431	C3S	O3-S1-O2	3.89	122.18	108.56	10	19
4	A	363	PX4	O7-C7-C8	3.89	122.30	108.34	16	6
4	A	370	PX4	C1-C2-N1	3.89	128.31	115.82	5	7
4	A	375	PX4	O5-C9-O6	3.89	113.90	123.63	19	8
4	A	350	PX4	C12-C11-C10	3.89	98.84	113.13	16	4
4	A	363	PX4	C4-N1-C3	3.89	98.76	108.98	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	331	PX4	O7-C7-C6	3.89	122.29	108.34	8	8
4	A	340	PX4	O1-P1-O2	3.89	130.53	112.44	7	9
4	A	354	PX4	P1-O3-C1	3.89	102.76	121.26	1	15
4	A	372	PX4	O1-P1-O2	3.89	130.52	112.44	3	10
4	A	400	PX4	P1-O4-C6	3.89	99.08	121.35	1	15
4	A	414	PX4	C5-N1-C4	3.89	98.76	108.98	20	4
5	A	435	C3S	C50-C48-C54	3.89	104.32	110.34	4	12
4	A	306	PX4	C5-N1-C3	3.88	98.77	108.98	8	2
5	A	431	C3S	C22-C20-C18	3.89	118.39	112.71	20	4
4	A	388	PX4	O7-C23-C24	3.88	119.88	111.48	7	7
4	A	395	PX4	P1-O4-C6	3.88	99.09	121.35	8	16
4	A	329	PX4	O1-P1-O2	3.88	130.50	112.44	17	12
4	A	396	PX4	P1-O4-C6	3.88	99.12	121.35	4	13
4	A	408	PX4	C5-N1-C4	3.88	98.78	108.98	5	5
4	A	338	PX4	P1-O3-C1	3.88	102.80	121.26	1	17
4	A	346	PX4	P1-O4-C6	3.88	99.14	121.35	20	13
4	A	347	PX4	C4-N1-C3	3.88	98.79	108.98	8	4
4	A	402	PX4	O4-P1-O2	3.88	124.31	108.94	2	4
4	A	409	PX4	C26-C25-C24	3.88	98.88	113.13	3	6
4	A	415	PX4	O7-C23-O8	3.88	114.64	123.70	6	8
4	A	335	PX4	C7-O7-C23	3.88	127.07	117.80	11	9
5	A	433	C3S	C23-C20-C18	3.88	106.37	111.78	7	11
4	A	319	PX4	O7-C7-C6	3.87	122.24	108.34	6	8
4	A	405	PX4	O5-C9-C10	3.87	123.65	111.83	11	7
4	A	379	PX4	O5-C9-C10	3.87	123.64	111.83	12	5
4	A	389	PX4	O7-C7-C6	3.87	122.23	108.34	17	10
4	A	329	PX4	C8-O5-C9	3.87	102.97	117.12	3	5
4	A	404	PX4	P1-O4-C6	3.87	99.17	121.35	18	14
4	A	408	PX4	O5-C9-O6	3.87	113.95	123.63	17	4
4	A	410	PX4	P1-O3-C1	3.87	102.85	121.26	17	14
4	A	331	PX4	P1-O4-C6	3.87	99.19	121.35	13	18
4	A	366	PX4	O4-P1-O2	3.87	124.26	108.94	19	5
5	A	435	C3S	C22-C12-C13	3.86	117.29	122.93	14	9
4	A	357	PX4	O7-C7-C6	3.86	122.19	108.34	10	8
4	A	313	PX4	C1-C2-N1	3.86	128.21	115.82	14	8
4	A	329	PX4	P1-O4-C6	3.86	99.24	121.35	9	14
4	A	307	PX4	C7-O7-C23	3.86	127.03	117.80	11	5
4	A	335	PX4	P1-O3-C1	3.86	102.90	121.26	16	16
4	A	345	PX4	O7-C7-C6	3.86	122.18	108.34	10	8
4	A	367	PX4	C1-C2-N1	3.86	128.21	115.82	15	6
4	A	425	PX4	C4-N1-C3	3.86	98.84	108.98	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	433	C3S	C15-C18-C20	3.86	114.18	109.72	9	9
4	A	417	PX4	P1-O3-C1	3.86	102.89	121.26	17	19
5	A	433	C3S	C22-C12-C13	3.86	117.30	122.93	18	6
4	A	333	PX4	C1-C2-N1	3.86	128.20	115.82	10	9
4	A	360	PX4	C1-C2-N1	3.86	128.20	115.82	6	4
4	A	368	PX4	O5-C9-O6	3.86	113.98	123.63	2	7
4	A	390	PX4	O5-C9-O6	3.86	113.98	123.63	17	5
4	A	418	PX4	C4-N1-C2	3.85	125.23	109.91	17	2
4	A	321	PX4	C12-C11-C10	3.85	98.97	113.13	2	2
4	A	381	PX4	P1-O3-C1	3.85	102.92	121.26	8	14
4	A	406	PX4	C7-O7-C23	3.85	127.02	117.80	11	7
4	A	424	PX4	O5-C8-C7	3.85	119.50	108.40	14	7
4	A	327	PX4	O7-C7-C8	3.85	122.15	108.34	20	11
4	A	351	PX4	O7-C7-C6	3.85	122.15	108.34	13	5
4	A	336	PX4	C1-C2-N1	3.85	128.17	115.82	16	6
5	A	431	C3S	C23-C20-C18	3.85	106.41	111.78	11	5
4	A	355	PX4	P1-O4-C6	3.85	99.31	121.35	8	13
5	A	434	C3S	C32-C35-C38	3.85	112.67	105.14	11	10
4	A	384	PX4	O7-C7-C6	3.84	122.13	108.34	19	7
4	A	325	PX4	P1-O3-C1	3.84	102.98	121.26	19	15
4	A	400	PX4	O7-C23-O8	3.84	114.72	123.70	4	4
4	A	316	PX4	O5-C9-O6	3.84	114.02	123.63	8	5
4	A	353	PX4	O5-C9-O6	3.84	114.02	123.63	4	5
4	A	384	PX4	O5-C9-O6	3.84	114.03	123.63	8	6
4	A	409	PX4	O7-C23-C24	3.84	119.79	111.48	2	13
4	A	417	PX4	P1-O4-C6	3.84	99.35	121.35	11	14
4	A	325	PX4	O3-P1-O2	3.84	93.72	108.94	20	2
4	A	350	PX4	P1-O4-C6	3.84	99.36	121.35	12	16
4	A	371	PX4	P1-O3-C1	3.84	102.99	121.26	15	12
4	A	377	PX4	C12-C11-C10	3.84	99.03	113.13	1	2
4	A	389	PX4	O7-C7-C8	3.84	122.11	108.34	3	10
4	A	332	PX4	C5-N1-C4	3.83	98.90	108.98	16	6
4	A	354	PX4	C11-C10-C9	3.83	99.64	113.69	8	5
4	A	390	PX4	O4-P1-O2	3.83	124.13	108.94	7	5
4	A	396	PX4	P1-O3-C1	3.84	103.00	121.26	19	15
4	A	339	PX4	O7-C23-O8	3.83	114.75	123.70	1	8
4	A	305	PX4	C25-C24-C23	3.83	99.67	113.69	1	1
4	A	346	PX4	O7-C7-C8	3.83	122.08	108.34	13	6
4	A	365	PX4	O7-C7-C6	3.83	122.08	108.34	4	10
4	A	369	PX4	C1-C2-N1	3.83	128.11	115.82	3	6
4	A	378	PX4	O5-C8-C7	3.83	119.43	108.40	6	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	424	PX4	O7-C7-C6	3.83	122.08	108.34	14	6
4	A	401	PX4	O5-C9-C10	3.83	123.50	111.83	4	8
5	A	433	C3S	C4-C1-C22	3.83	120.93	112.78	9	11
4	A	375	PX4	O1-P1-O2	3.83	130.24	112.44	13	13
4	A	384	PX4	O1-P1-O2	3.82	130.24	112.44	11	12
4	A	316	PX4	O4-P1-O2	3.82	124.09	108.94	3	5
4	A	413	PX4	C4-N1-C3	3.82	98.93	108.98	3	5
4	A	346	PX4	C1-C2-N1	3.82	128.09	115.82	6	4
4	A	413	PX4	C7-O7-C23	3.82	126.94	117.80	7	7
4	A	416	PX4	O5-C8-C7	3.82	119.41	108.40	17	14
4	A	355	PX4	O7-C23-O8	3.82	114.78	123.70	8	8
4	A	330	PX4	O7-C23-O8	3.82	114.78	123.70	11	7
4	A	361	PX4	C12-C11-C10	3.82	127.16	113.13	11	3
4	A	426	PX4	C5-N1-C3	3.82	98.95	108.98	18	3
4	A	374	PX4	C5-N1-C3	3.82	98.95	108.98	12	3
4	A	361	PX4	C4-N1-C3	3.81	98.96	108.98	9	8
4	A	332	PX4	C26-C25-C24	3.81	99.11	113.13	8	1
4	A	335	PX4	O5-C9-O6	3.81	114.09	123.63	10	9
4	A	395	PX4	O3-C1-C2	3.81	128.00	109.65	18	3
4	A	415	PX4	C28-C27-C26	3.81	95.10	114.37	10	1
4	A	322	PX4	O5-C9-O6	3.81	114.09	123.63	15	5
4	A	341	PX4	O7-C7-C8	3.81	122.01	108.34	9	10
4	A	407	PX4	C13-C12-C11	3.81	95.11	114.37	18	2
4	A	425	PX4	C7-O7-C23	3.81	126.92	117.80	20	4
4	A	342	PX4	O1-P1-O2	3.81	130.17	112.44	9	12
4	A	370	PX4	O7-C7-C8	3.81	122.00	108.34	11	6
4	A	382	PX4	O5-C8-C7	3.81	119.37	108.40	16	13
4	A	403	PX4	P1-O4-C6	3.81	99.54	121.35	8	11
4	A	424	PX4	O1-P1-O2	3.80	130.14	112.44	20	10
4	A	409	PX4	O7-C7-C6	3.80	121.98	108.34	1	9
4	A	411	PX4	O7-C23-C24	3.80	119.70	111.48	7	8
4	A	425	PX4	C5-N1-C4	3.80	98.99	108.98	20	2
4	A	386	PX4	O1-P1-O2	3.80	130.12	112.44	11	10
4	A	397	PX4	O1-P1-O3	3.80	90.35	107.57	3	3
4	A	310	PX4	O7-C7-C8	3.80	121.96	108.34	3	7
4	A	377	PX4	C13-C12-C11	3.80	95.18	114.37	9	4
4	A	319	PX4	O3-P1-O2	3.80	93.89	108.94	6	6
4	A	323	PX4	O7-C23-O8	3.80	114.83	123.70	4	8
5	A	433	C3S	C1-C22-C20	3.80	113.76	108.74	1	7
4	A	329	PX4	C5-N1-C4	3.79	118.94	108.98	14	3
4	A	361	PX4	O7-C23-O8	3.79	114.84	123.70	12	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	369	PX4	C12-C11-C10	3.79	99.19	113.13	20	3
4	A	377	PX4	O5-C8-C7	3.79	119.33	108.40	10	10
4	A	410	PX4	O4-P1-O2	3.79	123.96	108.94	7	2
4	A	347	PX4	O5-C8-C7	3.79	119.32	108.40	4	14
4	A	389	PX4	O1-P1-O4	3.79	124.75	107.57	19	4
4	A	391	PX4	O7-C23-C24	3.79	119.68	111.48	16	6
4	A	426	PX4	P1-O4-C6	3.79	99.63	121.35	15	11
4	A	336	PX4	C26-C25-C24	3.79	99.21	113.13	16	2
4	A	338	PX4	C5-N1-C4	3.79	99.03	108.98	6	8
4	A	358	PX4	O7-C7-C6	3.79	121.93	108.34	5	9
4	A	381	PX4	C7-O7-C23	3.79	108.73	117.80	20	3
4	A	373	PX4	O5-C9-C10	3.79	123.38	111.83	9	5
4	A	386	PX4	O7-C7-C8	3.79	121.93	108.34	16	8
4	A	388	PX4	O7-C7-C8	3.79	121.93	108.34	14	7
4	A	391	PX4	O5-C8-C7	3.79	119.31	108.40	19	8
4	A	411	PX4	C12-C11-C10	3.79	99.21	113.13	3	2
4	A	416	PX4	C5-N1-C3	3.79	99.03	108.98	5	4
4	A	312	PX4	C5-N1-C4	3.79	99.03	108.98	2	5
4	A	347	PX4	C4-N1-C2	3.79	94.86	109.91	2	2
4	A	356	PX4	C4-N1-C3	3.78	99.03	108.98	20	5
4	A	428	PX4	O7-C23-O8	3.79	114.86	123.70	8	5
4	A	383	PX4	O1-P1-O4	3.78	124.72	107.57	2	4
5	A	436	C3S	C20-C22-C12	3.78	115.19	109.65	7	8
4	A	328	PX4	O7-C23-C24	3.78	119.66	111.48	5	9
4	A	342	PX4	C5-N1-C4	3.78	99.05	108.98	13	4
4	A	418	PX4	O4-P1-O2	3.78	123.92	108.94	2	4
4	A	418	PX4	C12-C11-C10	3.78	99.24	113.13	12	4
4	A	345	PX4	O7-C7-C8	3.78	121.90	108.34	3	7
4	A	365	PX4	O3-P1-O2	3.78	93.96	108.94	2	5
4	A	381	PX4	O5-C9-C10	3.78	123.36	111.83	14	7
4	A	387	PX4	O5-C9-O6	3.78	114.18	123.63	19	6
5	A	431	C3S	O3-S1-O6	3.78	97.69	106.37	18	3
4	A	344	PX4	O1-P1-O2	3.78	130.01	112.44	18	10
4	A	319	PX4	O7-C7-C8	3.78	121.89	108.34	1	9
4	A	340	PX4	C4-N1-C3	3.78	99.06	108.98	17	2
4	A	328	PX4	O1-P1-O2	3.77	130.00	112.44	18	13
4	A	409	PX4	O5-C9-C10	3.77	123.34	111.83	11	8
4	A	314	PX4	C7-O7-C23	3.77	126.82	117.80	18	6
4	A	325	PX4	C26-C25-C24	3.77	126.98	113.13	8	7
4	A	326	PX4	C5-N1-C3	3.77	99.07	108.98	6	6
4	A	366	PX4	C11-C10-C9	3.77	99.88	113.69	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	369	PX4	P1-O4-C6	3.77	99.74	121.35	5	10
5	A	433	C3S	C23-C26-C29	3.77	119.10	112.74	13	7
4	A	306	PX4	O7-C7-C8	3.77	121.86	108.34	3	12
4	A	311	PX4	O5-C9-O6	3.77	114.20	123.63	18	4
4	A	385	PX4	P1-O4-C6	3.77	99.76	121.35	10	12
4	A	399	PX4	O1-P1-O3	3.77	90.49	107.57	16	5
4	A	307	PX4	C25-C24-C23	3.77	99.89	113.69	13	1
4	A	407	PX4	C4-N1-C3	3.77	99.08	108.98	11	5
4	A	318	PX4	C4-N1-C3	3.76	99.09	108.98	9	5
4	A	342	PX4	C7-O7-C23	3.76	126.81	117.80	16	6
5	A	432	C3S	C1-C22-C12	3.76	115.23	108.74	7	5
4	A	377	PX4	C26-C25-C24	3.76	99.30	113.13	16	4
4	A	383	PX4	C8-O5-C9	3.76	103.36	117.12	12	3
4	A	405	PX4	O7-C7-C6	3.76	121.84	108.34	18	7
4	A	343	PX4	C5-N1-C4	3.76	99.10	108.98	3	5
4	A	400	PX4	O7-C23-C24	3.76	119.62	111.48	20	10
4	A	364	PX4	O7-C23-O8	3.76	114.92	123.70	11	7
4	A	405	PX4	O5-C9-O6	3.76	114.22	123.63	9	7
4	A	399	PX4	C31-C30-C29	3.76	95.38	114.37	4	2
4	A	311	PX4	C29-C28-C27	3.75	95.40	114.37	18	1
4	A	416	PX4	C7-O7-C23	3.75	108.81	117.80	5	7
4	A	336	PX4	C8-O5-C9	3.75	103.41	117.12	8	4
4	A	350	PX4	C7-O7-C23	3.75	126.77	117.80	11	6
4	A	398	PX4	C4-N1-C3	3.75	99.13	108.98	15	6
4	A	394	PX4	C7-O7-C23	3.75	126.76	117.80	18	3
4	A	410	PX4	O7-C7-C6	3.75	121.78	108.34	2	8
4	A	314	PX4	P1-O4-C6	3.74	99.91	121.35	5	12
4	A	323	PX4	C4-N1-C3	3.74	99.15	108.98	18	3
4	A	335	PX4	P1-O4-C6	3.74	99.91	121.35	3	11
4	A	337	PX4	C4-N1-C3	3.74	118.80	108.98	18	7
4	A	341	PX4	O7-C23-O8	3.74	114.96	123.70	13	6
4	A	347	PX4	C1-C2-N1	3.74	127.83	115.82	14	2
4	A	374	PX4	O7-C7-C8	3.74	121.77	108.34	2	15
4	A	342	PX4	O7-C23-C24	3.74	119.57	111.48	4	9
4	A	398	PX4	O7-C7-C6	3.74	121.76	108.34	2	8
4	A	406	PX4	O4-P1-O2	3.74	123.76	108.94	5	2
4	A	358	PX4	O5-C9-C10	3.74	123.23	111.83	7	7
4	A	309	PX4	O3-P1-O2	3.74	94.13	108.94	2	3
4	A	398	PX4	O5-C9-O6	3.74	114.28	123.63	8	9
4	A	329	PX4	P1-O3-C1	3.73	103.49	121.26	3	14
4	A	365	PX4	O1-P1-O3	3.73	90.64	107.57	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	435	C3S	C4-C1-C22	3.73	120.73	112.78	12	10
4	A	400	PX4	O1-P1-O3	3.73	90.66	107.57	19	3
4	A	427	PX4	O4-P1-O2	3.73	123.72	108.94	7	2
4	A	364	PX4	C17-C16-C15	3.73	95.51	114.37	18	2
4	A	310	PX4	C5-N1-C3	3.73	118.77	108.98	3	3
4	A	394	PX4	C12-C11-C10	3.73	99.42	113.13	2	3
4	A	404	PX4	O7-C7-C8	3.73	121.72	108.34	8	4
4	A	310	PX4	C11-C10-C9	3.73	100.03	113.69	13	4
4	A	406	PX4	P1-O3-C1	3.73	103.51	121.26	13	12
4	A	410	PX4	P1-O4-C6	3.73	99.98	121.35	19	10
4	A	321	PX4	C3-N1-C2	3.73	124.72	109.91	3	2
4	A	321	PX4	O7-C7-C6	3.73	121.72	108.34	7	7
4	A	380	PX4	C7-O7-C23	3.73	126.72	117.80	16	6
4	A	318	PX4	P1-O3-C1	3.72	103.53	121.26	10	18
4	A	359	PX4	C4-N1-C3	3.73	99.19	108.98	1	5
4	A	360	PX4	O3-P1-O2	3.73	94.17	108.94	4	7
4	A	426	PX4	C4-N1-C3	3.73	99.19	108.98	4	4
4	A	395	PX4	O1-P1-O3	3.72	90.68	107.57	9	3
4	A	395	PX4	C31-C30-C29	3.72	95.55	114.37	19	1
4	A	424	PX4	O1-P1-O3	3.72	124.45	107.57	2	5
4	A	411	PX4	C4-N1-C3	3.72	118.75	108.98	18	6
4	A	343	PX4	P1-O3-C1	3.72	103.55	121.26	12	19
4	A	352	PX4	C5-N1-C4	3.72	118.75	108.98	7	4
4	A	424	PX4	C26-C25-C24	3.72	99.45	113.13	4	6
5	A	432	C3S	C26-C23-C20	3.72	119.46	113.14	13	5
4	A	410	PX4	O1-P1-O4	3.72	124.42	107.57	2	4
4	A	370	PX4	C7-O7-C23	3.72	126.69	117.80	13	4
4	A	382	PX4	O7-C23-O8	3.72	115.01	123.70	16	5
4	A	392	PX4	O7-C23-O8	3.72	115.02	123.70	11	9
4	A	429	PX4	C1-C2-N1	3.72	127.75	115.82	6	7
4	A	430	PX4	C5-N1-C3	3.72	99.21	108.98	10	3
4	A	305	PX4	C8-C7-C6	3.72	103.12	111.78	6	7
4	A	349	PX4	O7-C23-O8	3.71	115.02	123.70	7	7
4	A	382	PX4	P1-O4-C6	3.71	100.07	121.35	16	13
5	A	434	C3S	O4-S1-O2	3.71	126.56	112.24	6	3
4	A	400	PX4	O3-C1-C2	3.71	127.52	109.65	13	3
5	A	433	C3S	C26-C29-C30	3.71	101.69	107.25	4	5
4	A	314	PX4	C1-C2-N1	3.71	127.72	115.82	16	6
4	A	335	PX4	O1-P1-O2	3.71	129.69	112.44	13	9
4	A	337	PX4	P1-O4-C6	3.71	100.10	121.35	11	12
4	A	379	PX4	P1-O3-C1	3.71	103.61	121.26	9	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	394	PX4	O3-P1-O2	3.71	94.24	108.94	3	7
4	A	401	PX4	C7-O7-C23	3.71	126.67	117.80	10	7
4	A	344	PX4	C4-N1-C3	3.71	99.24	108.98	12	4
4	A	345	PX4	C5-N1-C3	3.70	118.71	108.98	10	7
4	A	333	PX4	O5-C9-C10	3.70	123.12	111.83	7	7
4	A	370	PX4	O1-P1-O2	3.70	129.67	112.44	16	11
4	A	358	PX4	O5-C9-O6	3.70	114.37	123.63	2	7
4	A	315	PX4	P1-O4-C6	3.70	100.15	121.35	4	15
4	A	336	PX4	O5-C9-O6	3.70	114.38	123.63	20	8
4	A	406	PX4	P1-O4-C6	3.70	100.15	121.35	1	15
5	A	434	C3S	C40-C29-C38	3.70	104.97	111.68	12	3
4	A	392	PX4	P1-O4-C6	3.70	100.16	121.35	11	11
4	A	393	PX4	O1-P1-O2	3.70	129.64	112.44	17	5
4	A	395	PX4	O5-C8-C7	3.70	119.05	108.40	16	14
4	A	403	PX4	O5-C9-O6	3.70	114.38	123.63	2	5
4	A	348	PX4	C5-N1-C4	3.69	99.27	108.98	4	4
4	A	354	PX4	C4-N1-C3	3.69	99.27	108.98	5	5
4	A	323	PX4	O7-C7-C6	3.69	121.59	108.34	9	6
4	A	401	PX4	C5-N1-C3	3.69	99.27	108.98	16	3
4	A	360	PX4	C5-N1-C4	3.69	118.68	108.98	16	4
4	A	385	PX4	C11-C10-C9	3.69	100.17	113.69	18	2
4	A	358	PX4	C5-N1-C3	3.69	118.67	108.98	16	5
4	A	333	PX4	O1-P1-O2	3.69	129.61	112.44	18	13
4	A	357	PX4	O5-C9-C10	3.69	123.08	111.83	13	6
4	A	316	PX4	C15-C14-C13	3.69	95.73	114.37	10	4
4	A	418	PX4	O5-C9-O6	3.69	114.41	123.63	13	4
5	A	431	C3S	C26-C23-C20	3.69	119.40	113.14	6	4
4	A	324	PX4	O4-P1-O2	3.68	123.54	108.94	18	3
4	A	331	PX4	C7-O7-C23	3.68	126.61	117.80	7	8
4	A	356	PX4	C1-C2-N1	3.68	127.64	115.82	11	9
4	A	360	PX4	C3-N1-C2	3.68	124.55	109.91	20	1
4	A	314	PX4	C26-C25-C24	3.68	99.60	113.13	10	3
4	A	316	PX4	P1-O4-C6	3.68	100.26	121.35	10	14
4	A	332	PX4	O4-P1-O2	3.68	123.52	108.94	17	3
4	A	348	PX4	C7-O7-C23	3.68	126.61	117.80	13	7
4	A	354	PX4	C25-C24-C23	3.68	100.20	113.69	15	2
4	A	366	PX4	O1-P1-O2	3.68	129.58	112.44	3	8
4	A	412	PX4	C5-N1-C4	3.68	99.30	108.98	14	6
4	A	377	PX4	O1-P1-O2	3.68	129.57	112.44	17	10
4	A	383	PX4	P1-O4-C6	3.68	100.25	121.35	1	13
4	A	402	PX4	C4-N1-C3	3.68	99.31	108.98	10	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	C5-N1-C4	3.68	99.31	108.98	1	3
4	A	383	PX4	C5-N1-C4	3.68	99.31	108.98	9	5
4	A	371	PX4	C7-O7-C23	3.68	109.00	117.80	3	6
4	A	388	PX4	P1-O4-C6	3.68	100.28	121.35	4	15
4	A	414	PX4	O7-C23-C24	3.68	119.43	111.48	10	8
4	A	338	PX4	O5-C9-C10	3.67	123.04	111.83	2	10
4	A	407	PX4	C1-C2-N1	3.67	127.62	115.82	6	5
4	A	391	PX4	O5-C9-O6	3.67	114.44	123.63	5	5
4	A	415	PX4	O7-C7-C6	3.67	121.53	108.34	18	9
4	A	310	PX4	O5-C9-O6	3.67	114.44	123.63	12	8
4	A	328	PX4	C4-N1-C3	3.67	99.33	108.98	11	6
4	A	330	PX4	O5-C9-C10	3.67	123.03	111.83	8	8
4	A	414	PX4	P1-O4-C6	3.67	100.31	121.35	7	14
4	A	344	PX4	P1-O4-C6	3.67	100.33	121.35	9	12
4	A	362	PX4	C4-N1-C2	3.67	124.49	109.91	5	3
4	A	379	PX4	C15-C14-C13	3.67	95.83	114.37	13	2
4	A	397	PX4	C12-C11-C10	3.67	99.65	113.13	17	3
4	A	430	PX4	O4-P1-O2	3.67	94.40	108.94	10	4
4	A	334	PX4	O5-C9-C10	3.67	123.01	111.83	6	7
5	A	435	C3S	C22-C20-C18	3.66	107.36	112.71	10	10
4	A	400	PX4	O5-C9-C10	3.66	123.00	111.83	9	8
4	A	410	PX4	C4-N1-C3	3.66	99.36	108.98	9	6
4	A	422	PX4	O1-P1-O2	3.66	129.48	112.44	10	12
4	A	427	PX4	C11-C10-C9	3.66	100.28	113.69	17	2
4	A	430	PX4	C1-C2-N1	3.66	127.57	115.82	8	8
5	A	435	C3S	C30-C29-C38	3.66	104.30	100.10	8	5
4	A	327	PX4	C4-N1-C3	3.66	99.37	108.98	1	2
4	A	351	PX4	C12-C11-C10	3.66	99.69	113.13	20	3
4	A	384	PX4	O7-C7-C8	3.66	121.46	108.34	8	10
4	A	404	PX4	O5-C9-O6	3.66	114.48	123.63	11	4
4	A	336	PX4	O7-C7-C6	3.66	121.46	108.34	15	9
4	A	317	PX4	C5-N1-C4	3.65	99.38	108.98	7	5
4	A	334	PX4	O1-P1-O2	3.65	129.43	112.44	2	12
4	A	392	PX4	C11-C10-C9	3.65	100.31	113.69	12	4
4	A	374	PX4	C26-C25-C24	3.65	99.71	113.13	11	2
4	A	314	PX4	O5-C8-C7	3.65	118.92	108.40	1	14
4	A	322	PX4	O7-C7-C8	3.65	121.44	108.34	1	7
4	A	350	PX4	C4-N1-C3	3.65	99.39	108.98	12	5
4	A	308	PX4	C1-C2-N1	3.65	127.53	115.82	19	6
4	A	310	PX4	P1-O4-C6	3.65	100.45	121.35	19	13
4	A	325	PX4	C12-C11-C10	3.65	99.72	113.13	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	334	PX4	C1-C2-N1	3.65	127.53	115.82	2	7
4	A	385	PX4	O5-C9-O6	3.65	114.50	123.63	1	6
4	A	367	PX4	O7-C7-C6	3.65	121.43	108.34	17	5
4	A	324	PX4	P1-O4-C6	3.65	100.46	121.35	13	12
4	A	336	PX4	O3-P1-O2	3.64	94.49	108.94	9	4
4	A	348	PX4	O7-C23-O8	3.65	115.18	123.70	10	7
4	A	382	PX4	C1-C2-N1	3.65	127.52	115.82	5	3
4	A	399	PX4	C7-O7-C23	3.65	126.52	117.80	3	8
4	A	429	PX4	P1-O4-C6	3.65	100.46	121.35	17	13
4	A	311	PX4	P1-O4-C6	3.64	100.47	121.35	15	16
4	A	368	PX4	C4-N1-C2	3.64	124.39	109.91	6	3
4	A	400	PX4	C25-C24-C23	3.64	100.34	113.69	15	1
4	A	400	PX4	O1-P1-O2	3.64	129.39	112.44	8	11
4	A	318	PX4	O7-C7-C6	3.64	121.40	108.34	8	9
4	A	401	PX4	O7-C23-O8	3.64	115.20	123.70	5	6
4	A	325	PX4	P1-O4-C6	3.64	100.51	121.35	14	15
4	A	367	PX4	C12-C11-C10	3.64	99.76	113.13	7	3
4	A	408	PX4	C4-N1-C3	3.64	99.42	108.98	7	5
4	A	415	PX4	C4-N1-C3	3.64	118.53	108.98	13	6
4	A	423	PX4	O3-P1-O2	3.64	94.52	108.94	13	5
4	A	361	PX4	C5-N1-C4	3.64	99.42	108.98	20	6
4	A	335	PX4	C4-N1-C3	3.64	118.53	108.98	19	6
4	A	371	PX4	O7-C23-O8	3.64	115.20	123.70	14	5
4	A	352	PX4	C7-O7-C23	3.63	126.49	117.80	10	5
4	A	397	PX4	O7-C23-O8	3.63	115.21	123.70	3	10
4	A	327	PX4	O1-P1-O2	3.63	129.34	112.44	19	8
4	A	355	PX4	C1-C2-N1	3.63	127.48	115.82	20	7
4	A	393	PX4	C12-C11-C10	3.63	99.78	113.13	5	3
4	A	396	PX4	O7-C7-C8	3.63	121.38	108.34	18	9
4	A	417	PX4	O5-C9-C10	3.63	122.91	111.83	18	7
4	A	311	PX4	C7-O7-C23	3.63	109.11	117.80	10	5
4	A	349	PX4	C12-C11-C10	3.63	99.80	113.13	17	2
4	A	353	PX4	O7-C7-C6	3.63	121.36	108.34	13	7
4	A	419	PX4	C26-C25-C24	3.63	99.80	113.13	13	1
4	A	326	PX4	C11-C10-C9	3.62	100.41	113.69	17	4
4	A	381	PX4	P1-O4-C6	3.62	100.58	121.35	19	16
4	A	388	PX4	O3-P1-O2	3.62	94.57	108.94	3	1
4	A	413	PX4	O5-C9-O6	3.62	114.56	123.63	20	4
5	A	435	C3S	C1-C4-C7	3.62	116.24	110.33	16	8
4	A	415	PX4	P1-O4-C6	3.62	100.59	121.35	7	14
4	A	372	PX4	O7-C7-C8	3.62	121.33	108.34	9	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	O3-C1-C2	3.62	127.07	109.65	19	3
5	A	432	C3S	C35-C38-C48	3.62	117.66	112.18	13	4
4	A	345	PX4	C4-N1-C3	3.62	118.48	108.98	18	7
4	A	351	PX4	P1-O4-C6	3.62	100.61	121.35	3	12
5	A	434	C3S	O3-S1-O2	3.62	121.22	108.56	11	17
4	A	331	PX4	O7-C23-O8	3.62	115.25	123.70	8	8
4	A	356	PX4	C14-C13-C12	3.62	96.08	114.37	9	1
4	A	423	PX4	O7-C23-O8	3.62	115.25	123.70	4	11
4	A	323	PX4	O1-P1-O2	3.62	129.27	112.44	14	12
4	A	353	PX4	C7-O7-C23	3.62	109.14	117.80	13	2
4	A	339	PX4	C7-O7-C23	3.61	126.45	117.80	17	5
4	A	387	PX4	P1-O4-C6	3.62	100.63	121.35	8	13
4	A	414	PX4	C5-N1-C3	3.62	99.48	108.98	11	4
4	A	310	PX4	O4-P1-O2	3.61	123.25	108.94	3	3
4	A	318	PX4	P1-O4-C6	3.61	100.65	121.35	2	12
4	A	421	PX4	C14-C13-C12	3.61	96.11	114.37	12	2
4	A	312	PX4	O1-P1-O2	3.61	129.23	112.44	8	8
4	A	374	PX4	P1-O3-C1	3.61	104.08	121.26	2	14
4	A	350	PX4	C5-N1-C4	3.61	99.50	108.98	16	3
4	A	383	PX4	O1-P1-O3	3.61	91.21	107.57	18	6
4	A	411	PX4	O3-P1-O2	3.61	94.63	108.94	13	5
4	A	408	PX4	C32-C31-C30	3.61	96.13	114.37	9	1
4	A	414	PX4	O7-C7-C8	3.61	121.28	108.34	1	11
4	A	380	PX4	C1-C2-N1	3.60	127.39	115.82	10	7
4	A	388	PX4	O1-P1-O2	3.60	129.21	112.44	5	13
4	A	393	PX4	O5-C9-C10	3.60	122.82	111.83	20	4
4	A	367	PX4	O1-P1-O2	3.60	129.20	112.44	7	10
4	A	417	PX4	O7-C23-O8	3.60	115.28	123.70	7	11
4	A	333	PX4	C5-N1-C3	3.60	99.52	108.98	11	4
4	A	345	PX4	O5-C9-C10	3.60	122.81	111.83	9	3
4	A	348	PX4	P1-O4-C6	3.60	100.72	121.35	17	11
4	A	427	PX4	O5-C9-C10	3.60	122.81	111.83	15	6
4	A	353	PX4	C12-C11-C10	3.60	99.91	113.13	17	3
4	A	410	PX4	C5-N1-C3	3.60	99.53	108.98	13	3
5	A	432	C3S	C44-C22-C1	3.60	103.96	109.43	5	7
4	A	331	PX4	O3-P1-O2	3.60	94.69	108.94	8	5
4	A	418	PX4	C17-C16-C15	3.59	96.20	114.37	9	6
4	A	314	PX4	C5-N1-C2	3.59	124.19	109.91	8	2
4	A	328	PX4	O3-P1-O2	3.59	94.69	108.94	9	5
4	A	326	PX4	O7-C7-C6	3.59	121.23	108.34	15	10
4	A	353	PX4	C1-C2-N1	3.59	127.35	115.82	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	C7-O7-C23	3.59	126.39	117.80	5	4
4	A	369	PX4	O5-C9-O6	3.59	114.65	123.63	14	6
4	A	371	PX4	O5-C9-C10	3.59	122.78	111.83	20	5
4	A	384	PX4	C4-N1-C3	3.59	99.55	108.98	17	4
4	A	412	PX4	P1-O4-C6	3.59	100.78	121.35	4	14
4	A	426	PX4	O1-P1-O2	3.59	129.14	112.44	14	10
4	A	321	PX4	O1-P1-O2	3.59	129.14	112.44	10	11
4	A	332	PX4	C1-C2-N1	3.59	127.34	115.82	14	7
4	A	344	PX4	O7-C7-C6	3.59	121.22	108.34	20	9
4	A	347	PX4	C5-N1-C3	3.59	99.56	108.98	17	2
4	A	411	PX4	C4-N1-C2	3.59	95.65	109.91	3	2
4	A	362	PX4	O7-C23-O8	3.59	115.32	123.70	9	5
4	A	413	PX4	O7-C7-C6	3.59	121.21	108.34	15	11
5	A	433	C3S	C35-C32-C30	3.59	98.13	105.14	3	7
5	A	433	C3S	C35-C38-C29	3.59	99.62	103.84	11	5
4	A	341	PX4	O7-C7-C6	3.58	121.20	108.34	2	9
4	A	350	PX4	O7-C23-O8	3.58	115.33	123.70	18	7
4	A	392	PX4	C8-O5-C9	3.58	104.02	117.12	1	4
4	A	411	PX4	C32-C31-C30	3.58	96.25	114.37	9	1
4	A	421	PX4	O7-C7-C8	3.58	121.20	108.34	14	5
4	A	332	PX4	C4-N1-C3	3.58	99.57	108.98	2	3
4	A	394	PX4	C16-C15-C14	3.58	96.27	114.37	13	3
4	A	399	PX4	P1-O4-C6	3.58	100.82	121.35	17	14
4	A	371	PX4	C8-O5-C9	3.58	130.21	117.12	12	5
4	A	312	PX4	O5-C9-O6	3.58	114.67	123.63	5	4
4	A	352	PX4	O7-C7-C6	3.58	121.19	108.34	3	5
4	A	406	PX4	O5-C9-O6	3.58	114.67	123.63	10	4
4	A	390	PX4	C8-O5-C9	3.58	130.20	117.12	19	5
4	A	307	PX4	C1-C2-N1	3.58	127.30	115.82	5	7
4	A	310	PX4	C17-C16-C15	3.58	96.30	114.37	13	1
4	A	339	PX4	C5-N1-C4	3.58	118.37	108.98	14	4
4	A	342	PX4	O3-P1-O2	3.58	94.76	108.94	13	4
4	A	389	PX4	C1-C2-N1	3.58	127.30	115.82	1	6
5	A	431	C3S	C40-C29-C38	3.58	118.16	111.68	8	6
4	A	330	PX4	O1-P1-O2	3.57	129.07	112.44	17	10
4	A	345	PX4	O1-P1-O2	3.57	129.07	112.44	14	10
4	A	339	PX4	O7-C7-C6	3.57	121.16	108.34	5	8
4	A	382	PX4	O3-P1-O2	3.57	94.78	108.94	15	5
4	A	412	PX4	O1-P1-O2	3.57	129.06	112.44	14	7
5	A	432	C3S	C23-C26-C29	3.57	118.77	112.74	17	3
4	A	386	PX4	O7-C23-O8	3.57	115.36	123.70	2	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	342	PX4	O7-C7-C8	3.57	121.15	108.34	18	9
4	A	306	PX4	O1-P1-O2	3.57	129.04	112.44	2	7
4	A	318	PX4	C1-C2-N1	3.57	127.27	115.82	2	6
4	A	424	PX4	O7-C7-C8	3.57	121.14	108.34	7	11
5	A	431	C3S	C7-C9-C12	3.56	116.72	111.45	2	10
4	A	309	PX4	O1-P1-O2	3.56	129.01	112.44	13	12
4	A	338	PX4	C26-C25-C24	3.56	100.04	113.13	3	2
4	A	385	PX4	C7-O7-C23	3.56	126.32	117.80	6	4
4	A	407	PX4	C7-O7-C23	3.56	126.32	117.80	6	5
4	A	416	PX4	C30-C29-C28	3.56	96.36	114.37	8	2
4	A	319	PX4	P1-O4-C6	3.56	100.95	121.35	9	18
4	A	374	PX4	P1-O4-C6	3.56	100.95	121.35	2	10
4	A	422	PX4	O7-C7-C6	3.56	121.12	108.34	10	10
4	A	397	PX4	O3-P1-O2	3.56	94.83	108.94	18	6
4	A	348	PX4	C5-N1-C3	3.56	99.63	108.98	8	3
4	A	385	PX4	C1-C2-N1	3.56	127.24	115.82	9	6
4	A	422	PX4	O7-C7-C8	3.56	121.10	108.34	11	4
4	A	323	PX4	C1-C2-N1	3.55	127.23	115.82	9	3
4	A	326	PX4	C3-N1-C2	3.55	95.78	109.91	7	2
4	A	387	PX4	O3-P1-O2	3.56	94.84	108.94	9	5
4	A	343	PX4	O7-C7-C8	3.55	121.09	108.34	17	11
4	A	361	PX4	C7-O7-C23	3.55	126.30	117.80	15	6
4	A	407	PX4	O5-C9-C10	3.55	122.67	111.83	16	5
4	A	343	PX4	C7-O7-C23	3.55	126.30	117.80	6	5
4	A	391	PX4	O5-C9-C10	3.55	122.66	111.83	15	5
4	A	330	PX4	O7-C7-C6	3.55	121.08	108.34	8	8
4	A	340	PX4	C7-O7-C23	3.55	126.29	117.80	17	6
4	A	372	PX4	P1-O4-C6	3.55	101.01	121.35	5	12
4	A	411	PX4	C5-N1-C3	3.55	99.65	108.98	16	6
4	A	408	PX4	C1-C2-N1	3.55	127.21	115.82	2	6
4	A	316	PX4	C5-N1-C3	3.55	99.66	108.98	2	4
5	A	435	C3S	C15-C18-C30	3.55	105.91	110.93	12	11
4	A	369	PX4	O7-C7-C8	3.55	121.06	108.34	8	12
4	A	360	PX4	O1-P1-O2	3.54	128.93	112.44	18	13
4	A	381	PX4	C4-N1-C3	3.54	99.67	108.98	16	5
4	A	386	PX4	C1-C2-N1	3.54	127.19	115.82	7	5
4	A	368	PX4	O7-C23-O8	3.54	115.43	123.70	16	3
4	A	388	PX4	O5-C9-C10	3.54	122.63	111.83	9	5
4	A	406	PX4	O1-P1-O2	3.54	128.91	112.44	15	15
4	A	310	PX4	P1-O3-C1	3.54	104.43	121.26	17	15
4	A	320	PX4	P1-O4-C6	3.54	101.09	121.35	14	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	425	PX4	O7-C7-C8	3.54	121.03	108.34	14	9
4	A	330	PX4	P1-O4-C6	3.53	101.10	121.35	10	12
4	A	305	PX4	C5-N1-C3	3.53	99.70	108.98	1	4
4	A	335	PX4	C1-C2-N1	3.53	127.16	115.82	11	7
4	A	352	PX4	P1-O3-C1	3.53	104.45	121.26	8	15
4	A	355	PX4	O1-P1-O2	3.53	128.88	112.44	1	9
4	A	392	PX4	O5-C9-C10	3.53	122.60	111.83	17	5
4	A	419	PX4	C20-C19-C18	3.53	96.51	114.37	16	2
4	A	405	PX4	O7-C7-C8	3.53	121.01	108.34	6	7
4	A	410	PX4	C7-O7-C23	3.53	109.35	117.80	19	4
4	A	363	PX4	P1-O4-C6	3.53	101.13	121.35	8	9
4	A	366	PX4	O7-C7-C8	3.53	121.00	108.34	9	9
4	A	419	PX4	P1-O4-C6	3.53	101.13	121.35	16	13
4	A	425	PX4	C1-C2-N1	3.53	127.15	115.82	7	6
4	A	347	PX4	C25-C24-C23	3.53	126.62	113.69	8	3
4	A	388	PX4	O5-C9-O6	3.53	114.81	123.63	9	6
4	A	393	PX4	O7-C7-C6	3.53	120.99	108.34	15	8
4	A	402	PX4	C5-N1-C2	3.53	123.93	109.91	19	2
4	A	430	PX4	O7-C7-C8	3.53	121.00	108.34	5	6
4	A	319	PX4	C3-N1-C2	3.53	123.92	109.91	18	1
4	A	319	PX4	O1-P1-O2	3.52	128.83	112.44	9	9
4	A	326	PX4	C17-C16-C15	3.52	96.56	114.37	2	3
4	A	344	PX4	C11-C10-C9	3.52	100.78	113.69	15	2
4	A	369	PX4	C4-N1-C3	3.52	99.72	108.98	13	2
4	A	373	PX4	C5-N1-C3	3.52	118.23	108.98	20	4
4	A	422	PX4	O3-P1-O2	3.52	94.97	108.94	13	6
4	A	316	PX4	O1-P1-O2	3.52	128.82	112.44	16	8
4	A	362	PX4	P1-O4-C6	3.52	101.17	121.35	14	15
4	A	320	PX4	O1-P1-O4	3.52	123.52	107.57	3	4
4	A	346	PX4	O7-C23-O8	3.52	115.48	123.70	3	7
4	A	383	PX4	C7-O7-C23	3.52	126.22	117.80	13	4
4	A	395	PX4	O1-P1-O4	3.52	123.52	107.57	2	2
4	A	321	PX4	C33-C32-C31	3.52	96.59	114.37	12	1
4	A	384	PX4	C33-C32-C31	3.52	96.59	114.37	12	2
4	A	311	PX4	C1-C2-N1	3.52	127.11	115.82	17	7
4	A	343	PX4	O4-P1-O2	3.52	122.87	108.94	20	3
4	A	347	PX4	O3-P1-O2	3.52	95.00	108.94	19	9
4	A	378	PX4	C5-N1-C4	3.52	99.74	108.98	11	4
4	A	383	PX4	O7-C7-C8	3.52	120.96	108.34	12	5
4	A	397	PX4	O5-C9-C10	3.51	122.55	111.83	4	7
4	A	417	PX4	O1-P1-O2	3.52	128.80	112.44	13	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	311	PX4	C5-N1-C3	3.51	118.20	108.98	5	6
4	A	313	PX4	C5-N1-C3	3.51	99.75	108.98	20	2
4	A	344	PX4	C16-C15-C14	3.51	96.62	114.37	3	4
4	A	346	PX4	O5-C9-O6	3.51	114.84	123.63	19	9
4	A	426	PX4	O3-P1-O2	3.51	95.01	108.94	18	4
4	A	374	PX4	C4-N1-C2	3.51	123.86	109.91	15	1
4	A	396	PX4	O5-C9-C10	3.51	122.54	111.83	1	6
4	A	380	PX4	C4-N1-C2	3.51	95.96	109.91	13	2
4	A	406	PX4	O1-P1-O3	3.51	91.66	107.57	1	3
4	A	427	PX4	C3-N1-C2	3.51	123.86	109.91	3	2
4	A	364	PX4	C7-O7-C23	3.51	109.40	117.80	16	8
4	A	366	PX4	C1-C2-N1	3.51	127.08	115.82	4	7
4	A	429	PX4	O7-C7-C6	3.51	120.92	108.34	2	12
4	A	309	PX4	C25-C24-C23	3.50	100.85	113.69	11	2
4	A	313	PX4	C12-C11-C10	3.50	100.25	113.13	17	5
4	A	358	PX4	O1-P1-O4	3.50	123.45	107.57	18	3
4	A	354	PX4	O1-P1-O2	3.50	128.74	112.44	6	10
4	A	374	PX4	O5-C8-C7	3.50	118.50	108.40	5	6
4	A	353	PX4	P1-O4-C6	3.50	101.28	121.35	9	13
4	A	354	PX4	C8-O5-C9	3.50	104.32	117.12	16	4
4	A	374	PX4	O3-C1-C2	3.50	126.50	109.65	11	3
4	A	380	PX4	C26-C25-C24	3.50	100.26	113.13	9	3
4	A	389	PX4	P1-O4-C6	3.50	101.28	121.35	19	7
4	A	407	PX4	C5-N1-C3	3.50	99.78	108.98	14	6
4	A	319	PX4	C34-C33-C32	3.50	96.67	114.37	7	2
4	A	383	PX4	O5-C9-C10	3.50	122.51	111.83	8	8
4	A	387	PX4	C12-C11-C10	3.50	100.27	113.13	16	3
4	A	403	PX4	C1-C2-N1	3.50	127.06	115.82	14	5
4	A	414	PX4	P1-O3-C1	3.50	104.59	121.26	5	13
4	A	314	PX4	O5-C9-C10	3.50	122.50	111.83	4	6
4	A	321	PX4	C29-C28-C27	3.50	96.69	114.37	13	3
4	A	372	PX4	C12-C11-C10	3.50	100.28	113.13	9	3
4	A	380	PX4	O5-C9-C10	3.50	122.50	111.83	4	2
4	A	386	PX4	P1-O4-C6	3.50	101.32	121.35	20	14
4	A	403	PX4	O7-C23-O8	3.50	115.53	123.70	18	4
4	A	413	PX4	C11-C10-C9	3.50	100.88	113.69	11	4
4	A	313	PX4	O7-C7-C6	3.50	120.89	108.34	17	9
4	A	328	PX4	O7-C7-C6	3.50	120.89	108.34	13	7
4	A	324	PX4	C25-C24-C23	3.49	100.89	113.69	7	2
4	A	355	PX4	C25-C24-C23	3.49	100.89	113.69	6	2
4	A	375	PX4	P1-O4-C6	3.49	101.32	121.35	16	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
5	A	435	C3S	C26-C29-C38	3.49	111.45	116.60	19	2
4	A	343	PX4	O5-C9-O6	3.49	114.89	123.63	13	6
4	A	350	PX4	O7-C7-C8	3.49	120.87	108.34	14	7
4	A	380	PX4	O7-C23-O8	3.49	115.54	123.70	17	8
4	A	388	PX4	C5-N1-C3	3.49	99.81	108.98	8	3
4	A	411	PX4	O7-C7-C6	3.49	120.87	108.34	17	11
4	A	421	PX4	C5-N1-C4	3.49	99.81	108.98	14	6
4	A	423	PX4	O1-P1-O2	3.49	128.69	112.44	1	10
4	A	315	PX4	O7-C7-C8	3.49	120.86	108.34	4	6
4	A	317	PX4	C12-C11-C10	3.49	125.94	113.13	13	6
4	A	320	PX4	O1-P1-O2	3.49	128.67	112.44	9	12
4	A	352	PX4	O1-P1-O2	3.49	128.66	112.44	6	9
4	A	357	PX4	C5-N1-C3	3.49	99.82	108.98	3	9
4	A	379	PX4	C17-C16-C15	3.49	96.75	114.37	20	2
4	A	359	PX4	O7-C7-C6	3.48	120.85	108.34	19	13
4	A	362	PX4	O7-C7-C6	3.48	120.84	108.34	4	6
4	A	326	PX4	C33-C32-C31	3.48	96.76	114.37	4	2
4	A	331	PX4	O7-C7-C8	3.48	120.84	108.34	6	8
4	A	381	PX4	C5-N1-C3	3.48	99.83	108.98	6	6
4	A	397	PX4	O4-P1-O2	3.48	122.74	108.94	3	1
4	A	343	PX4	O7-C23-O8	3.48	115.57	123.70	20	9
4	A	347	PX4	C12-C11-C10	3.48	100.34	113.13	9	2
4	A	411	PX4	C7-O7-C23	3.48	126.13	117.80	1	4
4	A	308	PX4	C12-C11-C10	3.48	100.35	113.13	9	3
4	A	308	PX4	O7-C7-C6	3.48	120.82	108.34	4	7
4	A	312	PX4	O5-C9-C10	3.48	122.44	111.83	10	6
4	A	331	PX4	O1-P1-O2	3.48	128.63	112.44	1	11
4	A	419	PX4	O7-C7-C8	3.48	120.83	108.34	6	8
4	A	400	PX4	O3-P1-O2	3.48	95.15	108.94	18	3
4	A	406	PX4	C26-C25-C24	3.48	100.35	113.13	20	6
4	A	318	PX4	O1-P1-O2	3.48	128.62	112.44	15	12
4	A	351	PX4	O1-P1-O2	3.48	128.62	112.44	2	9
4	A	360	PX4	C32-C31-C30	3.48	96.79	114.37	12	4
4	A	364	PX4	O7-C7-C8	3.48	120.82	108.34	18	9
4	A	345	PX4	O3-P1-O2	3.48	95.16	108.94	7	2
4	A	370	PX4	O4-P1-O2	3.48	122.71	108.94	19	3
4	A	393	PX4	C5-N1-C2	3.48	96.09	109.91	8	3
4	A	385	PX4	C4-N1-C3	3.48	99.85	108.98	17	3
4	A	389	PX4	C5-N1-C4	3.47	118.10	108.98	2	5
4	A	319	PX4	C4-N1-C3	3.47	99.86	108.98	18	3
4	A	336	PX4	P1-O4-C6	3.47	101.45	121.35	15	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	391	PX4	O7-C7-C8	3.47	120.80	108.34	13	5
4	A	352	PX4	P1-O4-C6	3.47	101.46	121.35	9	14
4	A	389	PX4	O7-C23-O8	3.47	115.59	123.70	2	2
4	A	424	PX4	O5-C9-O6	3.47	114.95	123.63	7	4
4	A	345	PX4	O7-C23-O8	3.47	115.60	123.70	1	7
4	A	365	PX4	O7-C7-C8	3.47	120.78	108.34	8	8
4	A	369	PX4	C5-N1-C3	3.47	99.87	108.98	2	3
4	A	382	PX4	O1-P1-O2	3.47	128.57	112.44	17	9
4	A	398	PX4	O5-C9-C10	3.47	122.41	111.83	12	7
4	A	419	PX4	C4-N1-C3	3.47	99.87	108.98	12	7
4	A	429	PX4	O5-C9-O6	3.47	114.95	123.63	2	7
5	A	434	C3S	C26-C23-C20	3.47	119.03	113.14	13	6
4	A	316	PX4	C18-C17-C16	3.46	96.86	114.37	19	5
4	A	317	PX4	C7-O7-C23	3.46	126.09	117.80	6	8
4	A	391	PX4	O1-P1-O2	3.47	128.56	112.44	12	11
4	A	396	PX4	C1-C2-N1	3.46	126.94	115.82	2	5
4	A	427	PX4	O1-P1-O4	3.46	123.27	107.57	11	4
4	A	321	PX4	O7-C7-C8	3.46	120.77	108.34	17	5
4	A	331	PX4	C4-N1-C3	3.46	99.88	108.98	7	4
4	A	367	PX4	O5-C9-C10	3.46	122.39	111.83	5	6
4	A	368	PX4	O5-C9-C10	3.46	122.39	111.83	1	8
4	A	414	PX4	O1-P1-O2	3.46	128.55	112.44	15	10
4	A	414	PX4	C1-C2-N1	3.46	126.94	115.82	12	4
4	A	429	PX4	C5-N1-C4	3.46	99.88	108.98	2	4
4	A	341	PX4	O1-P1-O2	3.46	128.54	112.44	1	9
4	A	409	PX4	P1-O4-C6	3.46	101.52	121.35	12	12
4	A	416	PX4	O1-P1-O2	3.46	128.55	112.44	8	11
4	A	425	PX4	O1-P1-O2	3.46	128.54	112.44	4	8
4	A	341	PX4	O5-C9-C10	3.46	122.38	111.83	13	5
4	A	332	PX4	O1-P1-O3	3.46	91.90	107.57	8	2
4	A	415	PX4	O7-C7-C8	3.46	120.74	108.34	20	10
4	A	429	PX4	C12-C11-C10	3.46	100.43	113.13	15	3
4	A	309	PX4	C4-N1-C3	3.46	118.05	108.98	19	7
4	A	315	PX4	C7-O7-C23	3.46	126.07	117.80	5	7
4	A	346	PX4	O7-C7-C6	3.45	120.74	108.34	9	5
4	A	408	PX4	P1-O4-C6	3.45	101.56	121.35	15	13
4	A	356	PX4	O3-P1-O2	3.45	95.26	108.94	19	1
4	A	367	PX4	C5-N1-C4	3.45	99.91	108.98	17	4
4	A	372	PX4	C26-C25-C24	3.45	100.45	113.13	8	4
4	A	416	PX4	O5-C9-C10	3.45	122.35	111.83	16	6
4	A	349	PX4	O7-C7-C6	3.45	120.72	108.34	6	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	378	PX4	C1-C2-N1	3.45	126.88	115.82	4	4
4	A	307	PX4	O7-C7-C6	3.44	120.70	108.34	8	7
4	A	369	PX4	C11-C10-C9	3.44	101.07	113.69	1	3
4	A	407	PX4	O1-P1-O4	3.44	123.18	107.57	15	2
4	A	386	PX4	C25-C24-C23	3.44	101.08	113.69	4	3
4	A	326	PX4	O5-C9-C10	3.44	122.32	111.83	14	7
4	A	335	PX4	O7-C7-C6	3.44	120.68	108.34	4	10
4	A	384	PX4	O5-C9-C10	3.44	122.32	111.83	15	5
4	A	389	PX4	O1-P1-O2	3.44	128.43	112.44	20	10
4	A	347	PX4	C28-C27-C26	3.43	97.01	114.37	14	2
4	A	372	PX4	C5-N1-C3	3.44	99.95	108.98	10	4
4	A	397	PX4	P1-O4-C6	3.44	101.67	121.35	13	12
4	A	414	PX4	O7-C7-C6	3.43	120.67	108.34	6	9
4	A	311	PX4	C15-C14-C13	3.43	97.02	114.37	19	1
4	A	318	PX4	O5-C9-O6	3.43	115.05	123.63	10	6
4	A	357	PX4	C1-C2-N1	3.43	126.84	115.82	2	6
4	A	359	PX4	O5-C9-C10	3.43	122.30	111.83	15	4
4	A	395	PX4	O5-C9-O6	3.43	115.04	123.63	19	4
4	A	351	PX4	O5-C9-O6	3.43	115.05	123.63	4	5
4	A	363	PX4	C5-N1-C4	3.43	99.96	108.98	16	6
4	A	367	PX4	O6-C9-C10	3.43	110.36	123.78	5	1
4	A	373	PX4	O5-C9-O6	3.43	115.05	123.63	9	4
4	A	411	PX4	C1-C2-N1	3.43	126.83	115.82	12	6
4	A	354	PX4	O5-C9-C10	3.43	122.29	111.83	4	6
4	A	356	PX4	C25-C24-C23	3.43	101.13	113.69	6	5
4	A	394	PX4	O7-C7-C6	3.43	120.64	108.34	16	6
4	A	332	PX4	O1-P1-O2	3.43	128.38	112.44	7	10
4	A	335	PX4	O4-P1-O2	3.43	122.52	108.94	20	4
4	A	376	PX4	O7-C7-C6	3.43	120.64	108.34	10	11
4	A	419	PX4	P1-O3-C1	3.43	104.94	121.26	8	14
4	A	310	PX4	O1-P1-O2	3.42	128.38	112.44	17	10
4	A	353	PX4	C11-C10-C9	3.43	126.25	113.69	2	4
4	A	343	PX4	C26-C25-C24	3.42	100.55	113.13	19	6
4	A	384	PX4	C15-C14-C13	3.42	97.06	114.37	11	5
5	A	434	C3S	C35-C32-C30	3.42	98.44	105.14	12	9
4	A	353	PX4	C5-N1-C3	3.42	99.99	108.98	14	2
4	A	374	PX4	C12-C11-C10	3.42	100.56	113.13	10	3
4	A	402	PX4	O1-P1-O2	3.42	128.36	112.44	19	9
4	A	370	PX4	O5-C9-O6	3.42	115.08	123.63	6	6
4	A	398	PX4	O3-P1-O2	3.42	95.38	108.94	18	5
4	A	399	PX4	O1-P1-O4	3.42	123.07	107.57	8	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	400	PX4	C1-C2-N1	3.42	126.80	115.82	15	3
4	A	305	PX4	P1-O4-C6	3.42	101.77	121.35	20	17
4	A	418	PX4	O1-P1-O2	3.42	128.34	112.44	16	9
4	A	343	PX4	C1-C2-N1	3.42	126.78	115.82	4	4
4	A	392	PX4	O4-P1-O2	3.42	95.40	108.94	5	4
4	A	422	PX4	P1-O4-C6	3.42	101.77	121.35	7	9
4	A	320	PX4	C14-C13-C12	3.41	97.11	114.37	3	2
4	A	338	PX4	O1-P1-O2	3.41	128.33	112.44	9	12
4	A	356	PX4	O7-C7-C6	3.41	120.59	108.34	16	10
4	A	360	PX4	O1-P1-O3	3.41	92.09	107.57	12	2
4	A	331	PX4	C26-C25-C24	3.41	100.59	113.13	8	4
4	A	332	PX4	O7-C7-C6	3.41	120.59	108.34	1	3
4	A	362	PX4	O1-P1-O2	3.41	128.32	112.44	6	7
4	A	390	PX4	C26-C25-C24	3.41	125.67	113.13	20	3
4	A	429	PX4	C30-C29-C28	3.41	97.12	114.37	16	2
4	A	396	PX4	O1-P1-O2	3.41	128.32	112.44	20	12
4	A	398	PX4	O1-P1-O2	3.41	128.31	112.44	11	12
4	A	426	PX4	O5-C9-C10	3.41	122.24	111.83	1	4
4	A	362	PX4	C11-C10-C9	3.41	101.20	113.69	10	1
5	A	433	C3S	C35-C38-C48	3.41	117.34	112.18	19	9
4	A	305	PX4	O7-C23-O8	3.41	115.74	123.70	4	7
4	A	321	PX4	C11-C10-C9	3.41	101.20	113.69	8	1
4	A	324	PX4	O1-P1-O2	3.41	128.30	112.44	13	10
4	A	330	PX4	O3-P1-O2	3.41	95.44	108.94	17	2
4	A	342	PX4	O7-C7-C6	3.41	120.56	108.34	9	10
4	A	383	PX4	C1-C2-N1	3.41	126.75	115.82	1	7
4	A	419	PX4	C5-N1-C2	3.41	96.37	109.91	15	3
4	A	402	PX4	C8-O5-C9	3.40	104.67	117.12	5	3
4	A	322	PX4	O4-P1-O2	3.40	95.45	108.94	16	3
4	A	326	PX4	C1-C2-N1	3.40	126.74	115.82	13	5
4	A	343	PX4	O1-P1-O2	3.40	128.28	112.44	4	14
4	A	385	PX4	O4-P1-O2	3.40	122.42	108.94	3	2
4	A	405	PX4	C4-N1-C3	3.40	100.04	108.98	5	6
4	A	370	PX4	O7-C23-C24	3.40	118.83	111.48	2	7
4	A	414	PX4	C16-C15-C14	3.40	97.19	114.37	1	2
4	A	354	PX4	C1-C2-N1	3.40	126.72	115.82	19	6
4	A	382	PX4	C29-C28-C27	3.40	97.20	114.37	8	1
4	A	395	PX4	C19-C18-C17	3.40	97.20	114.37	14	1
4	A	320	PX4	C4-N1-C3	3.39	100.07	108.98	19	6
5	A	433	C3S	C1-C22-C12	3.39	114.59	108.74	3	6
4	A	305	PX4	O5-C9-O6	3.39	115.15	123.63	8	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	O7-C23-O8	3.39	115.78	123.70	7	4
5	A	436	C3S	C4-C1-C22	3.39	120.01	112.78	16	10
4	A	386	PX4	C14-C13-C12	3.39	97.23	114.37	5	1
4	A	388	PX4	C28-C27-C26	3.39	97.23	114.37	15	2
4	A	341	PX4	C27-C26-C25	3.39	97.24	114.37	1	2
4	A	376	PX4	O7-C7-C8	3.39	120.50	108.34	11	6
4	A	397	PX4	O3-C1-C2	3.39	125.96	109.65	19	3
4	A	309	PX4	O4-P1-O2	3.39	122.36	108.94	20	2
4	A	402	PX4	O1-P1-O3	3.39	92.21	107.57	12	3
4	A	317	PX4	C27-C26-C25	3.38	97.26	114.37	8	2
4	A	348	PX4	O3-C1-C2	3.38	125.94	109.65	7	2
4	A	363	PX4	C25-C24-C23	3.38	101.29	113.69	9	3
4	A	364	PX4	O7-C7-C6	3.38	120.49	108.34	20	10
4	A	306	PX4	C4-N1-C3	3.38	100.09	108.98	13	3
4	A	320	PX4	C15-C14-C13	3.38	97.26	114.37	10	2
4	A	424	PX4	C1-C2-N1	3.38	126.69	115.82	11	5
4	A	373	PX4	C1-C2-N1	3.38	126.67	115.82	17	4
4	A	387	PX4	O1-P1-O2	3.38	128.18	112.44	9	9
4	A	333	PX4	C25-C24-C23	3.37	101.33	113.69	16	6
4	A	378	PX4	O7-C7-C6	3.37	120.44	108.34	17	9
4	A	394	PX4	P1-O4-C6	3.37	102.02	121.35	10	12
4	A	397	PX4	O7-C7-C6	3.37	120.45	108.34	2	10
4	A	401	PX4	O7-C7-C6	3.37	120.44	108.34	11	8
4	A	403	PX4	C4-N1-C3	3.37	100.11	108.98	2	4
5	A	433	C3S	C57-C54-C48	3.38	105.64	115.08	5	2
4	A	313	PX4	C26-C25-C24	3.37	100.73	113.13	11	3
4	A	413	PX4	P1-O4-C6	3.37	102.02	121.35	6	12
4	A	352	PX4	C1-C2-N1	3.37	126.65	115.82	4	4
4	A	357	PX4	O3-P1-O2	3.37	95.57	108.94	10	4
4	A	370	PX4	C5-N1-C2	3.37	123.31	109.91	9	3
4	A	374	PX4	O4-P1-O2	3.37	122.29	108.94	20	4
4	A	389	PX4	C20-C19-C18	3.37	97.33	114.37	11	2
5	A	435	C3S	C15-C13-C12	3.37	119.33	125.02	15	6
4	A	333	PX4	C5-N1-C4	3.37	117.82	108.98	5	6
4	A	337	PX4	O7-C7-C6	3.37	120.42	108.34	14	8
4	A	310	PX4	O7-C7-C6	3.36	120.42	108.34	9	7
4	A	323	PX4	O1-P1-O4	3.37	122.82	107.57	11	4
4	A	375	PX4	C5-N1-C3	3.37	100.13	108.98	19	7
4	A	405	PX4	P1-O4-C6	3.37	102.06	121.35	19	12
4	A	378	PX4	O7-C7-C8	3.36	120.42	108.34	18	6
4	A	377	PX4	O7-C7-C8	3.36	120.41	108.34	2	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	401	PX4	C3-N1-C2	3.36	123.28	109.91	16	3
4	A	416	PX4	C1-C2-N1	3.36	126.62	115.82	13	8
5	A	435	C3S	C32-C30-C18	3.36	124.47	119.10	11	5
4	A	430	PX4	O1-P1-O2	3.36	128.08	112.44	16	13
4	A	335	PX4	C8-O5-C9	3.36	129.40	117.12	13	4
4	A	392	PX4	O1-P1-O3	3.36	92.34	107.57	15	6
4	A	428	PX4	O1-P1-O2	3.36	128.08	112.44	6	13
4	A	326	PX4	C5-N1-C2	3.36	123.25	109.91	7	1
4	A	340	PX4	O5-C9-O6	3.36	115.23	123.63	19	5
4	A	399	PX4	O5-C9-C10	3.36	122.07	111.83	8	6
4	A	346	PX4	C5-N1-C4	3.36	100.16	108.98	17	4
4	A	323	PX4	O1-P1-O3	3.36	92.36	107.57	14	6
4	A	349	PX4	C5-N1-C3	3.36	117.79	108.98	20	3
4	A	351	PX4	C7-O7-C23	3.36	125.83	117.80	3	6
4	A	311	PX4	O3-P1-O2	3.35	95.64	108.94	15	6
4	A	320	PX4	C26-C25-C24	3.35	100.81	113.13	5	2
4	A	330	PX4	C4-N1-C3	3.35	100.17	108.98	6	3
4	A	346	PX4	C17-C16-C15	3.35	97.42	114.37	4	3
4	A	370	PX4	O3-P1-O2	3.35	95.65	108.94	16	5
4	A	357	PX4	C4-N1-C3	3.35	117.78	108.98	8	6
4	A	408	PX4	O7-C7-C6	3.35	120.36	108.34	14	8
5	A	435	C3S	C29-C30-C18	3.35	119.17	114.41	8	3
4	A	389	PX4	C27-C26-C25	3.35	97.44	114.37	5	1
4	A	331	PX4	C5-N1-C4	3.35	100.18	108.98	13	8
4	A	359	PX4	O7-C7-C8	3.35	120.35	108.34	3	10
4	A	378	PX4	C11-C10-C9	3.35	125.96	113.69	19	5
4	A	410	PX4	O7-C23-O8	3.35	115.88	123.70	14	8
5	A	432	C3S	C4-C1-C22	3.35	119.91	112.78	6	9
4	A	423	PX4	P1-O4-C6	3.34	102.18	121.35	1	11
4	A	381	PX4	C8-O5-C9	3.34	104.90	117.12	7	2
4	A	341	PX4	P1-O4-C6	3.34	102.20	121.35	20	13
4	A	376	PX4	O1-P1-O2	3.34	127.99	112.44	19	10
4	A	400	PX4	C5-N1-C4	3.34	100.20	108.98	18	7
4	A	402	PX4	C5-N1-C3	3.34	100.20	108.98	14	6
4	A	385	PX4	O3-P1-O2	3.34	95.70	108.94	2	5
4	A	370	PX4	C5-N1-C3	3.34	100.21	108.98	20	5
4	A	405	PX4	C1-C2-N1	3.34	126.53	115.82	18	7
4	A	359	PX4	C7-O7-C23	3.34	125.78	117.80	2	6
4	A	389	PX4	C11-C10-C9	3.34	101.47	113.69	15	1
4	A	421	PX4	O4-P1-O2	3.34	122.16	108.94	18	5
4	A	307	PX4	C26-C25-C24	3.33	100.88	113.13	15	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	406	PX4	C5-N1-C4	3.34	100.22	108.98	3	2
4	A	327	PX4	P1-O4-C6	3.33	102.25	121.35	9	9
4	A	390	PX4	O7-C23-O8	3.33	115.91	123.70	11	3
4	A	391	PX4	C18-C17-C16	3.33	97.52	114.37	16	3
4	A	392	PX4	O1-P1-O2	3.33	127.95	112.44	10	13
4	A	406	PX4	O7-C7-C6	3.33	120.31	108.34	1	6
4	A	349	PX4	C4-N1-C2	3.33	123.16	109.91	8	3
4	A	360	PX4	C26-C25-C24	3.33	100.88	113.13	9	6
4	A	320	PX4	C7-O7-C23	3.33	125.77	117.80	16	4
4	A	359	PX4	O5-C9-O6	3.33	115.30	123.63	1	5
4	A	394	PX4	C25-C24-C23	3.33	125.90	113.69	16	2
4	A	323	PX4	O4-P1-O2	3.33	122.13	108.94	12	5
4	A	407	PX4	C8-O5-C9	3.33	104.95	117.12	15	2
4	A	348	PX4	C11-C10-C9	3.33	101.50	113.69	6	3
4	A	342	PX4	P1-O4-C6	3.33	102.29	121.35	18	12
4	A	354	PX4	C32-C31-C30	3.33	97.55	114.37	6	2
4	A	377	PX4	O7-C7-C6	3.33	120.28	108.34	6	5
4	A	387	PX4	C11-C10-C9	3.33	101.51	113.69	13	2
4	A	422	PX4	O5-C9-C10	3.33	121.98	111.83	6	6
4	A	306	PX4	C1-C2-N1	3.32	126.49	115.82	16	7
4	A	409	PX4	C4-N1-C3	3.33	100.24	108.98	11	7
4	A	333	PX4	C12-C11-C10	3.32	100.92	113.13	14	4
4	A	373	PX4	O7-C7-C6	3.32	120.27	108.34	14	9
4	A	417	PX4	C7-O7-C23	3.32	125.75	117.80	14	6
4	A	338	PX4	C34-C33-C32	3.32	97.57	114.37	5	2
4	A	420	PX4	O7-C7-C6	3.32	120.27	108.34	10	4
4	A	321	PX4	O7-C23-O8	3.32	115.94	123.70	6	6
4	A	324	PX4	O5-C9-C10	3.32	121.96	111.83	14	5
4	A	346	PX4	C4-N1-C3	3.32	117.70	108.98	17	7
4	A	378	PX4	P1-O4-C6	3.32	102.32	121.35	8	13
4	A	422	PX4	C5-N1-C4	3.32	117.69	108.98	4	4
4	A	358	PX4	O4-P1-O2	3.32	95.79	108.94	8	3
4	A	326	PX4	C5-N1-C4	3.32	117.69	108.98	10	8
4	A	355	PX4	P1-O3-C1	3.32	105.48	121.26	17	14
4	A	407	PX4	O7-C7-C8	3.32	120.24	108.34	6	9
4	A	326	PX4	P1-O4-C6	3.31	102.36	121.35	5	11
4	A	392	PX4	C5-N1-C3	3.31	117.68	108.98	4	4
4	A	360	PX4	C5-N1-C3	3.31	100.28	108.98	11	5
4	A	314	PX4	C12-C11-C10	3.31	100.97	113.13	19	2
4	A	316	PX4	O7-C7-C6	3.31	120.22	108.34	5	7
4	A	324	PX4	C4-N1-C3	3.31	100.28	108.98	17	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	373	PX4	C8-O5-C9	3.31	129.21	117.12	18	1
4	A	423	PX4	O7-C7-C6	3.31	120.21	108.34	18	5
4	A	326	PX4	C18-C17-C16	3.31	97.66	114.37	20	1
4	A	352	PX4	O1-P1-O4	3.31	122.55	107.57	3	3
4	A	328	PX4	P1-O4-C6	3.30	102.42	121.35	13	9
4	A	417	PX4	O3-P1-O2	3.30	95.84	108.94	19	5
4	A	425	PX4	O1-P1-O4	3.30	122.55	107.57	8	1
4	A	329	PX4	C4-N1-C2	3.30	123.04	109.91	7	2
4	A	394	PX4	O7-C7-C8	3.30	120.19	108.34	16	6
4	A	386	PX4	O7-C7-C6	3.30	120.19	108.34	9	3
4	A	338	PX4	C32-C31-C30	3.30	97.69	114.37	1	1
4	A	426	PX4	C5-N1-C4	3.30	100.31	108.98	12	6
4	A	313	PX4	O1-P1-O2	3.30	127.78	112.44	19	11
4	A	328	PX4	C8-O5-C9	3.30	105.06	117.12	1	2
4	A	385	PX4	C30-C29-C28	3.30	97.69	114.37	15	1
4	A	411	PX4	C29-C28-C27	3.30	97.69	114.37	7	3
4	A	427	PX4	O3-P1-O2	3.30	95.86	108.94	2	6
4	A	340	PX4	O3-P1-O2	3.29	95.88	108.94	9	3
4	A	349	PX4	C26-C25-C24	3.29	101.02	113.13	17	2
4	A	361	PX4	O7-C7-C6	3.30	120.17	108.34	4	11
4	A	382	PX4	O7-C7-C6	3.30	120.17	108.34	15	7
4	A	419	PX4	C11-C10-C9	3.29	101.62	113.69	11	3
4	A	346	PX4	O1-P1-O2	3.29	127.77	112.44	9	10
4	A	305	PX4	C34-C33-C32	3.29	97.73	114.37	13	1
4	A	351	PX4	C20-C19-C18	3.29	97.73	114.37	2	1
4	A	377	PX4	C5-N1-C2	3.29	96.83	109.91	7	5
4	A	390	PX4	O3-P1-O2	3.29	95.89	108.94	3	6
4	A	315	PX4	O5-C9-C10	3.29	121.87	111.83	1	6
4	A	324	PX4	O7-C7-C6	3.29	120.15	108.34	8	7
4	A	334	PX4	O7-C7-C6	3.29	120.14	108.34	14	8
4	A	375	PX4	C8-O5-C9	3.29	129.14	117.12	12	2
4	A	395	PX4	C1-C2-N1	3.29	126.38	115.82	14	6
4	A	401	PX4	P1-O4-C6	3.29	102.50	121.35	13	11
4	A	321	PX4	C5-N1-C2	3.29	96.85	109.91	13	4
4	A	334	PX4	C15-C14-C13	3.29	97.75	114.37	13	2
4	A	364	PX4	O4-P1-O2	3.29	121.96	108.94	5	5
4	A	322	PX4	P1-O4-C6	3.28	102.53	121.35	4	13
4	A	412	PX4	O5-C9-C10	3.28	121.85	111.83	12	7
4	A	335	PX4	O7-C7-C8	3.28	120.11	108.34	2	10
4	A	413	PX4	O7-C7-C8	3.28	120.11	108.34	7	11
4	A	305	PX4	O1-P1-O3	3.28	92.70	107.57	6	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	427	PX4	O7-C7-C8	3.28	120.11	108.34	10	10
4	A	344	PX4	C1-C2-N1	3.28	126.35	115.82	2	8
4	A	314	PX4	O1-P1-O2	3.28	127.69	112.44	4	14
4	A	324	PX4	C26-C25-C24	3.28	101.08	113.13	5	3
4	A	394	PX4	O5-C9-C10	3.28	121.83	111.83	7	4
4	A	360	PX4	O5-C9-C10	3.28	121.82	111.83	12	6
4	A	380	PX4	C4-N1-C3	3.28	100.37	108.98	15	5
4	A	429	PX4	C7-O7-C23	3.28	125.64	117.80	3	3
4	A	380	PX4	O5-C9-O6	3.27	115.44	123.63	2	4
4	A	312	PX4	O3-P1-O2	3.27	95.96	108.94	12	5
4	A	322	PX4	O7-C7-C6	3.27	120.09	108.34	6	6
4	A	390	PX4	C4-N1-C3	3.27	100.38	108.98	6	4
4	A	320	PX4	C8-O5-C9	3.27	105.16	117.12	2	3
4	A	340	PX4	O1-P1-O3	3.27	92.73	107.57	7	2
4	A	365	PX4	C18-C17-C16	3.27	97.83	114.37	20	2
4	A	399	PX4	C4-N1-C3	3.27	117.57	108.98	12	7
4	A	325	PX4	C7-O7-C23	3.27	125.62	117.80	20	4
4	A	326	PX4	C12-C11-C10	3.27	101.10	113.13	11	2
4	A	430	PX4	C5-N1-C4	3.27	100.38	108.98	7	4
4	A	335	PX4	C12-C11-C10	3.27	101.11	113.13	9	5
4	A	425	PX4	C5-N1-C3	3.27	117.57	108.98	20	4
4	A	305	PX4	C33-C32-C31	3.27	97.85	114.37	14	2
4	A	369	PX4	C7-O7-C23	3.27	109.97	117.80	9	5
4	A	375	PX4	C33-C32-C31	3.27	97.85	114.37	12	1
4	A	402	PX4	C26-C25-C24	3.27	101.12	113.13	5	5
4	A	404	PX4	O7-C23-O8	3.27	116.06	123.70	18	6
4	A	428	PX4	O7-C7-C6	3.27	120.07	108.34	20	7
4	A	319	PX4	C8-O5-C9	3.27	105.18	117.12	5	3
4	A	402	PX4	O7-C7-C8	3.27	120.07	108.34	4	9
4	A	321	PX4	O1-P1-O3	3.27	92.77	107.57	3	2
4	A	380	PX4	O1-P1-O3	3.27	92.76	107.57	3	3
4	A	383	PX4	C28-C27-C26	3.27	97.86	114.37	18	1
4	A	324	PX4	O7-C23-O8	3.27	116.07	123.70	17	2
4	A	309	PX4	O5-C9-O6	3.26	115.47	123.63	3	3
4	A	320	PX4	C5-N1-C4	3.26	117.55	108.98	4	2
4	A	353	PX4	C5-N1-C4	3.26	100.40	108.98	20	5
4	A	360	PX4	P1-O3-C1	3.26	105.72	121.26	8	13
4	A	375	PX4	O3-P1-O2	3.26	96.00	108.94	5	6
4	A	392	PX4	C29-C28-C27	3.26	97.87	114.37	18	1
4	A	398	PX4	C7-O7-C23	3.26	125.61	117.80	12	8
4	A	418	PX4	C5-N1-C4	3.26	117.55	108.98	16	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	338	PX4	O3-P1-O2	3.26	96.01	108.94	7	4
4	A	338	PX4	C5-N1-C3	3.26	117.54	108.98	6	5
4	A	365	PX4	O4-P1-O2	3.26	121.86	108.94	7	3
4	A	378	PX4	O7-C23-O8	3.26	116.08	123.70	17	6
4	A	380	PX4	C5-N1-C3	3.26	117.53	108.98	13	5
4	A	410	PX4	O1-P1-O2	3.26	127.61	112.44	4	6
4	A	318	PX4	C7-O7-C23	3.26	125.59	117.80	18	8
4	A	336	PX4	C5-N1-C3	3.26	100.42	108.98	5	3
4	A	344	PX4	O7-C23-O8	3.26	116.09	123.70	6	5
4	A	363	PX4	O3-P1-O2	3.26	96.03	108.94	20	6
4	A	372	PX4	O3-P1-O2	3.26	96.03	108.94	10	9
4	A	389	PX4	C18-C17-C16	3.26	97.91	114.37	4	2
4	A	349	PX4	O1-P1-O4	3.25	122.32	107.57	3	4
4	A	410	PX4	C12-C11-C10	3.25	101.17	113.13	11	2
4	A	391	PX4	C1-C2-N1	3.25	126.26	115.82	10	5
4	A	419	PX4	O5-C9-C10	3.25	121.75	111.83	10	5
4	A	401	PX4	O1-P1-O4	3.25	122.30	107.57	17	6
4	A	337	PX4	C5-N1-C3	3.25	100.44	108.98	11	5
4	A	365	PX4	O1-P1-O2	3.25	127.55	112.44	16	8
4	A	372	PX4	C4-N1-C3	3.25	100.45	108.98	17	4
4	A	384	PX4	C27-C26-C25	3.24	97.97	114.37	9	2
4	A	307	PX4	C4-N1-C3	3.24	100.46	108.98	11	4
4	A	398	PX4	C1-C2-N1	3.24	126.23	115.82	13	6
4	A	317	PX4	C1-C2-N1	3.24	126.22	115.82	2	4
4	A	334	PX4	O3-P1-O2	3.24	96.10	108.94	8	4
4	A	356	PX4	C5-N1-C3	3.24	100.47	108.98	14	5
4	A	367	PX4	O5-C9-O6	3.24	115.53	123.63	11	7
4	A	403	PX4	C5-N1-C3	3.24	100.47	108.98	3	5
4	A	404	PX4	C5-N1-C4	3.24	100.47	108.98	8	4
4	A	322	PX4	C18-C17-C16	3.24	98.01	114.37	19	4
4	A	371	PX4	C5-N1-C4	3.24	117.48	108.98	1	3
4	A	369	PX4	O7-C7-C6	3.23	119.95	108.34	18	9
4	A	414	PX4	C26-C25-C24	3.24	101.24	113.13	6	2
4	A	311	PX4	O1-P1-O4	3.23	122.22	107.57	11	1
4	A	354	PX4	C12-C11-C10	3.23	101.25	113.13	5	3
4	A	369	PX4	O5-C9-C10	3.23	121.69	111.83	2	6
4	A	376	PX4	C1-C2-N1	3.23	126.20	115.82	17	5
4	A	317	PX4	C17-C16-C15	3.23	98.04	114.37	19	2
4	A	370	PX4	C12-C11-C10	3.23	101.25	113.13	19	4
4	A	386	PX4	C5-N1-C2	3.23	97.06	109.91	9	2
4	A	426	PX4	C27-C26-C25	3.23	98.03	114.37	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	326	PX4	O3-P1-O2	3.23	96.14	108.94	17	7
4	A	355	PX4	O1-P1-O4	3.23	122.21	107.57	6	4
4	A	358	PX4	O7-C7-C8	3.23	119.92	108.34	20	6
4	A	358	PX4	C5-N1-C4	3.23	117.45	108.98	10	4
4	A	426	PX4	C19-C18-C17	3.23	98.06	114.37	1	3
4	A	428	PX4	O1-P1-O3	3.23	122.20	107.57	13	1
4	A	372	PX4	C1-C2-N1	3.23	126.18	115.82	16	5
4	A	380	PX4	O3-P1-O2	3.23	96.15	108.94	18	3
4	A	328	PX4	O1-P1-O4	3.23	122.19	107.57	9	6
4	A	390	PX4	C5-N1-C4	3.23	117.45	108.98	11	2
4	A	355	PX4	O4-P1-O2	3.22	121.71	108.94	3	2
4	A	365	PX4	O3-C1-C2	3.22	125.16	109.65	13	4
4	A	398	PX4	O7-C23-C24	3.22	118.45	111.48	5	6
4	A	405	PX4	C12-C11-C10	3.22	101.29	113.13	5	3
4	A	428	PX4	C1-C2-N1	3.22	126.16	115.82	16	5
4	A	398	PX4	C25-C24-C23	3.22	101.89	113.69	18	1
4	A	350	PX4	O7-C7-C6	3.22	119.89	108.34	7	8
4	A	312	PX4	C5-N1-C3	3.22	117.43	108.98	13	3
4	A	397	PX4	O1-P1-O2	3.22	127.41	112.44	18	12
4	A	401	PX4	O7-C7-C8	3.22	119.89	108.34	4	8
4	A	314	PX4	O7-C7-C6	3.22	119.88	108.34	4	8
4	A	385	PX4	O7-C7-C6	3.22	119.89	108.34	9	8
4	A	332	PX4	C18-C17-C16	3.22	98.11	114.37	1	3
5	A	432	C3S	C40-C29-C38	3.22	117.51	111.68	13	5
4	A	328	PX4	O7-C23-O8	3.21	116.19	123.70	6	6
4	A	334	PX4	O7-C7-C8	3.21	119.87	108.34	4	10
4	A	338	PX4	C31-C30-C29	3.21	98.13	114.37	15	4
4	A	359	PX4	C1-C2-N1	3.21	126.13	115.82	1	3
4	A	418	PX4	O3-P1-O2	3.21	96.20	108.94	14	4
4	A	313	PX4	P1-O4-C6	3.21	102.95	121.35	1	12
4	A	379	PX4	C14-C13-C12	3.21	98.14	114.37	15	2
4	A	424	PX4	O5-C9-C10	3.21	121.62	111.83	7	4
4	A	347	PX4	C5-N1-C4	3.21	100.55	108.98	19	4
4	A	363	PX4	O1-P1-O2	3.21	127.38	112.44	7	10
4	A	394	PX4	C13-C12-C11	3.21	98.14	114.37	2	3
4	A	320	PX4	C1-C2-N1	3.21	126.12	115.82	19	1
4	A	371	PX4	O1-P1-O2	3.21	127.36	112.44	14	8
4	A	415	PX4	O1-P1-O4	3.21	122.10	107.57	4	3
4	A	309	PX4	P1-O4-C6	3.20	102.99	121.35	3	10
4	A	358	PX4	C17-C16-C15	3.20	98.17	114.37	3	1
4	A	392	PX4	O5-C9-O6	3.20	115.61	123.63	16	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C25-C24-C23	3.20	101.95	113.69	17	3
4	A	349	PX4	C29-C28-C27	3.20	98.18	114.37	10	2
4	A	414	PX4	O1-P1-O3	3.20	93.05	107.57	1	3
4	A	418	PX4	O7-C7-C6	3.20	119.83	108.34	19	6
4	A	427	PX4	C13-C12-C11	3.20	98.17	114.37	10	1
4	A	345	PX4	O5-C9-O6	3.20	115.62	123.63	12	4
4	A	363	PX4	O5-C9-O6	3.20	115.62	123.63	4	9
4	A	363	PX4	C5-N1-C3	3.20	100.57	108.98	11	4
5	A	434	C3S	C23-C26-C29	3.20	118.14	112.74	1	6
4	A	365	PX4	O8-C23-C24	3.20	111.27	123.78	14	3
4	A	312	PX4	O7-C7-C8	3.20	119.81	108.34	16	5
4	A	317	PX4	C26-C25-C24	3.20	101.38	113.13	20	1
4	A	412	PX4	C12-C11-C10	3.20	101.38	113.13	1	2
4	A	340	PX4	O4-P1-O2	3.20	121.61	108.94	14	2
4	A	309	PX4	C4-N1-C2	3.20	97.21	109.91	19	3
4	A	330	PX4	C5-N1-C4	3.20	100.58	108.98	9	4
4	A	357	PX4	O1-P1-O3	3.20	122.06	107.57	1	2
4	A	365	PX4	C5-N1-C2	3.20	97.21	109.91	11	3
4	A	396	PX4	C16-C15-C14	3.20	98.21	114.37	18	3
4	A	377	PX4	O5-C9-C10	3.19	121.58	111.83	16	7
4	A	414	PX4	C4-N1-C3	3.19	117.37	108.98	11	3
4	A	360	PX4	O7-C23-O8	3.19	116.24	123.70	17	4
4	A	368	PX4	O1-P1-O2	3.19	127.30	112.44	17	8
4	A	373	PX4	O1-P1-O4	3.19	93.10	107.57	14	2
4	A	387	PX4	O7-C23-O8	3.19	116.24	123.70	19	5
4	A	368	PX4	C5-N1-C3	3.19	100.60	108.98	17	6
4	A	324	PX4	C29-C28-C27	3.19	98.25	114.37	7	3
4	A	366	PX4	O7-C7-C6	3.19	119.78	108.34	14	8
4	A	410	PX4	C5-N1-C4	3.19	117.35	108.98	13	2
4	A	418	PX4	C25-C24-C23	3.19	102.01	113.69	10	5
4	A	357	PX4	C5-N1-C2	3.19	97.24	109.91	15	3
4	A	329	PX4	C5-N1-C3	3.19	100.61	108.98	19	5
4	A	420	PX4	O5-C9-O6	3.19	115.65	123.63	18	4
4	A	332	PX4	O8-C23-C24	3.18	111.33	123.78	17	2
4	A	359	PX4	O4-P1-O2	3.19	96.31	108.94	14	3
4	A	371	PX4	P1-O4-C6	3.19	103.09	121.35	4	12
4	A	388	PX4	O7-C7-C6	3.19	119.77	108.34	12	8
4	A	310	PX4	C4-N1-C3	3.18	117.34	108.98	5	3
4	A	313	PX4	C25-C24-C23	3.18	125.36	113.69	4	4
5	A	436	C3S	C29-C30-C18	3.18	109.89	114.41	20	7
4	A	347	PX4	C11-C10-C9	3.18	102.03	113.69	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	393	PX4	C1-C2-N1	3.18	126.03	115.82	9	4
4	A	314	PX4	C5-N1-C4	3.18	100.63	108.98	2	7
4	A	343	PX4	C11-C10-C9	3.18	102.04	113.69	8	5
4	A	386	PX4	O4-P1-O2	3.18	121.54	108.94	12	2
4	A	394	PX4	C11-C10-C9	3.18	102.04	113.69	2	5
4	A	415	PX4	C20-C19-C18	3.18	98.30	114.37	18	1
4	A	335	PX4	C5-N1-C2	3.18	122.54	109.91	5	2
4	A	337	PX4	O3-C1-C2	3.18	124.94	109.65	12	3
4	A	341	PX4	C4-N1-C2	3.18	122.54	109.91	13	3
4	A	335	PX4	O5-C9-C10	3.18	121.52	111.83	17	7
4	A	333	PX4	O5-C9-O6	3.17	115.69	123.63	20	6
4	A	351	PX4	O5-C9-C10	3.18	121.52	111.83	18	7
4	A	367	PX4	O4-P1-O2	3.17	96.35	108.94	11	2
4	A	334	PX4	C31-C30-C29	3.17	98.34	114.37	18	2
4	A	311	PX4	C5-N1-C4	3.17	100.65	108.98	13	4
4	A	338	PX4	C19-C18-C17	3.17	98.34	114.37	9	3
5	A	436	C3S	O4-S1-O2	3.17	124.47	112.24	16	7
4	A	324	PX4	C32-C31-C30	3.17	98.34	114.37	11	1
4	A	308	PX4	C33-C32-C31	3.17	98.35	114.37	5	1
4	A	396	PX4	O7-C7-C6	3.17	119.71	108.34	13	8
4	A	357	PX4	O4-P1-O2	3.17	121.49	108.94	10	3
4	A	411	PX4	C26-C25-C24	3.17	101.49	113.13	5	3
4	A	374	PX4	O7-C7-C6	3.17	119.70	108.34	13	9
4	A	394	PX4	C5-N1-C3	3.17	100.66	108.98	13	3
4	A	394	PX4	C31-C30-C29	3.17	98.36	114.37	18	1
4	A	404	PX4	C34-C33-C32	3.16	98.37	114.37	10	2
4	A	424	PX4	O7-C23-O8	3.17	116.30	123.70	15	5
4	A	307	PX4	C34-C33-C32	3.16	98.38	114.37	18	2
4	A	310	PX4	C30-C29-C28	3.16	98.37	114.37	5	1
4	A	354	PX4	O1-P1-O3	3.16	93.23	107.57	7	2
4	A	340	PX4	C20-C19-C18	3.16	98.38	114.37	8	1
4	A	364	PX4	C1-C2-N1	3.16	125.97	115.82	11	4
4	A	413	PX4	C25-C24-C23	3.16	102.10	113.69	5	5
4	A	305	PX4	O7-C7-C6	3.16	119.69	108.34	19	6
4	A	307	PX4	O5-C9-O6	3.16	115.72	123.63	7	6
4	A	342	PX4	O7-C23-O8	3.16	116.32	123.70	18	5
4	A	381	PX4	C27-C26-C25	3.16	98.39	114.37	17	1
4	A	312	PX4	O4-P1-O2	3.16	121.45	108.94	15	2
4	A	319	PX4	C26-C25-C24	3.16	101.52	113.13	18	5
4	A	325	PX4	C5-N1-C2	3.16	97.35	109.91	13	2
4	A	352	PX4	C15-C14-C13	3.16	98.40	114.37	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	360	PX4	O1-P1-O4	3.16	121.88	107.57	12	3
4	A	335	PX4	C31-C30-C29	3.16	98.41	114.37	13	1
4	A	416	PX4	C31-C30-C29	3.16	98.41	114.37	11	3
4	A	311	PX4	O1-P1-O2	3.15	127.12	112.44	17	10
4	A	320	PX4	O5-C9-C10	3.15	121.45	111.83	1	7
4	A	350	PX4	C29-C28-C27	3.15	98.42	114.37	20	1
4	A	359	PX4	C19-C18-C17	3.15	98.42	114.37	11	2
4	A	388	PX4	C3-N1-C2	3.16	97.37	109.91	12	1
4	A	405	PX4	C25-C24-C23	3.16	102.13	113.69	14	3
5	A	435	C3S	O4-S1-O2	3.16	124.41	112.24	11	10
4	A	373	PX4	O1-P1-O2	3.15	127.11	112.44	10	11
4	A	341	PX4	O3-C1-C2	3.15	124.81	109.65	4	1
4	A	375	PX4	C26-C25-C24	3.15	101.55	113.13	12	5
4	A	406	PX4	O5-C9-C10	3.15	121.45	111.83	20	6
4	A	408	PX4	O1-P1-O4	3.15	121.85	107.57	19	3
4	A	411	PX4	C25-C24-C23	3.15	125.24	113.69	18	4
4	A	413	PX4	C1-C2-N1	3.15	125.94	115.82	20	6
5	A	433	C3S	C26-C23-C20	3.15	118.49	113.14	5	8
4	A	322	PX4	C25-C24-C23	3.15	102.16	113.69	10	3
4	A	353	PX4	O4-P1-O2	3.15	96.46	108.94	10	4
4	A	370	PX4	O7-C7-C6	3.15	119.64	108.34	4	6
4	A	428	PX4	O7-C7-C8	3.15	119.64	108.34	3	6
4	A	371	PX4	C26-C25-C24	3.15	101.56	113.13	3	4
4	A	378	PX4	C12-C11-C10	3.15	101.56	113.13	16	5
4	A	412	PX4	C1-C2-N1	3.15	125.92	115.82	9	3
4	A	322	PX4	C1-C2-N1	3.14	125.92	115.82	15	1
4	A	326	PX4	O1-P1-O2	3.15	127.08	112.44	8	7
4	A	384	PX4	P1-O4-C6	3.15	103.33	121.35	8	9
4	A	421	PX4	O5-C9-C10	3.15	121.42	111.83	2	3
4	A	397	PX4	C4-N1-C3	3.14	117.23	108.98	18	2
4	A	318	PX4	C31-C30-C29	3.14	98.48	114.37	9	1
4	A	426	PX4	C12-C11-C10	3.14	101.58	113.13	4	5
5	A	432	C3S	C23-C20-C18	3.14	107.39	111.78	17	3
4	A	329	PX4	O7-C7-C6	3.14	119.61	108.34	4	5
4	A	368	PX4	C32-C31-C30	3.14	98.49	114.37	14	2
4	A	405	PX4	O4-P1-O2	3.14	121.38	108.94	6	3
4	A	430	PX4	O7-C7-C6	3.14	119.61	108.34	17	5
4	A	366	PX4	C4-N1-C2	3.14	97.43	109.91	7	1
4	A	374	PX4	O1-P1-O3	3.14	93.34	107.57	20	4
4	A	404	PX4	C12-C11-C10	3.14	124.66	113.13	9	7
4	A	309	PX4	O5-C9-C10	3.14	121.40	111.83	15	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	350	PX4	O1-P1-O2	3.14	127.04	112.44	19	8
4	A	415	PX4	O1-P1-O2	3.14	127.04	112.44	14	7
4	A	314	PX4	C5-N1-C3	3.14	100.74	108.98	19	4
4	A	373	PX4	C20-C19-C18	3.14	98.51	114.37	17	3
4	A	380	PX4	C11-C10-C9	3.14	102.20	113.69	18	3
4	A	390	PX4	O1-P1-O4	3.14	121.79	107.57	14	2
4	A	363	PX4	O5-C9-C10	3.13	121.39	111.83	3	3
4	A	306	PX4	C11-C10-C9	3.13	102.21	113.69	10	5
4	A	318	PX4	O3-C1-C2	3.13	124.73	109.65	20	5
4	A	418	PX4	C4-N1-C3	3.13	100.74	108.98	8	4
4	A	384	PX4	C26-C25-C24	3.13	101.61	113.13	6	3
4	A	429	PX4	C4-N1-C3	3.13	100.74	108.98	12	3
4	A	327	PX4	C5-N1-C4	3.13	100.75	108.98	12	5
4	A	346	PX4	C19-C18-C17	3.13	98.53	114.37	2	2
4	A	402	PX4	P1-O4-C6	3.13	103.40	121.35	17	15
4	A	374	PX4	C25-C24-C23	3.13	102.22	113.69	12	2
4	A	376	PX4	O5-C9-C10	3.13	121.38	111.83	6	8
4	A	402	PX4	C30-C29-C28	3.13	98.54	114.37	6	2
4	A	364	PX4	C32-C31-C30	3.13	98.54	114.37	1	3
4	A	394	PX4	O3-C1-C2	3.13	124.71	109.65	11	3
4	A	361	PX4	O3-P1-O2	3.13	121.33	108.94	6	2
4	A	407	PX4	C34-C33-C32	3.13	98.56	114.37	3	2
4	A	382	PX4	O7-C7-C8	3.13	119.56	108.34	19	6
4	A	376	PX4	P1-O4-C6	3.12	103.45	121.35	14	14
4	A	420	PX4	P1-O4-C6	3.12	103.45	121.35	9	15
4	A	330	PX4	O5-C9-O6	3.12	115.82	123.63	14	8
4	A	350	PX4	C5-N1-C3	3.12	100.77	108.98	6	4
4	A	325	PX4	O4-P1-O2	3.12	121.30	108.94	8	2
4	A	345	PX4	O1-P1-O4	3.12	121.71	107.57	16	3
4	A	350	PX4	C28-C27-C26	3.12	98.60	114.37	15	3
4	A	422	PX4	C1-C2-N1	3.12	125.83	115.82	6	7
4	A	425	PX4	C11-C10-C9	3.12	102.26	113.69	3	4
4	A	322	PX4	O1-P1-O3	3.12	93.43	107.57	20	3
4	A	349	PX4	C5-N1-C4	3.12	100.79	108.98	8	3
4	A	350	PX4	O4-P1-O2	3.12	121.29	108.94	13	5
4	A	359	PX4	O1-P1-O3	3.12	93.43	107.57	5	3
4	A	391	PX4	O1-P1-O3	3.12	93.44	107.57	12	1
4	A	401	PX4	O1-P1-O2	3.12	126.94	112.44	9	8
4	A	411	PX4	O5-C9-C10	3.12	121.34	111.83	7	7
4	A	328	PX4	C31-C30-C29	3.12	98.62	114.37	4	5
4	A	420	PX4	C5-N1-C3	3.12	100.79	108.98	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	337	PX4	C5-N1-C2	3.11	97.53	109.91	4	2
4	A	363	PX4	C32-C31-C30	3.11	98.62	114.37	8	4
4	A	374	PX4	O1-P1-O2	3.11	126.93	112.44	17	7
4	A	422	PX4	C33-C32-C31	3.11	98.63	114.37	15	2
4	A	391	PX4	P1-O4-C6	3.11	103.52	121.35	7	12
4	A	407	PX4	O3-P1-O2	3.11	96.60	108.94	15	3
4	A	421	PX4	C3-N1-C2	3.11	122.28	109.91	14	1
4	A	309	PX4	C26-C25-C24	3.11	101.69	113.13	1	2
4	A	338	PX4	C4-N1-C3	3.11	100.80	108.98	6	2
4	A	311	PX4	O4-P1-O2	3.11	121.26	108.94	5	4
4	A	340	PX4	O5-C9-C10	3.11	121.32	111.83	12	7
4	A	341	PX4	O5-C9-O6	3.11	115.85	123.63	10	7
4	A	353	PX4	C25-C24-C23	3.11	102.30	113.69	15	4
4	A	395	PX4	O5-C9-C10	3.11	121.32	111.83	19	7
4	A	343	PX4	O5-C9-C10	3.11	121.32	111.83	13	4
4	A	376	PX4	O5-C9-O6	3.11	115.85	123.63	14	3
4	A	317	PX4	O4-P1-O2	3.11	96.63	108.94	13	3
4	A	336	PX4	O5-C9-C10	3.11	121.31	111.83	7	4
4	A	385	PX4	O5-C9-C10	3.11	121.31	111.83	4	5
4	A	390	PX4	O7-C7-C6	3.11	119.48	108.34	8	7
4	A	423	PX4	C8-O5-C9	3.11	105.76	117.12	12	5
4	A	317	PX4	O5-C9-C10	3.10	121.30	111.83	10	4
4	A	370	PX4	O5-C9-C10	3.10	121.30	111.83	17	4
4	A	395	PX4	C8-O5-C9	3.10	105.78	117.12	5	2
4	A	397	PX4	C11-C10-C9	3.10	102.32	113.69	13	1
5	A	434	C3S	C32-C30-C29	3.10	100.19	103.84	20	7
4	A	314	PX4	C4-N1-C2	3.10	97.58	109.91	16	2
4	A	334	PX4	P1-O4-C6	3.10	103.57	121.35	17	10
4	A	363	PX4	C1-C2-N1	3.10	125.78	115.82	20	5
4	A	381	PX4	O5-C9-O6	3.10	115.87	123.63	20	7
4	A	412	PX4	O7-C7-C8	3.10	119.47	108.34	8	7
4	A	344	PX4	C5-N1-C4	3.10	117.12	108.98	1	2
4	A	344	PX4	O5-C9-O6	3.10	115.87	123.63	18	10
4	A	347	PX4	C31-C30-C29	3.10	98.70	114.37	17	1
4	A	379	PX4	O4-P1-O2	3.10	121.22	108.94	8	2
4	A	385	PX4	C26-C25-C24	3.10	101.74	113.13	16	2
4	A	400	PX4	C12-C11-C10	3.10	101.74	113.13	13	4
4	A	355	PX4	C12-C11-C10	3.10	101.75	113.13	8	2
4	A	363	PX4	C8-O5-C9	3.10	105.80	117.12	19	2
4	A	424	PX4	C27-C26-C25	3.10	98.71	114.37	13	1
4	A	425	PX4	C30-C29-C28	3.10	98.72	114.37	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	310	PX4	C34-C33-C32	3.09	98.73	114.37	5	4
4	A	323	PX4	C26-C25-C24	3.09	101.76	113.13	12	2
4	A	386	PX4	C11-C10-C9	3.10	102.35	113.69	15	3
4	A	365	PX4	C8-O5-C9	3.09	105.82	117.12	18	1
4	A	368	PX4	O3-P1-O2	3.09	96.68	108.94	20	2
4	A	424	PX4	C3-N1-C2	3.09	122.20	109.91	6	1
4	A	352	PX4	C4-N1-C3	3.09	100.86	108.98	17	5
4	A	409	PX4	C1-C2-N1	3.09	125.74	115.82	7	6
5	A	434	C3S	C1-C22-C12	3.09	103.41	108.74	14	3
4	A	381	PX4	C1-C2-N1	3.09	125.74	115.82	3	8
4	A	310	PX4	O1-P1-O3	3.09	93.57	107.57	2	2
4	A	311	PX4	C4-N1-C3	3.09	117.09	108.98	2	3
4	A	363	PX4	C7-O7-C23	3.09	110.41	117.80	2	7
4	A	406	PX4	C11-C10-C9	3.09	102.38	113.69	13	3
4	A	427	PX4	O7-C7-C6	3.09	119.42	108.34	6	12
4	A	324	PX4	C5-N1-C4	3.09	100.87	108.98	6	4
4	A	330	PX4	O7-C7-C8	3.08	119.41	108.34	2	6
4	A	383	PX4	C5-N1-C3	3.09	100.87	108.98	14	6
4	A	393	PX4	C20-C19-C18	3.09	98.77	114.37	10	3
4	A	397	PX4	C5-N1-C3	3.09	100.87	108.98	11	4
4	A	423	PX4	O7-C7-C8	3.09	119.41	108.34	17	7
4	A	340	PX4	C5-N1-C3	3.08	100.88	108.98	3	3
4	A	354	PX4	O1-P1-O4	3.08	121.54	107.57	3	4
4	A	359	PX4	O3-C1-C2	3.08	124.49	109.65	4	3
4	A	371	PX4	C3-N1-C2	3.08	97.66	109.91	19	5
4	A	377	PX4	C5-N1-C3	3.08	117.07	108.98	17	5
4	A	417	PX4	O6-C9-C10	3.08	111.73	123.78	19	3
4	A	421	PX4	C5-N1-C2	3.08	122.16	109.91	3	2
4	A	375	PX4	C5-N1-C4	3.08	117.07	108.98	14	5
4	A	391	PX4	C4-N1-C2	3.08	97.67	109.91	15	1
4	A	330	PX4	C16-C15-C14	3.08	98.81	114.37	3	3
4	A	366	PX4	C4-N1-C3	3.08	100.89	108.98	5	5
4	A	406	PX4	O1-P1-O4	3.08	121.52	107.57	17	1
4	A	351	PX4	O3-P1-O2	3.08	121.13	108.94	6	3
4	A	384	PX4	C11-C10-C9	3.07	102.43	113.69	6	3
4	A	399	PX4	O7-C23-O8	3.08	116.51	123.70	16	5
4	A	307	PX4	C4-N1-C2	3.07	122.13	109.91	4	1
4	A	420	PX4	O7-C23-O8	3.08	116.52	123.70	19	7
4	A	411	PX4	O1-P1-O4	3.07	121.50	107.57	1	4
4	A	422	PX4	O1-P1-O4	3.07	121.50	107.57	20	1
4	A	429	PX4	C11-C10-C9	3.07	102.43	113.69	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	307	PX4	C29-C28-C27	3.07	98.84	114.37	19	2
4	A	328	PX4	C12-C11-C10	3.07	101.83	113.13	11	4
4	A	343	PX4	O3-P1-O2	3.07	96.76	108.94	10	5
4	A	381	PX4	O3-P1-O2	3.07	96.76	108.94	7	4
4	A	400	PX4	C26-C25-C24	3.07	101.84	113.13	20	2
4	A	406	PX4	C1-C2-N1	3.07	125.69	115.82	8	5
4	A	349	PX4	O1-P1-O2	3.07	126.73	112.44	11	11
4	A	361	PX4	C5-N1-C3	3.07	100.91	108.98	8	3
4	A	382	PX4	O5-C9-C10	3.07	121.20	111.83	16	2
4	A	398	PX4	C5-N1-C3	3.07	100.91	108.98	15	4
4	A	309	PX4	C14-C13-C12	3.07	98.85	114.37	18	3
4	A	310	PX4	O3-P1-O2	3.07	96.77	108.94	11	3
4	A	379	PX4	C8-O5-C9	3.07	105.89	117.12	14	4
4	A	355	PX4	C30-C29-C28	3.07	98.85	114.37	20	2
4	A	423	PX4	O5-C9-O6	3.07	115.95	123.63	3	6
4	A	306	PX4	C18-C17-C16	3.07	98.86	114.37	9	3
4	A	397	PX4	O1-P1-O4	3.07	121.47	107.57	13	2
4	A	404	PX4	O3-P1-O2	3.07	96.77	108.94	15	5
4	A	409	PX4	O1-P1-O4	3.07	121.48	107.57	18	4
4	A	327	PX4	C1-C2-N1	3.07	125.67	115.82	7	4
4	A	333	PX4	C14-C13-C12	3.07	98.86	114.37	17	2
4	A	362	PX4	O5-C9-O6	3.07	115.96	123.63	2	3
4	A	307	PX4	O5-C9-C10	3.06	121.18	111.83	7	4
4	A	308	PX4	O7-C7-C8	3.06	119.34	108.34	3	9
4	A	316	PX4	O3-C1-C2	3.06	124.40	109.65	17	3
4	A	331	PX4	C5-N1-C2	3.07	122.10	109.91	10	3
4	A	394	PX4	C33-C32-C31	3.06	98.88	114.37	16	1
5	A	436	C3S	C1-C22-C12	3.07	103.46	108.74	16	5
4	A	328	PX4	O5-C9-C10	3.06	121.18	111.83	9	6
4	A	363	PX4	C20-C19-C18	3.06	98.88	114.37	2	1
4	A	318	PX4	C25-C24-C23	3.06	102.47	113.69	5	1
4	A	373	PX4	C19-C18-C17	3.06	98.89	114.37	17	1
4	A	379	PX4	C32-C31-C30	3.06	98.89	114.37	1	1
4	A	321	PX4	C5-N1-C3	3.06	100.93	108.98	10	3
4	A	415	PX4	O3-C1-C2	3.06	124.39	109.65	15	1
4	A	322	PX4	C12-C11-C10	3.06	101.88	113.13	16	3
4	A	328	PX4	O1-P1-O3	3.06	93.69	107.57	19	4
4	A	418	PX4	C26-C25-C24	3.06	124.38	113.13	13	5
4	A	415	PX4	O5-C9-O6	3.06	115.97	123.63	13	4
4	A	317	PX4	O7-C23-O8	3.06	116.56	123.70	13	6
4	A	343	PX4	O3-C1-C2	3.06	124.36	109.65	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	349	PX4	C31-C30-C29	3.06	98.92	114.37	19	3
5	A	433	C3S	C32-C35-C38	3.06	111.13	105.14	3	4
4	A	348	PX4	O5-C9-C10	3.06	121.15	111.83	14	6
4	A	387	PX4	C28-C27-C26	3.06	98.92	114.37	17	2
4	A	410	PX4	O7-C7-C8	3.06	119.31	108.34	12	13
4	A	424	PX4	C4-N1-C3	3.05	100.95	108.98	9	3
4	A	365	PX4	O5-C9-O6	3.05	131.26	123.63	19	4
4	A	387	PX4	O5-C9-C10	3.05	121.14	111.83	4	7
4	A	392	PX4	C5-N1-C4	3.05	116.99	108.98	11	5
4	A	326	PX4	O5-C9-O6	3.05	116.00	123.63	14	9
4	A	337	PX4	C5-N1-C4	3.05	100.97	108.98	19	4
4	A	359	PX4	C26-C25-C24	3.05	124.33	113.13	10	4
4	A	364	PX4	O3-P1-O2	3.05	96.85	108.94	7	3
4	A	366	PX4	C28-C27-C26	3.05	98.95	114.37	16	1
4	A	392	PX4	O7-C7-C6	3.05	119.28	108.34	12	7
4	A	384	PX4	O8-C23-C24	3.05	111.86	123.78	1	1
4	A	315	PX4	O5-C9-O6	3.05	116.01	123.63	16	11
4	A	357	PX4	C26-C25-C24	3.05	101.93	113.13	9	4
4	A	317	PX4	C3-N1-C2	3.05	122.02	109.91	10	5
4	A	368	PX4	C33-C32-C31	3.04	98.98	114.37	2	2
4	A	306	PX4	C5-N1-C4	3.04	100.98	108.98	18	2
4	A	320	PX4	C20-C19-C18	3.04	98.98	114.37	14	3
4	A	328	PX4	C1-C2-N1	3.04	125.59	115.82	8	7
4	A	333	PX4	C31-C30-C29	3.04	98.98	114.37	18	2
4	A	390	PX4	O5-C9-C10	3.04	121.12	111.83	17	3
4	A	399	PX4	O5-C9-O6	3.04	116.02	123.63	9	5
4	A	409	PX4	C14-C13-C12	3.04	98.98	114.37	18	1
4	A	417	PX4	O7-C7-C6	3.04	119.26	108.34	11	11
4	A	348	PX4	C28-C27-C26	3.04	98.99	114.37	19	2
4	A	340	PX4	O7-C7-C8	3.04	119.25	108.34	2	4
4	A	366	PX4	C32-C31-C30	3.04	99.00	114.37	1	1
4	A	410	PX4	O5-C9-C10	3.04	121.10	111.83	18	9
4	A	305	PX4	C1-C2-N1	3.04	125.57	115.82	19	6
4	A	321	PX4	C4-N1-C3	3.04	101.00	108.98	14	2
4	A	359	PX4	C31-C30-C29	3.04	99.02	114.37	13	3
4	A	359	PX4	C12-C11-C10	3.04	124.28	113.13	16	6
4	A	364	PX4	C11-C10-C9	3.04	102.57	113.69	14	3
4	A	380	PX4	C5-N1-C2	3.04	121.98	109.91	6	1
4	A	396	PX4	C4-N1-C3	3.04	101.00	108.98	2	2
4	A	377	PX4	O5-C9-O6	3.03	116.04	123.63	11	8
4	A	417	PX4	O5-C9-O6	3.03	116.04	123.63	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	424	PX4	C4-N1-C2	3.03	97.85	109.91	3	4
4	A	428	PX4	O5-C9-C10	3.03	121.09	111.83	12	8
4	A	322	PX4	C4-N1-C2	3.03	121.97	109.91	13	1
4	A	397	PX4	O7-C7-C8	3.03	119.22	108.34	18	6
4	A	371	PX4	C32-C31-C30	3.03	99.05	114.37	4	1
4	A	323	PX4	C4-N1-C2	3.03	121.95	109.91	16	2
4	A	331	PX4	C1-C2-N1	3.03	125.55	115.82	20	6
4	A	351	PX4	C26-C25-C24	3.03	101.99	113.13	2	2
4	A	372	PX4	C32-C31-C30	3.03	99.05	114.37	7	2
4	A	415	PX4	C12-C11-C10	3.03	102.00	113.13	2	6
4	A	319	PX4	O8-C23-C24	3.03	111.94	123.78	6	2
4	A	379	PX4	O8-C23-C24	3.03	111.94	123.78	3	1
4	A	338	PX4	O7-C7-C8	3.03	119.20	108.34	3	6
4	A	346	PX4	C11-C10-C9	3.03	102.61	113.69	15	2
4	A	353	PX4	C16-C15-C14	3.03	99.07	114.37	2	2
4	A	358	PX4	C11-C10-C9	3.03	102.61	113.69	20	5
4	A	373	PX4	C11-C10-C9	3.03	102.61	113.69	11	2
4	A	417	PX4	C11-C10-C9	3.02	102.61	113.69	18	4
4	A	316	PX4	C25-C24-C23	3.02	102.61	113.69	6	4
4	A	342	PX4	C5-N1-C2	3.02	121.93	109.91	18	2
4	A	352	PX4	C33-C32-C31	3.02	99.09	114.37	8	3
4	A	313	PX4	C3-N1-C2	3.02	121.92	109.91	4	2
4	A	332	PX4	C33-C32-C31	3.02	99.09	114.37	1	1
4	A	384	PX4	O3-P1-O2	3.02	96.95	108.94	15	5
4	A	324	PX4	O5-C9-O6	3.02	116.07	123.63	11	6
4	A	332	PX4	C8-O5-C9	3.02	106.07	117.12	14	2
4	A	394	PX4	O8-C23-C24	3.02	111.96	123.78	4	1
4	A	372	PX4	C28-C27-C26	3.02	99.10	114.37	3	2
4	A	381	PX4	C26-C25-C24	3.02	102.03	113.13	16	5
4	A	374	PX4	C5-N1-C4	3.02	101.05	108.98	19	4
4	A	384	PX4	C5-N1-C4	3.02	101.05	108.98	6	8
4	A	425	PX4	C25-C24-C23	3.02	102.63	113.69	14	2
4	A	326	PX4	C20-C19-C18	3.02	99.11	114.37	16	3
4	A	417	PX4	C5-N1-C4	3.02	101.05	108.98	2	5
4	A	426	PX4	O7-C23-O8	3.02	116.65	123.70	8	7
4	A	305	PX4	C4-N1-C3	3.01	116.89	108.98	8	5
4	A	367	PX4	C33-C32-C31	3.01	99.14	114.37	11	2
4	A	412	PX4	C17-C16-C15	3.01	99.14	114.37	7	1
4	A	413	PX4	C32-C31-C30	3.01	99.13	114.37	20	4
4	A	401	PX4	C19-C18-C17	3.01	99.14	114.37	16	3
4	A	373	PX4	C26-C25-C24	3.01	102.06	113.13	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	416	PX4	C11-C10-C9	3.01	124.72	113.69	12	4
4	A	315	PX4	C8-O5-C9	3.01	106.12	117.12	14	3
4	A	372	PX4	C25-C24-C23	3.01	102.67	113.69	8	2
4	A	372	PX4	C5-N1-C2	3.01	97.95	109.91	20	1
4	A	381	PX4	C30-C29-C28	3.01	99.16	114.37	19	1
4	A	420	PX4	O1-P1-O3	3.01	93.93	107.57	1	3
4	A	335	PX4	C11-C10-C9	3.01	124.71	113.69	6	3
4	A	404	PX4	C17-C16-C15	3.01	99.17	114.37	18	2
4	A	326	PX4	C4-N1-C3	3.00	101.08	108.98	7	4
4	A	344	PX4	C5-N1-C3	3.00	101.08	108.98	7	2
4	A	367	PX4	C34-C33-C32	3.01	99.18	114.37	16	1
4	A	375	PX4	C12-C11-C10	3.00	102.09	113.13	12	3
4	A	407	PX4	C4-N1-C2	3.00	121.85	109.91	8	3
4	A	419	PX4	C5-N1-C3	3.00	116.86	108.98	17	3
4	A	420	PX4	C5-N1-C4	3.00	101.09	108.98	3	5
4	A	347	PX4	O5-C9-O6	3.00	116.12	123.63	14	7
4	A	305	PX4	C3-N1-C2	3.00	97.98	109.91	13	3
4	A	353	PX4	O1-P1-O3	3.00	93.96	107.57	17	4
4	A	355	PX4	C4-N1-C3	3.00	101.09	108.98	19	6
4	A	387	PX4	O4-P1-O2	3.00	120.82	108.94	18	5
4	A	395	PX4	C26-C25-C24	3.00	102.11	113.13	8	4
4	A	406	PX4	C5-N1-C3	3.00	116.85	108.98	15	3
4	A	328	PX4	C25-C24-C23	3.00	102.72	113.69	6	3
4	A	374	PX4	O5-C9-C10	3.00	120.97	111.83	9	4
4	A	387	PX4	O1-P1-O3	3.00	93.99	107.57	9	4
4	A	347	PX4	C19-C18-C17	3.00	99.23	114.37	20	1
4	A	316	PX4	O3-P1-O2	2.99	97.07	108.94	14	6
4	A	349	PX4	C4-N1-C3	2.99	101.11	108.98	9	6
4	A	364	PX4	C30-C29-C28	3.00	129.51	114.37	10	3
4	A	421	PX4	O8-C23-C24	3.00	112.06	123.78	1	1
4	A	375	PX4	O7-C7-C6	2.99	119.09	108.34	11	7
4	A	391	PX4	O6-C9-C10	2.99	112.07	123.78	4	2
4	A	400	PX4	O7-C7-C6	2.99	119.08	108.34	7	8
4	A	429	PX4	C26-C25-C24	2.99	102.13	113.13	4	2
4	A	397	PX4	C25-C24-C23	2.99	102.73	113.69	5	3
4	A	391	PX4	C26-C25-C24	2.99	102.14	113.13	18	5
4	A	428	PX4	C26-C25-C24	2.99	102.14	113.13	15	3
4	A	332	PX4	C19-C18-C17	2.99	99.26	114.37	7	2
4	A	338	PX4	O4-P1-O2	2.99	120.78	108.94	7	4
4	A	348	PX4	O7-C7-C6	2.99	119.06	108.34	15	11
4	A	368	PX4	C20-C19-C18	2.99	99.26	114.37	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C4-N1-C3	2.99	101.13	108.98	5	2
4	A	312	PX4	C29-C28-C27	2.99	99.28	114.37	5	5
4	A	414	PX4	C31-C30-C29	2.99	99.27	114.37	2	2
4	A	324	PX4	C5-N1-C3	2.98	116.81	108.98	17	3
4	A	331	PX4	C28-C27-C26	2.98	99.28	114.37	17	1
4	A	344	PX4	O3-P1-O2	2.98	97.11	108.94	11	6
4	A	347	PX4	O3-C1-C2	2.98	124.01	109.65	9	2
4	A	414	PX4	O3-C1-C2	2.98	124.01	109.65	8	5
4	A	422	PX4	O5-C9-O6	2.99	116.16	123.63	10	3
4	A	348	PX4	C3-N1-C2	2.98	121.77	109.91	8	1
4	A	385	PX4	C12-C11-C10	2.98	102.16	113.13	10	4
4	A	388	PX4	C16-C15-C14	2.98	99.28	114.37	2	2
4	A	425	PX4	O7-C7-C6	2.98	119.05	108.34	13	9
4	A	351	PX4	C5-N1-C3	2.98	101.14	108.98	10	4
4	A	319	PX4	O5-C9-C10	2.98	120.93	111.83	4	5
4	A	336	PX4	C12-C11-C10	2.98	102.17	113.13	6	2
4	A	339	PX4	C11-C10-C9	2.98	102.77	113.69	1	2
4	A	393	PX4	C33-C32-C31	2.98	99.29	114.37	17	4
4	A	395	PX4	C30-C29-C28	2.98	99.29	114.37	2	2
4	A	403	PX4	O3-P1-O2	2.98	97.11	108.94	3	2
4	A	409	PX4	C27-C26-C25	2.98	99.29	114.37	18	3
4	A	310	PX4	C26-C25-C24	2.98	102.18	113.13	7	5
4	A	335	PX4	C5-N1-C4	2.98	116.81	108.98	15	3
4	A	383	PX4	O7-C7-C6	2.98	119.04	108.34	3	8
4	A	399	PX4	O1-P1-O2	2.98	126.31	112.44	5	9
4	A	316	PX4	C4-N1-C3	2.98	101.15	108.98	5	1
4	A	338	PX4	C33-C32-C31	2.98	99.31	114.37	6	2
4	A	396	PX4	C26-C25-C24	2.98	102.18	113.13	9	2
4	A	387	PX4	C32-C31-C30	2.98	99.32	114.37	6	4
4	A	312	PX4	C26-C25-C24	2.98	102.19	113.13	4	3
4	A	330	PX4	C26-C25-C24	2.98	102.19	113.13	19	2
4	A	404	PX4	C4-N1-C3	2.98	101.16	108.98	17	5
4	A	413	PX4	O5-C9-C10	2.98	120.91	111.83	20	6
4	A	332	PX4	C31-C30-C29	2.98	99.32	114.37	11	3
4	A	330	PX4	C1-C2-N1	2.97	125.37	115.82	18	4
4	A	382	PX4	O1-P1-O3	2.97	94.10	107.57	17	1
4	A	402	PX4	C16-C15-C14	2.97	99.34	114.37	16	3
4	A	411	PX4	C28-C27-C26	2.97	99.34	114.37	5	3
4	A	428	PX4	O3-C1-C2	2.97	123.96	109.65	16	1
4	A	339	PX4	O1-P1-O4	2.97	121.04	107.57	19	2
4	A	330	PX4	C3-N1-C2	2.97	121.72	109.91	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	337	PX4	O7-C23-O8	2.97	116.76	123.70	4	7
4	A	342	PX4	C32-C31-C30	2.97	99.35	114.37	15	3
4	A	352	PX4	C12-C11-C10	2.97	102.21	113.13	9	5
4	A	348	PX4	C30-C29-C28	2.97	99.36	114.37	1	1
4	A	361	PX4	O1-P1-O2	2.97	126.26	112.44	17	6
4	A	362	PX4	C8-O5-C9	2.97	127.98	117.12	6	2
4	A	393	PX4	C26-C25-C24	2.97	102.21	113.13	2	3
4	A	387	PX4	O7-C7-C6	2.97	119.00	108.34	10	8
4	A	376	PX4	C18-C17-C16	2.97	99.37	114.37	8	1
4	A	378	PX4	C5-N1-C2	2.97	121.71	109.91	18	2
4	A	393	PX4	O7-C23-O8	2.97	116.76	123.70	18	4
4	A	408	PX4	C5-N1-C3	2.97	101.18	108.98	8	4
4	A	411	PX4	O5-C9-O6	2.97	116.20	123.63	19	5
4	A	318	PX4	C5-N1-C4	2.97	116.77	108.98	5	2
4	A	328	PX4	C11-C10-C9	2.97	124.57	113.69	8	4
4	A	391	PX4	O7-C23-O8	2.97	116.77	123.70	9	4
4	A	401	PX4	C34-C33-C32	2.97	99.37	114.37	2	2
4	A	418	PX4	C20-C19-C18	2.97	99.37	114.37	8	1
4	A	430	PX4	C32-C31-C30	2.97	99.37	114.37	11	1
4	A	340	PX4	P1-O4-C6	2.97	104.36	121.35	14	12
4	A	350	PX4	O5-C9-C10	2.97	120.88	111.83	2	4
4	A	361	PX4	C18-C17-C16	2.96	99.38	114.37	11	2
4	A	380	PX4	C25-C24-C23	2.96	102.83	113.69	15	3
4	A	391	PX4	C11-C10-C9	2.97	102.83	113.69	18	2
4	A	324	PX4	C1-C2-N1	2.96	125.33	115.82	5	9
4	A	367	PX4	C18-C17-C16	2.96	99.38	114.37	7	6
4	A	390	PX4	O1-P1-O3	2.96	94.13	107.57	7	3
4	A	397	PX4	C8-O5-C9	2.97	106.28	117.12	14	2
4	A	401	PX4	C16-C15-C14	2.96	99.38	114.37	11	4
5	A	432	C3S	C32-C35-C38	2.96	110.94	105.14	14	12
5	A	432	C3S	C26-C29-C30	2.96	102.81	107.25	4	4
4	A	391	PX4	C12-C11-C10	2.96	124.01	113.13	19	4
4	A	394	PX4	O1-P1-O3	2.96	94.14	107.57	3	2
4	A	401	PX4	C1-C2-N1	2.96	125.33	115.82	7	6
4	A	408	PX4	O3-C1-C2	2.96	123.91	109.65	19	3
4	A	338	PX4	C1-C2-N1	2.96	125.33	115.82	20	6
4	A	412	PX4	O1-P1-O4	2.96	121.00	107.57	6	3
4	A	379	PX4	C30-C29-C28	2.96	99.40	114.37	14	2
4	A	388	PX4	C15-C14-C13	2.96	99.40	114.37	13	3
4	A	420	PX4	O5-C9-C10	2.96	120.86	111.83	10	4
4	A	342	PX4	C4-N1-C3	2.96	101.20	108.98	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	345	PX4	C1-C2-N1	2.96	125.32	115.82	20	3
4	A	353	PX4	C32-C31-C30	2.96	99.40	114.37	7	3
4	A	393	PX4	O1-P1-O3	2.96	94.15	107.57	14	4
4	A	317	PX4	O1-P1-O2	2.96	126.20	112.44	6	12
4	A	320	PX4	C3-N1-C2	2.96	98.16	109.91	18	1
4	A	344	PX4	C15-C14-C13	2.96	99.42	114.37	20	3
5	A	432	C3S	C22-C20-C18	2.96	117.04	112.71	9	2
4	A	313	PX4	O5-C9-C10	2.96	120.85	111.83	20	4
4	A	332	PX4	C13-C12-C11	2.95	99.43	114.37	18	2
4	A	335	PX4	C3-N1-C2	2.95	121.66	109.91	1	4
4	A	365	PX4	C22-C21-C20	2.95	93.41	113.36	7	1
4	A	384	PX4	C31-C30-C29	2.95	99.44	114.37	12	2
4	A	390	PX4	C3-N1-C2	2.95	98.17	109.91	13	1
4	A	319	PX4	C7-O7-C23	2.95	110.73	117.80	9	5
4	A	339	PX4	O5-C9-C10	2.95	120.84	111.83	8	5
4	A	340	PX4	C4-N1-C2	2.95	121.65	109.91	20	2
4	A	369	PX4	O3-P1-O2	2.95	97.23	108.94	14	4
4	A	377	PX4	O8-C23-C24	2.95	112.24	123.78	4	3
4	A	337	PX4	C11-C10-C9	2.95	102.89	113.69	12	2
4	A	350	PX4	O3-P1-O2	2.95	97.24	108.94	19	8
4	A	397	PX4	C26-C25-C24	2.95	102.29	113.13	1	2
4	A	347	PX4	C33-C32-C31	2.95	99.47	114.37	15	1
4	A	406	PX4	C34-C33-C32	2.95	99.47	114.37	3	2
4	A	305	PX4	C15-C14-C13	2.94	99.48	114.37	7	4
4	A	312	PX4	C13-C12-C11	2.94	99.48	114.37	13	2
4	A	317	PX4	O7-C7-C6	2.95	118.91	108.34	3	4
4	A	323	PX4	C3-N1-C2	2.95	121.62	109.91	8	2
4	A	329	PX4	C1-C2-N1	2.95	125.28	115.82	16	4
5	A	431	C3S	C29-C30-C18	2.95	118.60	114.41	4	5
4	A	314	PX4	C20-C19-C18	2.94	99.49	114.37	7	1
4	A	324	PX4	C11-C10-C9	2.94	102.91	113.69	1	5
4	A	338	PX4	C15-C14-C13	2.94	99.49	114.37	10	2
4	A	422	PX4	C30-C29-C28	2.94	99.49	114.37	11	3
4	A	366	PX4	C7-O7-C23	2.94	124.84	117.80	15	5
4	A	379	PX4	C5-N1-C4	2.94	101.25	108.98	13	5
4	A	417	PX4	O3-C1-C2	2.94	123.81	109.65	10	2
4	A	395	PX4	C15-C14-C13	2.94	99.50	114.37	14	2
4	A	422	PX4	C18-C17-C16	2.94	99.50	114.37	19	1
4	A	364	PX4	C4-N1-C2	2.94	121.60	109.91	4	2
4	A	380	PX4	O1-P1-O4	2.94	120.89	107.57	13	2
4	A	413	PX4	O3-C1-C2	2.94	123.80	109.65	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	414	PX4	C5-N1-C2	2.94	98.22	109.91	8	3
4	A	370	PX4	C4-N1-C3	2.94	101.26	108.98	9	4
4	A	331	PX4	C25-C24-C23	2.94	102.93	113.69	5	3
4	A	359	PX4	C27-C26-C25	2.94	99.52	114.37	5	2
4	A	311	PX4	C3-N1-C2	2.94	98.24	109.91	6	1
4	A	364	PX4	C5-N1-C4	2.94	101.26	108.98	12	3
4	A	386	PX4	C3-N1-C2	2.94	121.58	109.91	9	4
4	A	407	PX4	C18-C17-C16	2.94	99.53	114.37	12	2
4	A	370	PX4	C18-C17-C16	2.93	99.54	114.37	18	3
4	A	404	PX4	C18-C17-C16	2.93	99.54	114.37	19	3
4	A	422	PX4	C19-C18-C17	2.93	99.53	114.37	12	1
4	A	305	PX4	O7-C7-C8	2.93	118.86	108.34	4	5
4	A	389	PX4	O5-C9-O6	2.93	116.29	123.63	1	3
4	A	420	PX4	O3-P1-O2	2.93	97.31	108.94	19	4
4	A	308	PX4	C5-N1-C2	2.93	98.26	109.91	18	3
4	A	319	PX4	O5-C9-O6	2.93	116.30	123.63	17	6
4	A	326	PX4	C15-C14-C13	2.93	99.56	114.37	12	2
4	A	352	PX4	C11-C10-C9	2.93	102.96	113.69	6	4
4	A	365	PX4	C1-C2-N1	2.93	125.23	115.82	12	6
4	A	403	PX4	C11-C10-C9	2.93	102.96	113.69	12	2
4	A	406	PX4	C18-C17-C16	2.93	99.55	114.37	12	3
4	A	429	PX4	O4-P1-O2	2.93	97.32	108.94	7	2
4	A	429	PX4	C31-C30-C29	2.93	99.55	114.37	17	3
4	A	308	PX4	O1-P1-O2	2.93	126.06	112.44	17	12
4	A	352	PX4	C5-N1-C2	2.93	121.55	109.91	17	1
4	A	402	PX4	C12-C11-C10	2.93	102.36	113.13	4	5
4	A	334	PX4	C30-C29-C28	2.93	99.57	114.37	10	3
4	A	376	PX4	C5-N1-C4	2.93	116.67	108.98	9	3
4	A	393	PX4	C27-C26-C25	2.93	99.57	114.37	16	3
4	A	400	PX4	O7-C7-C8	2.93	118.85	108.34	2	6
4	A	309	PX4	O1-P1-O3	2.93	94.31	107.57	20	3
4	A	330	PX4	C15-C14-C13	2.93	99.58	114.37	3	2
4	A	416	PX4	O7-C7-C6	2.93	118.84	108.34	14	6
4	A	420	PX4	C29-C28-C27	2.93	99.58	114.37	5	2
4	A	401	PX4	C18-C17-C16	2.93	99.58	114.37	8	1
4	A	349	PX4	C17-C16-C15	2.92	99.59	114.37	9	3
4	A	355	PX4	O3-P1-O2	2.92	97.35	108.94	5	3
4	A	390	PX4	O7-C7-C8	2.92	118.83	108.34	13	5
4	A	409	PX4	C5-N1-C2	2.92	98.29	109.91	4	2
4	A	398	PX4	O4-P1-O2	2.92	97.35	108.94	14	2
4	A	422	PX4	C11-C10-C9	2.92	102.98	113.69	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	318	PX4	O4-P1-O2	2.92	97.36	108.94	14	1
4	A	421	PX4	C30-C29-C28	2.92	99.60	114.37	20	1
4	A	350	PX4	C32-C31-C30	2.92	99.61	114.37	1	1
4	A	314	PX4	O6-C9-C10	2.92	112.36	123.78	4	1
4	A	317	PX4	O5-C9-O6	2.92	116.32	123.63	6	4
4	A	391	PX4	O1-P1-O4	2.92	120.80	107.57	7	2
4	A	402	PX4	O7-C23-O8	2.92	116.88	123.70	14	3
4	A	414	PX4	O4-P1-O2	2.92	120.51	108.94	6	5
4	A	421	PX4	O1-P1-O4	2.92	120.80	107.57	11	4
4	A	312	PX4	O7-C7-C6	2.92	118.81	108.34	17	5
4	A	338	PX4	C25-C24-C23	2.92	103.01	113.69	1	1
4	A	420	PX4	C32-C31-C30	2.92	99.63	114.37	2	3
4	A	305	PX4	O1-P1-O4	2.91	120.77	107.57	3	3
4	A	333	PX4	O3-P1-O2	2.91	97.39	108.94	1	4
4	A	353	PX4	O5-C9-C10	2.91	120.72	111.83	17	3
4	A	363	PX4	C26-C25-C24	2.91	123.84	113.13	1	4
4	A	396	PX4	O1-P1-O3	2.92	94.35	107.57	12	2
4	A	419	PX4	C8-O5-C9	2.91	106.46	117.12	13	3
4	A	429	PX4	C25-C24-C23	2.91	103.01	113.69	10	4
4	A	388	PX4	C31-C30-C29	2.91	99.65	114.37	8	2
4	A	419	PX4	O1-P1-O4	2.91	94.36	107.57	17	5
4	A	307	PX4	C20-C19-C18	2.91	99.66	114.37	15	2
4	A	310	PX4	C20-C19-C18	2.91	99.66	114.37	13	2
4	A	321	PX4	C18-C17-C16	2.91	99.65	114.37	16	6
4	A	342	PX4	C4-N1-C2	2.91	98.34	109.91	5	3
4	A	353	PX4	C33-C32-C31	2.91	99.66	114.37	11	2
4	A	427	PX4	C32-C31-C30	2.91	99.66	114.37	12	3
4	A	316	PX4	C8-O5-C9	2.91	127.74	117.12	15	4
4	A	371	PX4	C5-N1-C3	2.91	116.61	108.98	4	7
4	A	315	PX4	C3-N1-C2	2.91	121.46	109.91	7	4
4	A	362	PX4	C25-C24-C23	2.90	103.05	113.69	14	4
4	A	322	PX4	C5-N1-C2	2.90	121.45	109.91	8	4
4	A	369	PX4	O1-P1-O2	2.90	125.95	112.44	13	12
4	A	380	PX4	O1-P1-O2	2.90	125.96	112.44	4	6
4	A	405	PX4	C8-O5-C9	2.90	106.50	117.12	12	2
4	A	416	PX4	C19-C18-C17	2.90	99.69	114.37	5	1
4	A	328	PX4	C32-C31-C30	2.90	99.69	114.37	5	2
4	A	314	PX4	C19-C18-C17	2.90	99.70	114.37	18	3
4	A	379	PX4	C1-C2-N1	2.90	125.13	115.82	8	5
4	A	307	PX4	O3-P1-O2	2.90	97.45	108.94	9	3
4	A	311	PX4	O6-C9-C10	2.90	112.44	123.78	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	326	PX4	O1-P1-O4	2.90	120.71	107.57	1	2
4	A	336	PX4	O8-C23-C24	2.90	112.44	123.78	5	2
4	A	361	PX4	C25-C24-C23	2.90	103.07	113.69	12	4
4	A	392	PX4	C12-C11-C10	2.90	102.47	113.13	5	2
4	A	416	PX4	O4-P1-O2	2.90	120.42	108.94	14	3
4	A	308	PX4	O5-C9-C10	2.90	120.67	111.83	2	4
4	A	339	PX4	C32-C31-C30	2.90	99.73	114.37	6	1
4	A	370	PX4	C16-C15-C14	2.90	99.73	114.37	15	1
4	A	395	PX4	O7-C7-C8	2.90	118.73	108.34	12	5
4	A	382	PX4	C8-O5-C9	2.90	106.53	117.12	8	3
4	A	404	PX4	O5-C9-C10	2.90	120.67	111.83	12	3
4	A	428	PX4	C11-C10-C9	2.90	124.31	113.69	8	4
4	A	349	PX4	C8-O5-C9	2.89	106.54	117.12	8	2
4	A	400	PX4	C28-C27-C26	2.89	99.74	114.37	13	4
4	A	419	PX4	O6-C9-C10	2.89	135.10	123.78	7	1
4	A	310	PX4	C1-C2-N1	2.89	125.11	115.82	4	5
4	A	318	PX4	C19-C18-C17	2.89	99.74	114.37	20	1
4	A	363	PX4	C13-C12-C11	2.89	99.75	114.37	16	2
5	A	435	C3S	C40-C29-C38	2.89	116.92	111.68	19	5
4	A	321	PX4	O3-P1-O2	2.89	97.47	108.94	16	2
4	A	372	PX4	C33-C32-C31	2.89	99.75	114.37	10	2
4	A	326	PX4	C26-C25-C24	2.89	102.51	113.13	2	1
4	A	337	PX4	C8-O5-C9	2.89	106.56	117.12	10	2
4	A	345	PX4	C33-C32-C31	2.89	99.76	114.37	10	4
4	A	394	PX4	O5-C9-O6	2.89	116.40	123.63	3	5
4	A	412	PX4	O5-C9-O6	2.89	116.40	123.63	12	5
4	A	415	PX4	C8-O5-C9	2.89	127.68	117.12	9	2
4	A	429	PX4	C33-C32-C31	2.89	99.76	114.37	16	1
5	A	435	C3S	C26-C23-C20	2.89	108.22	113.14	11	5
4	A	306	PX4	C28-C27-C26	2.89	99.78	114.37	4	2
4	A	322	PX4	O3-P1-O2	2.89	97.50	108.94	10	4
4	A	340	PX4	C14-C13-C12	2.89	99.78	114.37	6	4
4	A	346	PX4	C14-C13-C12	2.89	99.78	114.37	5	1
4	A	357	PX4	C8-O5-C9	2.89	106.57	117.12	17	3
4	A	365	PX4	C11-C10-C9	2.89	103.12	113.69	9	3
4	A	391	PX4	C14-C13-C12	2.89	99.78	114.37	9	1
4	A	424	PX4	O4-P1-O2	2.89	120.37	108.94	3	4
4	A	368	PX4	O1-P1-O4	2.88	120.64	107.57	20	2
4	A	423	PX4	C7-O7-C23	2.88	124.70	117.80	16	3
4	A	308	PX4	C5-N1-C4	2.88	101.41	108.98	20	5
4	A	319	PX4	O1-P1-O4	2.88	120.63	107.57	18	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	325	PX4	C8-O5-C9	2.88	106.58	117.12	12	1
4	A	392	PX4	O8-C23-C24	2.88	135.06	123.78	11	3
4	A	372	PX4	C4-N1-C2	2.88	121.36	109.91	6	3
4	A	384	PX4	C28-C27-C26	2.88	99.81	114.37	16	1
4	A	393	PX4	C34-C33-C32	2.88	99.81	114.37	8	3
4	A	411	PX4	P1-O4-C6	2.88	104.84	121.35	3	13
4	A	308	PX4	C4-N1-C3	2.88	101.42	108.98	6	3
4	A	308	PX4	C32-C31-C30	2.88	99.82	114.37	9	2
4	A	333	PX4	C8-O5-C9	2.88	106.60	117.12	13	2
4	A	335	PX4	O3-P1-O2	2.88	97.52	108.94	20	6
4	A	366	PX4	O5-C9-O6	2.88	116.43	123.63	2	3
4	A	376	PX4	O3-C1-C2	2.88	123.50	109.65	5	6
4	A	381	PX4	C32-C31-C30	2.88	99.82	114.37	18	1
4	A	416	PX4	C26-C25-C24	2.88	102.55	113.13	20	3
4	A	362	PX4	C4-N1-C3	2.88	116.53	108.98	1	5
4	A	381	PX4	C13-C12-C11	2.88	99.83	114.37	3	3
4	A	386	PX4	O1-P1-O4	2.88	120.61	107.57	20	7
4	A	413	PX4	O3-P1-O2	2.88	97.54	108.94	16	4
4	A	342	PX4	C25-C24-C23	2.87	103.16	113.69	9	5
4	A	319	PX4	O7-C23-O8	2.87	116.99	123.70	8	5
4	A	332	PX4	O5-C9-C10	2.87	120.59	111.83	18	3
4	A	367	PX4	O1-P1-O4	2.87	120.59	107.57	14	2
4	A	398	PX4	C5-N1-C4	2.87	116.52	108.98	7	4
4	A	374	PX4	C32-C31-C30	2.87	99.85	114.37	15	5
4	A	384	PX4	O3-C1-C2	2.87	123.47	109.65	16	3
4	A	308	PX4	C26-C25-C24	2.87	102.58	113.13	18	2
4	A	345	PX4	O1-P1-O3	2.87	94.56	107.57	6	1
4	A	348	PX4	O1-P1-O4	2.87	94.56	107.57	2	2
4	A	361	PX4	C5-N1-C2	2.87	121.32	109.91	14	2
4	A	419	PX4	C25-C24-C23	2.87	103.17	113.69	6	2
4	A	428	PX4	C19-C18-C17	2.87	99.85	114.37	10	2
4	A	317	PX4	C14-C13-C12	2.87	99.87	114.37	1	2
4	A	340	PX4	O7-C7-C6	2.87	118.63	108.34	18	7
4	A	346	PX4	O4-P1-O2	2.87	97.57	108.94	7	2
4	A	354	PX4	C14-C13-C12	2.87	99.86	114.37	4	4
4	A	401	PX4	C4-N1-C3	2.87	101.44	108.98	2	3
4	A	355	PX4	C26-C25-C24	2.87	102.59	113.13	19	4
4	A	369	PX4	C18-C17-C16	2.87	99.87	114.37	16	1
4	A	371	PX4	O7-C7-C6	2.87	118.63	108.34	18	7
4	A	382	PX4	O5-C9-O6	2.87	116.45	123.63	14	6
4	A	414	PX4	O1-P1-O4	2.87	120.57	107.57	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	423	PX4	O5-C9-C10	2.87	120.58	111.83	9	5
4	A	426	PX4	C4-N1-C2	2.87	121.31	109.91	9	6
4	A	320	PX4	C25-C24-C23	2.86	103.20	113.69	8	3
4	A	325	PX4	C1-C2-N1	2.86	125.02	115.82	2	4
4	A	337	PX4	O5-C9-C10	2.86	120.57	111.83	3	4
4	A	342	PX4	C34-C33-C32	2.87	99.89	114.37	5	3
4	A	348	PX4	C14-C13-C12	2.87	99.88	114.37	17	3
4	A	309	PX4	C12-C11-C10	2.86	102.61	113.13	20	3
4	A	366	PX4	C15-C14-C13	2.86	99.89	114.37	10	1
4	A	370	PX4	C30-C29-C28	2.86	99.89	114.37	6	2
4	A	346	PX4	C20-C19-C18	2.86	99.90	114.37	1	2
4	A	399	PX4	C15-C14-C13	2.86	99.90	114.37	11	2
4	A	341	PX4	C8-O5-C9	2.86	106.66	117.12	3	2
4	A	400	PX4	C33-C32-C31	2.86	99.90	114.37	16	3
4	A	423	PX4	O1-P1-O4	2.86	120.54	107.57	18	2
4	A	356	PX4	C12-C11-C10	2.86	102.62	113.13	7	4
4	A	305	PX4	C12-C11-C10	2.86	123.63	113.13	9	3
4	A	369	PX4	C19-C18-C17	2.86	99.91	114.37	6	4
4	A	375	PX4	C25-C24-C23	2.86	103.21	113.69	6	3
4	A	323	PX4	C7-O7-C23	2.86	124.64	117.80	4	3
4	A	332	PX4	O5-C9-O6	2.86	116.48	123.63	15	3
4	A	386	PX4	C5-N1-C4	2.86	101.47	108.98	7	6
4	A	407	PX4	C29-C28-C27	2.86	99.92	114.37	15	2
4	A	423	PX4	C32-C31-C30	2.86	99.92	114.37	8	3
4	A	325	PX4	C4-N1-C2	2.86	121.27	109.91	7	3
4	A	341	PX4	C30-C29-C28	2.86	99.93	114.37	8	2
4	A	407	PX4	O1-P1-O2	2.86	125.74	112.44	2	5
4	A	426	PX4	O7-C7-C8	2.86	118.59	108.34	8	7
4	A	344	PX4	C13-C12-C11	2.86	128.80	114.37	16	2
4	A	321	PX4	C30-C29-C28	2.85	99.94	114.37	5	1
4	A	335	PX4	O8-C23-C24	2.85	112.62	123.78	2	1
4	A	336	PX4	C5-N1-C2	2.85	121.25	109.91	2	2
4	A	340	PX4	O7-C23-O8	2.85	117.03	123.70	4	5
4	A	346	PX4	O3-C1-C2	2.86	123.39	109.65	6	5
4	A	377	PX4	O3-P1-O2	2.86	97.62	108.94	1	1
4	A	339	PX4	C25-C24-C23	2.85	103.24	113.69	8	1
4	A	344	PX4	O5-C9-C10	2.85	120.53	111.83	4	5
4	A	425	PX4	C12-C11-C10	2.85	102.64	113.13	11	1
4	A	428	PX4	C31-C30-C29	2.85	99.94	114.37	5	1
4	A	313	PX4	O1-P1-O4	2.85	120.49	107.57	18	2
4	A	332	PX4	C4-N1-C2	2.85	121.25	109.91	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	355	PX4	O6-C9-C10	2.85	112.63	123.78	19	1
4	A	356	PX4	O4-P1-O2	2.85	120.24	108.94	11	3
4	A	373	PX4	C31-C30-C29	2.85	99.95	114.37	5	2
4	A	367	PX4	C14-C13-C12	2.85	99.95	114.37	2	3
4	A	394	PX4	C20-C19-C18	2.85	128.78	114.37	20	2
4	A	409	PX4	C4-N1-C2	2.85	121.25	109.91	4	2
4	A	393	PX4	O4-P1-O2	2.85	120.23	108.94	14	3
4	A	393	PX4	O8-C23-C24	2.85	112.63	123.78	11	3
4	A	338	PX4	C27-C26-C25	2.85	99.97	114.37	14	1
4	A	398	PX4	C8-O5-C9	2.85	106.70	117.12	2	3
4	A	423	PX4	C1-C2-N1	2.85	124.97	115.82	20	5
4	A	346	PX4	C26-C25-C24	2.85	102.66	113.13	8	2
4	A	352	PX4	C13-C12-C11	2.85	99.97	114.37	10	3
4	A	393	PX4	O1-P1-O4	2.85	120.47	107.57	11	3
4	A	409	PX4	O4-P1-O2	2.85	120.22	108.94	9	2
4	A	327	PX4	O5-C9-O6	2.85	116.51	123.63	7	4
4	A	330	PX4	C5-N1-C2	2.85	98.60	109.91	7	2
4	A	359	PX4	C34-C33-C32	2.85	99.98	114.37	3	3
4	A	360	PX4	C33-C32-C31	2.85	99.98	114.37	13	2
4	A	397	PX4	C15-C14-C13	2.85	99.98	114.37	16	3
4	A	427	PX4	O5-C9-O6	2.85	116.51	123.63	3	5
4	A	308	PX4	O3-C1-C2	2.84	123.34	109.65	15	2
4	A	333	PX4	C11-C10-C9	2.85	103.27	113.69	8	2
4	A	351	PX4	O4-P1-O2	2.85	97.66	108.94	14	2
4	A	365	PX4	C29-C28-C27	2.85	99.98	114.37	12	3
4	A	317	PX4	O7-C7-C8	2.84	118.54	108.34	2	6
4	A	338	PX4	O7-C23-O8	2.84	117.06	123.70	5	6
4	A	342	PX4	C26-C25-C24	2.84	102.68	113.13	3	3
4	A	338	PX4	C29-C28-C27	2.84	100.00	114.37	18	2
4	A	384	PX4	O1-P1-O3	2.84	94.68	107.57	15	1
4	A	390	PX4	C5-N1-C2	2.84	98.61	109.91	12	3
4	A	413	PX4	C19-C18-C17	2.84	100.01	114.37	9	2
4	A	311	PX4	O7-C7-C8	2.84	118.53	108.34	13	5
4	A	325	PX4	C27-C26-C25	2.84	100.02	114.37	16	5
4	A	342	PX4	C30-C29-C28	2.84	100.02	114.37	1	3
4	A	352	PX4	C31-C30-C29	2.84	100.02	114.37	18	3
4	A	370	PX4	C8-O5-C9	2.84	106.74	117.12	7	1
4	A	311	PX4	C18-C17-C16	2.84	100.03	114.37	18	2
4	A	374	PX4	C18-C17-C16	2.84	100.03	114.37	16	3
4	A	392	PX4	C28-C27-C26	2.84	100.03	114.37	17	1
4	A	334	PX4	O1-P1-O4	2.84	120.42	107.57	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	341	PX4	C11-C10-C9	2.84	103.30	113.69	9	1
4	A	347	PX4	C3-N1-C2	2.83	121.18	109.91	3	2
4	A	354	PX4	C30-C29-C28	2.84	100.04	114.37	9	3
4	A	384	PX4	C4-N1-C2	2.84	121.18	109.91	7	2
4	A	407	PX4	O1-P1-O3	2.84	94.71	107.57	19	3
4	A	414	PX4	C33-C32-C31	2.84	100.04	114.37	9	1
4	A	312	PX4	C33-C32-C31	2.83	100.05	114.37	14	3
4	A	375	PX4	C1-C2-N1	2.83	124.91	115.82	15	5
4	A	375	PX4	O4-P1-O2	2.83	120.17	108.94	5	3
4	A	392	PX4	C17-C16-C15	2.83	100.05	114.37	17	1
4	A	408	PX4	C31-C30-C29	2.83	100.04	114.37	10	1
4	A	343	PX4	O1-P1-O4	2.83	120.41	107.57	10	2
4	A	422	PX4	O3-C1-C2	2.83	123.28	109.65	3	3
4	A	334	PX4	O1-P1-O3	2.83	94.73	107.57	10	2
4	A	344	PX4	O4-P1-O2	2.83	120.16	108.94	7	3
4	A	364	PX4	O8-C23-C24	2.83	112.70	123.78	18	1
4	A	337	PX4	C3-N1-C2	2.83	98.66	109.91	3	2
4	A	347	PX4	O5-C9-C10	2.83	120.46	111.83	17	5
4	A	369	PX4	C3-N1-C2	2.83	121.16	109.91	2	2
4	A	416	PX4	C17-C16-C15	2.83	100.06	114.37	11	3
4	A	347	PX4	O1-P1-O3	2.83	94.74	107.57	9	3
4	A	361	PX4	O4-P1-O2	2.83	120.14	108.94	20	2
4	A	418	PX4	C8-O5-C9	2.83	106.78	117.12	12	3
4	A	323	PX4	C13-C12-C11	2.83	100.08	114.37	12	1
4	A	422	PX4	C4-N1-C3	2.83	101.55	108.98	2	4
4	A	378	PX4	C5-N1-C3	2.83	101.55	108.98	18	4
4	A	408	PX4	C3-N1-C2	2.83	121.14	109.91	8	1
4	A	414	PX4	O5-C9-C10	2.83	120.45	111.83	1	5
4	A	363	PX4	O7-C7-C6	2.82	118.48	108.34	3	10
4	A	364	PX4	C29-C28-C27	2.82	100.09	114.37	17	2
4	A	378	PX4	C4-N1-C3	2.82	116.40	108.98	8	5
4	A	309	PX4	C1-C2-N1	2.82	124.88	115.82	1	5
4	A	361	PX4	C11-C10-C9	2.82	103.36	113.69	6	3
4	A	365	PX4	C14-C13-C12	2.82	100.10	114.37	20	1
4	A	380	PX4	O7-C7-C6	2.82	118.47	108.34	15	5
4	A	380	PX4	C14-C13-C12	2.82	100.11	114.37	15	1
4	A	407	PX4	C5-N1-C4	2.82	116.39	108.98	11	4
4	A	414	PX4	C3-N1-C2	2.82	121.12	109.91	8	2
4	A	420	PX4	C5-N1-C2	2.82	98.69	109.91	7	1
4	A	320	PX4	O7-C7-C8	2.82	118.46	108.34	19	7
4	A	342	PX4	O1-P1-O3	2.82	120.35	107.57	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	399	PX4	O8-C23-C24	2.82	112.75	123.78	8	2
4	A	414	PX4	C32-C31-C30	2.82	100.11	114.37	18	1
4	A	421	PX4	C15-C14-C13	2.82	100.11	114.37	9	2
4	A	425	PX4	O3-P1-O2	2.82	97.76	108.94	18	4
4	A	339	PX4	O4-P1-O2	2.82	120.10	108.94	1	5
4	A	421	PX4	C20-C19-C18	2.82	100.12	114.37	10	3
4	A	322	PX4	C5-N1-C3	2.82	101.58	108.98	2	4
4	A	380	PX4	C27-C26-C25	2.82	100.13	114.37	5	2
4	A	415	PX4	C31-C30-C29	2.82	100.13	114.37	8	1
4	A	310	PX4	C15-C14-C13	2.81	100.14	114.37	13	1
4	A	323	PX4	C32-C31-C30	2.81	100.14	114.37	5	3
4	A	322	PX4	C29-C28-C27	2.81	100.14	114.37	4	3
4	A	354	PX4	C5-N1-C4	2.81	116.37	108.98	20	3
4	A	386	PX4	C12-C11-C10	2.81	123.47	113.13	10	5
4	A	314	PX4	C30-C29-C28	2.81	100.15	114.37	5	1
4	A	319	PX4	C15-C14-C13	2.81	100.15	114.37	2	2
4	A	335	PX4	O1-P1-O4	2.81	120.31	107.57	5	3
4	A	364	PX4	C5-N1-C3	2.81	101.59	108.98	14	5
4	A	327	PX4	O7-C7-C6	2.81	118.42	108.34	11	6
4	A	329	PX4	C12-C11-C10	2.81	102.80	113.13	16	6
4	A	335	PX4	C30-C29-C28	2.81	100.16	114.37	7	1
4	A	385	PX4	C27-C26-C25	2.81	100.16	114.37	18	1
4	A	399	PX4	C18-C17-C16	2.81	100.16	114.37	11	4
4	A	387	PX4	C1-C2-N1	2.81	124.83	115.82	16	5
4	A	390	PX4	O1-P1-O2	2.81	125.51	112.44	12	8
4	A	394	PX4	C26-C25-C24	2.81	123.45	113.13	1	2
4	A	417	PX4	C33-C32-C31	2.81	100.17	114.37	9	1
4	A	351	PX4	C5-N1-C4	2.81	116.35	108.98	15	1
4	A	371	PX4	C15-C14-C13	2.81	100.18	114.37	11	2
4	A	344	PX4	C18-C17-C16	2.81	100.19	114.37	5	2
4	A	381	PX4	C12-C11-C10	2.80	102.82	113.13	13	2
4	A	382	PX4	C11-C10-C9	2.81	103.41	113.69	18	3
4	A	398	PX4	C32-C31-C30	2.81	100.19	114.37	7	2
4	A	319	PX4	C4-N1-C2	2.80	121.06	109.91	11	3
4	A	330	PX4	C8-O5-C9	2.80	106.87	117.12	8	4
4	A	350	PX4	C17-C16-C15	2.80	100.19	114.37	18	2
4	A	358	PX4	O3-P1-O2	2.80	97.83	108.94	11	4
4	A	308	PX4	O5-C9-O6	2.80	116.62	123.63	11	2
4	A	330	PX4	C5-N1-C3	2.80	101.62	108.98	8	7
4	A	348	PX4	O1-P1-O3	2.80	120.27	107.57	1	4
4	A	410	PX4	C30-C29-C28	2.80	100.20	114.37	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	312	PX4	C3-N1-C2	2.80	98.78	109.91	17	6
4	A	350	PX4	C25-C24-C23	2.80	103.43	113.69	20	1
4	A	354	PX4	O8-C23-C24	2.80	112.84	123.78	12	2
4	A	375	PX4	C29-C28-C27	2.80	100.22	114.37	17	1
4	A	399	PX4	C5-N1-C2	2.80	98.79	109.91	16	1
4	A	380	PX4	C15-C14-C13	2.80	100.23	114.37	8	3
4	A	325	PX4	O3-C1-C2	2.79	123.10	109.65	11	2
4	A	347	PX4	C16-C15-C14	2.79	100.24	114.37	16	4
4	A	363	PX4	C33-C32-C31	2.80	100.24	114.37	12	6
4	A	392	PX4	C25-C24-C23	2.80	103.45	113.69	18	3
4	A	358	PX4	O1-P1-O2	2.79	125.44	112.44	3	15
4	A	366	PX4	O3-P1-O2	2.79	97.86	108.94	3	5
4	A	405	PX4	C33-C32-C31	2.79	100.24	114.37	12	3
4	A	372	PX4	C8-O5-C9	2.79	106.91	117.12	19	2
4	A	315	PX4	C25-C24-C23	2.79	103.47	113.69	19	2
4	A	381	PX4	O1-P1-O2	2.79	125.43	112.44	7	11
4	A	389	PX4	O3-P1-O2	2.79	97.87	108.94	13	5
4	A	416	PX4	C33-C32-C31	2.79	100.26	114.37	10	3
4	A	426	PX4	O5-C9-O6	2.79	116.64	123.63	8	4
4	A	333	PX4	C5-N1-C2	2.79	98.82	109.91	15	1
4	A	337	PX4	O4-P1-O2	2.79	119.99	108.94	13	2
4	A	370	PX4	C11-C10-C9	2.79	123.92	113.69	6	3
4	A	371	PX4	O4-P1-O2	2.79	119.99	108.94	12	1
4	A	425	PX4	C8-O5-C9	2.79	106.92	117.12	7	2
4	A	352	PX4	C26-C25-C24	2.79	102.88	113.13	7	2
4	A	378	PX4	O6-C9-C10	2.79	112.88	123.78	19	3
4	A	404	PX4	C32-C31-C30	2.79	100.27	114.37	5	1
4	A	313	PX4	C33-C32-C31	2.79	100.28	114.37	1	4
4	A	357	PX4	C28-C27-C26	2.79	100.28	114.37	17	2
4	A	322	PX4	C27-C26-C25	2.79	100.29	114.37	14	3
4	A	381	PX4	O4-P1-O2	2.79	119.98	108.94	13	3
4	A	371	PX4	O1-P1-O4	2.78	120.19	107.57	20	4
4	A	325	PX4	C15-C14-C13	2.78	100.30	114.37	17	1
4	A	337	PX4	C25-C24-C23	2.78	103.49	113.69	3	2
4	A	424	PX4	C31-C30-C29	2.79	100.29	114.37	12	1
4	A	311	PX4	C28-C27-C26	2.78	100.30	114.37	5	3
4	A	335	PX4	C16-C15-C14	2.78	128.44	114.37	9	6
4	A	337	PX4	O5-C9-O6	2.78	116.67	123.63	12	5
4	A	343	PX4	C13-C12-C11	2.78	100.30	114.37	1	3
4	A	360	PX4	C20-C19-C18	2.78	100.30	114.37	15	2
4	A	361	PX4	O3-C1-C2	2.78	123.05	109.65	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	400	PX4	O4-P1-O2	2.78	119.97	108.94	15	5
4	A	376	PX4	O4-P1-O2	2.78	97.90	108.94	19	5
4	A	339	PX4	O3-C1-C2	2.78	123.03	109.65	5	3
4	A	367	PX4	C31-C30-C29	2.78	100.31	114.37	16	4
4	A	388	PX4	O4-P1-O2	2.78	119.96	108.94	8	1
4	A	389	PX4	C33-C32-C31	2.78	100.31	114.37	1	2
4	A	403	PX4	O1-P1-O2	2.78	125.38	112.44	14	9
4	A	327	PX4	O5-C9-C10	2.78	120.31	111.83	4	4
4	A	334	PX4	C3-N1-C2	2.78	120.96	109.91	12	1
4	A	338	PX4	O1-P1-O3	2.78	94.97	107.57	7	2
4	A	381	PX4	C11-C10-C9	2.78	103.51	113.69	18	4
4	A	404	PX4	O4-P1-O2	2.78	119.95	108.94	17	2
4	A	420	PX4	C17-C16-C15	2.78	100.31	114.37	5	1
4	A	314	PX4	O7-C23-O8	2.78	117.21	123.70	7	5
4	A	336	PX4	C16-C15-C14	2.78	100.33	114.37	6	1
4	A	355	PX4	C5-N1-C3	2.78	116.27	108.98	12	4
4	A	356	PX4	C13-C12-C11	2.78	100.33	114.37	15	2
4	A	360	PX4	C12-C11-C10	2.78	123.33	113.13	14	2
4	A	386	PX4	C34-C33-C32	2.78	100.33	114.37	15	2
4	A	371	PX4	C16-C15-C14	2.78	100.34	114.37	7	1
4	A	375	PX4	C11-C10-C9	2.78	123.87	113.69	17	2
4	A	384	PX4	C1-C2-N1	2.78	124.73	115.82	1	6
4	A	394	PX4	C1-C2-N1	2.78	124.73	115.82	8	4
4	A	325	PX4	C4-N1-C3	2.77	101.69	108.98	6	5
4	A	362	PX4	O7-C7-C8	2.78	118.30	108.34	8	5
4	A	402	PX4	O3-P1-O2	2.78	97.93	108.94	16	6
4	A	345	PX4	O4-P1-O2	2.77	97.94	108.94	5	3
4	A	372	PX4	O7-C7-C6	2.77	118.29	108.34	13	5
4	A	390	PX4	C1-C2-N1	2.77	124.73	115.82	18	4
4	A	343	PX4	C5-N1-C2	2.77	98.89	109.91	2	1
4	A	351	PX4	O7-C23-O8	2.77	117.22	123.70	6	3
4	A	394	PX4	O4-P1-O2	2.77	119.93	108.94	17	5
4	A	349	PX4	C1-C2-N1	2.77	124.72	115.82	14	2
4	A	398	PX4	O3-C1-C2	2.77	122.99	109.65	13	2
4	A	422	PX4	O4-P1-O2	2.77	97.95	108.94	5	2
4	A	430	PX4	C7-O7-C23	2.77	124.43	117.80	12	4
4	A	312	PX4	C4-N1-C3	2.77	116.25	108.98	17	5
4	A	348	PX4	C4-N1-C3	2.77	101.70	108.98	14	4
4	A	356	PX4	C11-C10-C9	2.77	103.54	113.69	5	4
4	A	364	PX4	O1-P1-O3	2.77	95.02	107.57	15	4
4	A	400	PX4	C30-C29-C28	2.77	100.37	114.37	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	418	PX4	C11-C10-C9	2.77	103.55	113.69	20	2
4	A	347	PX4	C17-C16-C15	2.77	100.38	114.37	8	1
4	A	367	PX4	C4-N1-C3	2.77	101.71	108.98	7	7
4	A	306	PX4	C32-C31-C30	2.76	100.40	114.37	1	2
4	A	325	PX4	C32-C31-C30	2.76	100.40	114.37	20	3
4	A	409	PX4	O1-P1-O2	2.76	125.30	112.44	7	9
4	A	335	PX4	C28-C27-C26	2.76	100.41	114.37	20	2
4	A	340	PX4	C11-C10-C9	2.76	103.57	113.69	16	2
4	A	331	PX4	C31-C30-C29	2.76	100.41	114.37	20	4
4	A	416	PX4	C16-C15-C14	2.76	100.41	114.37	17	1
4	A	328	PX4	O3-C1-C2	2.76	122.93	109.65	1	1
4	A	365	PX4	C7-O7-C23	2.76	111.19	117.80	6	5
4	A	371	PX4	C1-C2-N1	2.76	124.68	115.82	15	2
4	A	374	PX4	C5-N1-C2	2.76	120.88	109.91	1	1
4	A	385	PX4	O1-P1-O3	2.76	120.08	107.57	8	3
4	A	399	PX4	C34-C33-C32	2.76	100.42	114.37	18	2
4	A	306	PX4	C30-C29-C28	2.76	100.43	114.37	11	2
4	A	315	PX4	C30-C29-C28	2.76	100.43	114.37	1	5
4	A	319	PX4	C13-C12-C11	2.76	100.44	114.37	20	2
4	A	349	PX4	C20-C19-C18	2.76	100.43	114.37	2	2
4	A	390	PX4	C28-C27-C26	2.76	100.43	114.37	6	1
4	A	347	PX4	O8-C23-C24	2.76	113.00	123.78	15	2
4	A	418	PX4	O5-C9-C10	2.76	120.24	111.83	7	3
4	A	325	PX4	C33-C32-C31	2.75	100.44	114.37	10	3
4	A	343	PX4	C4-N1-C2	2.75	120.86	109.91	2	4
4	A	324	PX4	O6-C9-C10	2.75	113.02	123.78	14	3
4	A	353	PX4	O3-C1-C2	2.75	122.90	109.65	5	4
4	A	365	PX4	C5-N1-C3	2.75	116.21	108.98	19	2
4	A	389	PX4	O3-C1-C2	2.75	122.90	109.65	5	4
4	A	346	PX4	C32-C31-C30	2.75	100.46	114.37	7	4
4	A	369	PX4	C32-C31-C30	2.75	100.46	114.37	18	4
4	A	378	PX4	C13-C12-C11	2.75	100.46	114.37	3	3
4	A	387	PX4	O3-C1-C2	2.75	122.89	109.65	12	4
4	A	410	PX4	C1-C2-N1	2.75	124.65	115.82	7	5
4	A	429	PX4	C34-C33-C32	2.75	100.46	114.37	10	1
4	A	429	PX4	C8-O5-C9	2.75	107.07	117.12	3	3
4	A	353	PX4	C18-C17-C16	2.75	100.47	114.37	14	3
4	A	407	PX4	O7-C7-C6	2.75	118.20	108.34	12	5
4	A	429	PX4	O1-P1-O4	2.75	120.02	107.57	18	3
4	A	320	PX4	C12-C11-C10	2.75	103.04	113.13	4	3
4	A	349	PX4	C14-C13-C12	2.75	100.49	114.37	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	413	PX4	C27-C26-C25	2.75	100.48	114.37	12	2
4	A	422	PX4	C26-C25-C24	2.75	103.04	113.13	6	3
4	A	351	PX4	C28-C27-C26	2.74	100.49	114.37	9	3
4	A	393	PX4	C25-C24-C23	2.74	103.64	113.69	10	1
4	A	422	PX4	C32-C31-C30	2.74	100.49	114.37	1	1
4	A	329	PX4	C3-N1-C2	2.74	99.01	109.91	6	2
4	A	334	PX4	C19-C18-C17	2.74	100.50	114.37	1	1
4	A	371	PX4	C27-C26-C25	2.74	100.50	114.37	5	3
4	A	306	PX4	C3-N1-C2	2.74	120.81	109.91	8	2
4	A	360	PX4	C19-C18-C17	2.74	100.51	114.37	9	2
4	A	383	PX4	C29-C28-C27	2.74	100.51	114.37	14	4
4	A	420	PX4	C1-C2-N1	2.74	124.62	115.82	8	5
4	A	325	PX4	O1-P1-O2	2.74	125.18	112.44	3	11
4	A	340	PX4	O1-P1-O4	2.74	119.98	107.57	9	3
4	A	341	PX4	C12-C11-C10	2.74	103.06	113.13	16	4
4	A	369	PX4	C8-O5-C9	2.74	107.11	117.12	17	4
4	A	370	PX4	C17-C16-C15	2.74	100.53	114.37	3	2
4	A	428	PX4	O3-P1-O2	2.74	98.08	108.94	6	4
4	A	314	PX4	C32-C31-C30	2.74	100.54	114.37	1	2
4	A	315	PX4	C14-C13-C12	2.74	100.54	114.37	4	1
4	A	317	PX4	C5-N1-C2	2.74	120.78	109.91	19	3
4	A	351	PX4	C34-C33-C32	2.74	100.54	114.37	13	3
4	A	354	PX4	C29-C28-C27	2.74	100.54	114.37	11	1
4	A	376	PX4	C32-C31-C30	2.74	100.53	114.37	2	2
4	A	396	PX4	C28-C27-C26	2.74	100.53	114.37	6	3
4	A	369	PX4	C5-N1-C4	2.73	116.16	108.98	20	2
4	A	398	PX4	C4-N1-C2	2.74	120.78	109.91	2	1
4	A	404	PX4	C28-C27-C26	2.73	100.55	114.37	3	1
4	A	407	PX4	C26-C25-C24	2.73	103.08	113.13	17	1
4	A	321	PX4	O1-P1-O4	2.73	119.95	107.57	13	5
4	A	327	PX4	O3-P1-O2	2.73	98.10	108.94	19	3
4	A	328	PX4	C18-C17-C16	2.73	100.56	114.37	5	2
4	A	348	PX4	C8-O5-C9	2.73	107.14	117.12	9	1
4	A	391	PX4	C16-C15-C14	2.73	100.56	114.37	9	2
4	A	396	PX4	C25-C24-C23	2.73	103.69	113.69	16	4
4	A	419	PX4	C14-C13-C12	2.73	100.56	114.37	12	2
4	A	310	PX4	C3-N1-C2	2.73	120.76	109.91	9	2
4	A	312	PX4	O3-C1-C2	2.73	122.78	109.65	18	3
4	A	337	PX4	C19-C18-C17	2.73	100.58	114.37	11	1
4	A	404	PX4	C1-C2-N1	2.73	124.58	115.82	2	6
4	A	375	PX4	C4-N1-C2	2.73	120.75	109.91	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	C11-C10-C9	2.73	103.70	113.69	3	3
4	A	375	PX4	C15-C14-C13	2.73	100.59	114.37	16	5
4	A	387	PX4	C13-C12-C11	2.73	100.59	114.37	20	2
4	A	391	PX4	C15-C14-C13	2.73	100.58	114.37	5	3
4	A	345	PX4	C5-N1-C2	2.73	120.74	109.91	8	1
4	A	430	PX4	C15-C14-C13	2.73	100.59	114.37	5	1
4	A	311	PX4	C17-C16-C15	2.72	100.60	114.37	3	1
4	A	359	PX4	C11-C10-C9	2.72	103.71	113.69	14	2
4	A	382	PX4	C4-N1-C2	2.72	120.74	109.91	4	1
4	A	316	PX4	C3-N1-C2	2.72	120.73	109.91	16	2
4	A	306	PX4	O4-P1-O2	2.72	98.15	108.94	16	2
4	A	308	PX4	C25-C24-C23	2.72	103.72	113.69	7	2
4	A	353	PX4	C8-O5-C9	2.72	107.17	117.12	7	3
4	A	365	PX4	O1-P1-O4	2.72	119.90	107.57	2	2
4	A	412	PX4	O8-C23-C24	2.72	113.14	123.78	8	3
4	A	326	PX4	O3-C1-C2	2.72	122.74	109.65	6	1
4	A	310	PX4	C33-C32-C31	2.72	100.63	114.37	2	1
4	A	353	PX4	O8-C23-C24	2.72	113.15	123.78	7	1
4	A	420	PX4	C26-C25-C24	2.72	103.14	113.13	14	2
4	A	421	PX4	C4-N1-C3	2.72	101.83	108.98	17	5
4	A	423	PX4	C25-C24-C23	2.72	103.73	113.69	15	1
4	A	426	PX4	C33-C32-C31	2.72	100.62	114.37	6	4
4	A	313	PX4	C11-C10-C9	2.72	103.74	113.69	19	3
4	A	389	PX4	C8-O5-C9	2.72	107.18	117.12	20	2
4	A	391	PX4	O4-P1-O2	2.72	119.71	108.94	1	2
4	A	428	PX4	C14-C13-C12	2.72	100.63	114.37	11	1
4	A	423	PX4	C5-N1-C4	2.72	116.11	108.98	6	3
4	A	338	PX4	O6-C9-C10	2.71	113.17	123.78	14	3
4	A	305	PX4	C5-N1-C2	2.71	120.69	109.91	13	1
4	A	312	PX4	C11-C10-C9	2.71	103.75	113.69	13	3
4	A	326	PX4	C29-C28-C27	2.71	100.66	114.37	7	3
4	A	334	PX4	C16-C15-C14	2.71	100.65	114.37	3	3
4	A	368	PX4	C29-C28-C27	2.71	100.65	114.37	17	2
5	A	432	C3S	O4-S1-O2	2.71	122.70	112.24	14	6
4	A	369	PX4	O1-P1-O4	2.71	119.86	107.57	14	1
4	A	373	PX4	C17-C16-C15	2.71	100.66	114.37	3	1
4	A	417	PX4	C12-C11-C10	2.71	103.16	113.13	18	2
4	A	361	PX4	O7-C7-C8	2.71	118.07	108.34	10	5
4	A	379	PX4	C12-C11-C10	2.71	103.17	113.13	20	4
4	A	405	PX4	O1-P1-O3	2.71	95.28	107.57	20	6
4	A	419	PX4	C12-C11-C10	2.71	103.16	113.13	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	308	PX4	O3-P1-O2	2.71	98.20	108.94	18	3
4	A	341	PX4	C32-C31-C30	2.71	100.67	114.37	5	1
4	A	341	PX4	C4-N1-C3	2.71	116.09	108.98	10	3
4	A	426	PX4	O1-P1-O4	2.71	119.85	107.57	7	2
4	A	369	PX4	C13-C12-C11	2.71	100.68	114.37	11	2
4	A	379	PX4	C5-N1-C3	2.71	101.86	108.98	10	5
4	A	420	PX4	O3-C1-C2	2.71	122.68	109.65	10	2
4	A	427	PX4	C18-C17-C16	2.71	100.68	114.37	8	1
4	A	366	PX4	C27-C26-C25	2.71	100.69	114.37	19	2
4	A	307	PX4	C8-O5-C9	2.70	107.23	117.12	5	4
4	A	315	PX4	O3-C1-C2	2.70	122.66	109.65	12	3
4	A	318	PX4	C8-O5-C9	2.70	107.23	117.12	7	3
4	A	346	PX4	C8-O5-C9	2.70	107.23	117.12	3	3
4	A	391	PX4	C30-C29-C28	2.70	100.70	114.37	10	2
4	A	395	PX4	C5-N1-C3	2.70	101.87	108.98	3	2
4	A	339	PX4	C14-C13-C12	2.70	100.71	114.37	11	3
4	A	395	PX4	C3-N1-C2	2.70	120.66	109.91	20	2
4	A	367	PX4	C11-C10-C9	2.70	103.79	113.69	10	3
4	A	339	PX4	O5-C9-O6	2.70	116.87	123.63	4	2
4	A	410	PX4	C15-C14-C13	2.70	100.72	114.37	8	2
4	A	410	PX4	C5-N1-C2	2.70	99.17	109.91	3	1
4	A	429	PX4	C17-C16-C15	2.70	100.72	114.37	10	1
4	A	307	PX4	C5-N1-C4	2.70	101.89	108.98	14	4
4	A	313	PX4	C4-N1-C3	2.70	101.89	108.98	6	2
4	A	389	PX4	C26-C25-C24	2.70	103.21	113.13	9	1
4	A	412	PX4	C19-C18-C17	2.70	100.73	114.37	12	1
4	A	310	PX4	O1-P1-O4	2.70	119.79	107.57	8	3
4	A	316	PX4	O1-P1-O4	2.70	119.79	107.57	13	3
4	A	426	PX4	O7-C7-C6	2.70	118.02	108.34	4	4
4	A	364	PX4	C26-C25-C24	2.70	103.22	113.13	18	2
4	A	310	PX4	O5-C9-C10	2.69	120.05	111.83	9	5
4	A	333	PX4	C27-C26-C25	2.69	100.75	114.37	15	2
4	A	357	PX4	C14-C13-C12	2.69	100.75	114.37	3	3
4	A	364	PX4	O5-C9-C10	2.69	120.05	111.83	10	4
4	A	389	PX4	C25-C24-C23	2.69	103.82	113.69	11	3
5	A	436	C3S	C22-C20-C18	2.69	116.65	112.71	19	3
4	A	343	PX4	C31-C30-C29	2.69	100.76	114.37	14	3
4	A	367	PX4	C20-C19-C18	2.69	100.75	114.37	16	2
4	A	386	PX4	C5-N1-C3	2.69	116.05	108.98	13	2
4	A	387	PX4	C27-C26-C25	2.69	100.76	114.37	2	3
4	A	393	PX4	C11-C10-C9	2.69	103.83	113.69	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	420	PX4	C14-C13-C12	2.69	100.75	114.37	1	1
5	A	436	C3S	C40-C29-C38	2.69	116.56	111.68	12	2
4	A	361	PX4	C13-C12-C11	2.69	100.77	114.37	9	1
4	A	348	PX4	C31-C30-C29	2.69	100.78	114.37	18	5
4	A	362	PX4	C5-N1-C2	2.69	99.22	109.91	8	2
4	A	373	PX4	O8-C23-C24	2.69	113.26	123.78	12	2
4	A	401	PX4	C31-C30-C29	2.69	100.77	114.37	9	4
4	A	430	PX4	O1-P1-O3	2.69	95.37	107.57	7	4
4	A	424	PX4	C11-C10-C9	2.69	123.55	113.69	9	2
5	A	431	C3S	O3-S1-O4	2.69	117.97	108.56	3	1
4	A	309	PX4	O7-C7-C6	2.69	117.99	108.34	14	5
4	A	340	PX4	C5-N1-C2	2.69	120.59	109.91	10	2
4	A	357	PX4	C11-C10-C9	2.69	103.85	113.69	1	4
4	A	323	PX4	C25-C24-C23	2.69	103.85	113.69	12	2
4	A	372	PX4	C19-C18-C17	2.69	100.79	114.37	12	2
4	A	421	PX4	C4-N1-C2	2.69	99.23	109.91	14	3
4	A	323	PX4	C28-C27-C26	2.68	100.80	114.37	14	3
4	A	334	PX4	C26-C25-C24	2.68	103.26	113.13	15	4
4	A	368	PX4	C25-C24-C23	2.68	103.86	113.69	3	1
4	A	395	PX4	C13-C12-C11	2.68	100.80	114.37	5	3
4	A	404	PX4	C3-N1-C2	2.68	120.58	109.91	1	2
4	A	335	PX4	C15-C14-C13	2.68	100.80	114.37	16	2
4	A	404	PX4	C27-C26-C25	2.68	127.94	114.37	9	1
4	A	346	PX4	C27-C26-C25	2.68	100.80	114.37	2	2
4	A	347	PX4	O4-P1-O2	2.68	119.57	108.94	17	3
4	A	422	PX4	C34-C33-C32	2.68	100.81	114.37	11	3
5	A	435	C3S	C1-C22-C12	2.68	113.37	108.74	6	4
4	A	348	PX4	C27-C26-C25	2.68	100.82	114.37	14	3
4	A	415	PX4	C25-C24-C23	2.68	123.52	113.69	7	3
4	A	314	PX4	C25-C24-C23	2.68	103.88	113.69	5	3
4	A	389	PX4	O1-P1-O3	2.68	95.42	107.57	20	2
4	A	390	PX4	C31-C30-C29	2.68	100.82	114.37	7	3
4	A	309	PX4	C11-C10-C9	2.68	103.88	113.69	1	2
4	A	362	PX4	O1-P1-O4	2.68	119.71	107.57	4	2
4	A	396	PX4	O5-C9-O6	2.68	116.92	123.63	9	3
4	A	403	PX4	C14-C13-C12	2.68	100.83	114.37	12	2
4	A	419	PX4	C5-N1-C4	2.68	101.94	108.98	2	3
4	A	316	PX4	C4-N1-C2	2.68	120.55	109.91	19	2
4	A	331	PX4	O4-P1-O2	2.68	119.54	108.94	8	2
4	A	339	PX4	O7-C7-C8	2.68	117.95	108.34	15	3
4	A	345	PX4	C19-C18-C17	2.68	100.84	114.37	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	361	PX4	C29-C28-C27	2.68	100.84	114.37	10	3
4	A	378	PX4	C8-O5-C9	2.68	107.34	117.12	3	1
4	A	404	PX4	O1-P1-O2	2.68	124.89	112.44	3	13
4	A	330	PX4	C33-C32-C31	2.67	100.85	114.37	1	5
4	A	334	PX4	C17-C16-C15	2.67	100.86	114.37	3	3
4	A	420	PX4	C18-C17-C16	2.67	100.85	114.37	17	2
4	A	334	PX4	O4-P1-O2	2.67	119.53	108.94	5	1
4	A	337	PX4	C32-C31-C30	2.67	100.87	114.37	8	1
4	A	375	PX4	O1-P1-O4	2.67	119.67	107.57	1	3
4	A	399	PX4	C25-C24-C23	2.67	103.91	113.69	16	3
4	A	342	PX4	C15-C14-C13	2.67	100.87	114.37	9	2
4	A	344	PX4	C30-C29-C28	2.67	100.88	114.37	13	1
4	A	383	PX4	C4-N1-C2	2.67	120.52	109.91	4	1
4	A	390	PX4	C11-C10-C9	2.67	103.92	113.69	10	3
4	A	395	PX4	C29-C28-C27	2.67	100.88	114.37	14	1
4	A	412	PX4	C31-C30-C29	2.67	100.87	114.37	10	3
4	A	418	PX4	C15-C14-C13	2.67	100.87	114.37	17	2
4	A	322	PX4	C8-O5-C9	2.67	107.37	117.12	2	2
4	A	328	PX4	C33-C32-C31	2.67	100.89	114.37	16	4
4	A	400	PX4	C17-C16-C15	2.67	100.90	114.37	11	2
4	A	404	PX4	C4-N1-C2	2.67	99.31	109.91	20	3
4	A	405	PX4	C26-C25-C24	2.67	103.33	113.13	1	4
4	A	405	PX4	O3-C1-C2	2.67	122.48	109.65	4	1
4	A	406	PX4	C27-C26-C25	2.67	100.88	114.37	15	2
4	A	359	PX4	C30-C29-C28	2.67	100.89	114.37	1	4
4	A	362	PX4	C3-N1-C2	2.67	120.51	109.91	18	3
4	A	311	PX4	C34-C33-C32	2.66	100.90	114.37	15	1
4	A	317	PX4	O1-P1-O3	2.67	119.65	107.57	15	1
4	A	317	PX4	C29-C28-C27	2.67	100.89	114.37	18	1
4	A	331	PX4	O8-C23-C24	2.67	113.35	123.78	9	2
4	A	412	PX4	O3-C1-C2	2.67	122.48	109.65	3	2
4	A	407	PX4	C32-C31-C30	2.67	100.89	114.37	20	4
4	A	412	PX4	O3-P1-O2	2.67	119.50	108.94	7	5
4	A	422	PX4	C7-O7-C23	2.67	124.18	117.80	18	3
4	A	428	PX4	C13-C12-C11	2.67	100.89	114.37	16	1
4	A	337	PX4	C1-C2-N1	2.67	124.38	115.82	4	4
4	A	319	PX4	C20-C19-C18	2.66	100.90	114.37	4	2
4	A	418	PX4	C16-C15-C14	2.67	100.89	114.37	12	1
4	A	348	PX4	C1-C2-N1	2.66	124.37	115.82	7	3
4	A	428	PX4	C5-N1-C2	2.66	120.50	109.91	14	1
4	A	336	PX4	C15-C14-C13	2.66	100.91	114.37	10	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	363	PX4	C16-C15-C14	2.66	100.91	114.37	6	1
4	A	374	PX4	C14-C13-C12	2.66	100.91	114.37	19	1
4	A	391	PX4	C33-C32-C31	2.66	100.91	114.37	7	5
4	A	395	PX4	C33-C32-C31	2.66	100.92	114.37	2	3
4	A	401	PX4	O3-P1-O2	2.66	98.39	108.94	18	4
4	A	427	PX4	O6-C9-C10	2.66	113.37	123.78	5	1
4	A	320	PX4	C5-N1-C3	2.66	101.99	108.98	4	3
4	A	339	PX4	C33-C32-C31	2.66	100.92	114.37	6	2
4	A	394	PX4	C3-N1-C2	2.66	99.34	109.91	19	3
4	A	399	PX4	C3-N1-C2	2.66	120.48	109.91	17	4
4	A	413	PX4	C30-C29-C28	2.66	100.92	114.37	13	1
4	A	426	PX4	O4-P1-O2	2.66	119.48	108.94	11	3
4	A	352	PX4	O1-P1-O3	2.66	95.52	107.57	1	5
4	A	376	PX4	C12-C11-C10	2.66	103.36	113.13	16	2
4	A	391	PX4	C5-N1-C3	2.66	101.99	108.98	18	2
4	A	322	PX4	O1-P1-O4	2.66	119.61	107.57	18	2
4	A	331	PX4	C19-C18-C17	2.66	100.94	114.37	16	2
4	A	347	PX4	O1-P1-O4	2.66	119.60	107.57	6	4
4	A	349	PX4	C16-C15-C14	2.66	100.94	114.37	2	3
4	A	315	PX4	O7-C7-C6	2.65	117.86	108.34	5	7
4	A	365	PX4	C27-C26-C25	2.65	100.95	114.37	16	1
4	A	387	PX4	C5-N1-C2	2.65	120.46	109.91	15	1
4	A	420	PX4	C8-O5-C9	2.65	107.42	117.12	3	2
4	A	420	PX4	O4-P1-O2	2.65	119.46	108.94	11	2
4	A	425	PX4	C13-C12-C11	2.65	100.95	114.37	10	2
4	A	427	PX4	C28-C27-C26	2.65	100.95	114.37	9	2
4	A	376	PX4	O1-P1-O4	2.65	119.58	107.57	16	2
4	A	403	PX4	O3-C1-C2	2.65	122.41	109.65	11	2
4	A	405	PX4	C15-C14-C13	2.65	100.97	114.37	17	1
4	A	416	PX4	O3-C1-C2	2.65	122.41	109.65	4	2
4	A	429	PX4	C32-C31-C30	2.65	100.96	114.37	19	1
4	A	309	PX4	C15-C14-C13	2.65	100.97	114.37	12	3
4	A	329	PX4	O4-P1-O2	2.65	119.44	108.94	3	2
4	A	330	PX4	C18-C17-C16	2.65	100.97	114.37	20	3
4	A	397	PX4	C18-C17-C16	2.65	100.97	114.37	13	2
4	A	399	PX4	C5-N1-C3	2.65	102.01	108.98	9	2
4	A	430	PX4	C14-C13-C12	2.65	100.97	114.37	6	1
4	A	353	PX4	C20-C19-C18	2.65	100.98	114.37	5	3
4	A	383	PX4	O3-C1-C2	2.65	122.39	109.65	8	1
4	A	391	PX4	C17-C16-C15	2.65	100.98	114.37	1	1
4	A	405	PX4	O3-P1-O2	2.65	98.44	108.94	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	406	PX4	C8-O5-C9	2.65	126.80	117.12	12	1
4	A	420	PX4	C3-N1-C2	2.65	120.44	109.91	7	1
4	A	319	PX4	C32-C31-C30	2.65	100.98	114.37	4	1
4	A	405	PX4	C13-C12-C11	2.65	100.99	114.37	20	1
4	A	414	PX4	C25-C24-C23	2.65	103.99	113.69	18	2
4	A	331	PX4	O3-C1-C2	2.65	122.38	109.65	18	1
4	A	340	PX4	C12-C11-C10	2.65	103.40	113.13	12	1
4	A	374	PX4	C30-C29-C28	2.65	100.99	114.37	8	1
4	A	395	PX4	C27-C26-C25	2.65	100.99	114.37	11	1
4	A	414	PX4	C28-C27-C26	2.65	100.99	114.37	3	2
4	A	419	PX4	C16-C15-C14	2.65	100.99	114.37	16	2
4	A	308	PX4	C20-C19-C18	2.64	101.00	114.37	14	1
4	A	336	PX4	O1-P1-O3	2.64	95.59	107.57	11	2
4	A	358	PX4	C1-C2-N1	2.64	124.31	115.82	9	4
4	A	373	PX4	C33-C32-C31	2.64	101.00	114.37	1	1
4	A	414	PX4	C8-O5-C9	2.64	107.45	117.12	14	2
4	A	367	PX4	C19-C18-C17	2.64	101.01	114.37	14	2
4	A	369	PX4	C4-N1-C2	2.64	99.40	109.91	9	2
4	A	380	PX4	O4-P1-O2	2.64	119.40	108.94	9	2
4	A	384	PX4	O1-P1-O4	2.64	119.54	107.57	16	5
4	A	398	PX4	O6-C9-C10	2.64	113.45	123.78	6	1
4	A	408	PX4	O1-P1-O3	2.64	95.59	107.57	11	1
4	A	417	PX4	C4-N1-C3	2.64	115.92	108.98	7	4
4	A	310	PX4	C18-C17-C16	2.64	101.02	114.37	15	2
4	A	328	PX4	C20-C19-C18	2.64	101.02	114.37	4	3
4	A	420	PX4	C16-C15-C14	2.64	101.01	114.37	1	1
4	A	323	PX4	C14-C13-C12	2.64	101.03	114.37	7	3
4	A	324	PX4	C12-C11-C10	2.64	103.43	113.13	6	2
4	A	350	PX4	C31-C30-C29	2.64	101.03	114.37	5	2
4	A	363	PX4	C29-C28-C27	2.64	101.03	114.37	14	1
4	A	386	PX4	C32-C31-C30	2.64	101.02	114.37	1	2
4	A	386	PX4	C13-C12-C11	2.64	101.03	114.37	7	2
4	A	416	PX4	C20-C19-C18	2.64	101.02	114.37	13	4
4	A	321	PX4	C8-O5-C9	2.64	107.48	117.12	19	3
4	A	335	PX4	C29-C28-C27	2.64	101.03	114.37	18	1
4	A	378	PX4	O1-P1-O4	2.64	119.52	107.57	18	5
4	A	414	PX4	C19-C18-C17	2.64	101.03	114.37	13	1
4	A	306	PX4	C31-C30-C29	2.64	101.04	114.37	1	2
4	A	357	PX4	O1-P1-O4	2.64	119.52	107.57	8	4
5	A	431	C3S	C57-C54-C48	2.64	107.70	115.08	11	1
4	A	318	PX4	C13-C12-C11	2.63	101.05	114.37	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	358	PX4	C18-C17-C16	2.63	101.05	114.37	14	2
4	A	365	PX4	O6-C9-C10	2.63	113.48	123.78	8	2
4	A	410	PX4	C18-C17-C16	2.63	101.06	114.37	13	2
4	A	412	PX4	O6-C9-C10	2.63	113.48	123.78	6	4
4	A	413	PX4	C20-C19-C18	2.63	101.05	114.37	4	2
4	A	313	PX4	O7-C7-C8	2.63	117.79	108.34	17	7
4	A	318	PX4	C14-C13-C12	2.63	101.06	114.37	17	1
4	A	388	PX4	C12-C11-C10	2.63	103.46	113.13	12	2
4	A	423	PX4	C11-C10-C9	2.63	104.05	113.69	15	4
4	A	367	PX4	C27-C26-C25	2.63	101.07	114.37	15	1
4	A	307	PX4	O1-P1-O2	2.63	124.68	112.44	17	11
4	A	309	PX4	C34-C33-C32	2.63	101.08	114.37	17	1
4	A	312	PX4	O1-P1-O4	2.63	119.49	107.57	20	2
4	A	327	PX4	O1-P1-O3	2.63	119.49	107.57	20	2
4	A	314	PX4	O5-C9-O6	2.63	117.05	123.63	20	4
4	A	334	PX4	O6-C9-C10	2.63	113.50	123.78	17	1
4	A	336	PX4	C32-C31-C30	2.63	101.08	114.37	2	1
4	A	345	PX4	C26-C25-C24	2.63	103.46	113.13	1	2
4	A	333	PX4	C4-N1-C2	2.63	120.36	109.91	19	1
4	A	335	PX4	C26-C25-C24	2.63	103.47	113.13	4	2
4	A	368	PX4	C12-C11-C10	2.63	103.47	113.13	6	3
4	A	375	PX4	O5-C9-C10	2.63	103.82	111.83	4	5
4	A	393	PX4	O3-C1-C2	2.63	122.30	109.65	14	4
4	A	320	PX4	C19-C18-C17	2.63	101.08	114.37	17	1
4	A	322	PX4	C33-C32-C31	2.63	101.09	114.37	18	2
4	A	367	PX4	O8-C23-C24	2.63	113.51	123.78	4	1
4	A	425	PX4	C28-C27-C26	2.63	101.08	114.37	2	2
4	A	318	PX4	C15-C14-C13	2.62	101.10	114.37	1	1
4	A	323	PX4	C33-C32-C31	2.62	101.10	114.37	13	2
4	A	345	PX4	O6-C9-C10	2.63	113.52	123.78	8	1
4	A	340	PX4	C25-C24-C23	2.62	123.31	113.69	11	3
4	A	367	PX4	O3-P1-O2	2.62	98.53	108.94	8	3
4	A	391	PX4	C5-N1-C2	2.63	99.48	109.91	14	2
4	A	380	PX4	C16-C15-C14	2.62	101.11	114.37	20	2
5	A	433	C3S	O4-S1-O2	2.62	122.36	112.24	10	7
4	A	309	PX4	C3-N1-C2	2.62	120.33	109.91	11	3
4	A	371	PX4	C19-C18-C17	2.62	101.11	114.37	19	1
4	A	372	PX4	C13-C12-C11	2.62	101.11	114.37	10	3
4	A	401	PX4	C30-C29-C28	2.62	101.11	114.37	18	1
4	A	410	PX4	C33-C32-C31	2.62	101.11	114.37	15	2
4	A	316	PX4	C29-C28-C27	2.62	101.12	114.37	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	341	PX4	C18-C17-C16	2.62	101.12	114.37	8	2
4	A	405	PX4	O1-P1-O4	2.62	119.44	107.57	20	1
4	A	365	PX4	C33-C32-C31	2.62	101.13	114.37	15	2
4	A	376	PX4	C11-C10-C9	2.62	123.29	113.69	19	8
4	A	397	PX4	C19-C18-C17	2.62	101.13	114.37	18	1
4	A	407	PX4	C25-C24-C23	2.62	104.10	113.69	2	3
4	A	410	PX4	C11-C10-C9	2.62	104.10	113.69	20	4
4	A	378	PX4	C26-C25-C24	2.62	103.51	113.13	18	3
4	A	379	PX4	C4-N1-C3	2.62	102.10	108.98	14	2
4	A	340	PX4	C31-C30-C29	2.62	101.14	114.37	6	2
4	A	341	PX4	C5-N1-C2	2.62	120.31	109.91	5	4
4	A	380	PX4	O3-C1-C2	2.62	122.24	109.65	2	4
4	A	380	PX4	C20-C19-C18	2.62	101.14	114.37	20	1
4	A	323	PX4	O7-C7-C8	2.61	117.72	108.34	4	5
4	A	340	PX4	C3-N1-C2	2.61	120.30	109.91	9	2
4	A	397	PX4	C5-N1-C4	2.62	102.11	108.98	19	6
4	A	386	PX4	C26-C25-C24	2.61	103.52	113.13	6	2
4	A	428	PX4	C17-C16-C15	2.61	101.15	114.37	1	3
4	A	355	PX4	C11-C10-C9	2.61	123.27	113.69	11	3
4	A	312	PX4	O1-P1-O3	2.61	95.73	107.57	15	1
4	A	319	PX4	C33-C32-C31	2.61	101.17	114.37	5	2
4	A	329	PX4	C20-C19-C18	2.61	101.16	114.37	5	1
4	A	365	PX4	C26-C25-C24	2.61	103.53	113.13	12	2
4	A	368	PX4	O4-P1-O2	2.61	98.58	108.94	6	1
4	A	403	PX4	C20-C19-C18	2.61	101.17	114.37	9	2
4	A	412	PX4	O7-C7-C6	2.61	117.72	108.34	12	7
4	A	344	PX4	C32-C31-C30	2.61	101.17	114.37	7	1
4	A	355	PX4	C5-N1-C4	2.61	102.12	108.98	7	1
4	A	358	PX4	C13-C12-C11	2.61	101.17	114.37	17	1
4	A	425	PX4	C14-C13-C12	2.61	101.17	114.37	20	3
4	A	316	PX4	O1-P1-O3	2.61	95.74	107.57	18	3
4	A	330	PX4	C25-C24-C23	2.61	104.13	113.69	16	3
4	A	369	PX4	C14-C13-C12	2.61	101.18	114.37	6	1
4	A	383	PX4	C5-N1-C2	2.61	99.54	109.91	19	3
4	A	393	PX4	C5-N1-C4	2.61	115.83	108.98	17	2
4	A	415	PX4	C1-C2-N1	2.61	124.20	115.82	17	5
4	A	415	PX4	O4-P1-O2	2.61	119.28	108.94	15	2
4	A	314	PX4	C8-O5-C9	2.61	126.65	117.12	9	1
4	A	344	PX4	C31-C30-C29	2.61	101.19	114.37	15	2
4	A	316	PX4	C32-C31-C30	2.61	101.19	114.37	13	3
4	A	327	PX4	C14-C13-C12	2.61	101.19	114.37	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	320	PX4	C11-C10-C9	2.60	104.15	113.69	9	2
4	A	330	PX4	O8-C23-C24	2.60	113.60	123.78	19	1
4	A	333	PX4	O4-P1-O2	2.60	98.61	108.94	8	3
4	A	403	PX4	C12-C11-C10	2.60	103.56	113.13	6	1
4	A	405	PX4	C17-C16-C15	2.60	101.20	114.37	6	1
4	A	306	PX4	C20-C19-C18	2.60	101.21	114.37	17	2
4	A	417	PX4	C32-C31-C30	2.60	101.21	114.37	2	2
4	A	309	PX4	C30-C29-C28	2.60	101.22	114.37	4	2
4	A	334	PX4	C8-O5-C9	2.60	107.61	117.12	11	2
4	A	356	PX4	C5-N1-C4	2.60	115.81	108.98	2	2
4	A	359	PX4	C25-C24-C23	2.60	104.16	113.69	15	4
4	A	426	PX4	C7-O7-C23	2.60	124.02	117.80	18	1
4	A	386	PX4	O3-C1-C2	2.60	122.16	109.65	13	1
4	A	408	PX4	C4-N1-C2	2.60	120.25	109.91	11	3
4	A	322	PX4	C14-C13-C12	2.60	101.23	114.37	2	1
4	A	355	PX4	C13-C12-C11	2.60	101.23	114.37	19	2
4	A	387	PX4	C29-C28-C27	2.60	101.23	114.37	11	3
4	A	405	PX4	C19-C18-C17	2.60	101.23	114.37	5	2
4	A	306	PX4	O1-P1-O4	2.60	119.34	107.57	16	1
4	A	318	PX4	C4-N1-C2	2.60	99.59	109.91	3	3
4	A	330	PX4	C34-C33-C32	2.60	101.24	114.37	1	1
4	A	397	PX4	C3-N1-C2	2.60	99.58	109.91	5	3
4	A	398	PX4	C13-C12-C11	2.60	101.24	114.37	7	2
4	A	343	PX4	C36-C35-C34	2.60	95.83	113.36	16	1
4	A	352	PX4	C29-C28-C27	2.60	101.25	114.37	11	1
4	A	325	PX4	O8-C23-C24	2.59	113.63	123.78	15	2
4	A	336	PX4	O3-C1-C2	2.59	122.14	109.65	12	4
4	A	381	PX4	O1-P1-O4	2.60	119.33	107.57	2	1
4	A	406	PX4	C4-N1-C3	2.59	102.16	108.98	9	1
4	A	409	PX4	C18-C17-C16	2.60	101.25	114.37	2	4
4	A	312	PX4	O8-C23-C24	2.59	113.64	123.78	10	1
4	A	405	PX4	C5-N1-C4	2.59	102.16	108.98	10	5
4	A	350	PX4	C34-C33-C32	2.59	101.26	114.37	18	1
4	A	366	PX4	C8-O5-C9	2.59	107.64	117.12	7	1
4	A	412	PX4	C28-C27-C26	2.59	101.26	114.37	16	1
4	A	348	PX4	C20-C19-C18	2.59	101.27	114.37	11	2
4	A	402	PX4	C14-C13-C12	2.59	101.27	114.37	8	1
4	A	416	PX4	C4-N1-C2	2.59	120.21	109.91	1	1
4	A	419	PX4	C32-C31-C30	2.59	101.27	114.37	11	1
4	A	424	PX4	C32-C31-C30	2.59	101.27	114.37	19	3
4	A	353	PX4	C14-C13-C12	2.59	101.27	114.37	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	377	PX4	C31-C30-C29	2.59	101.27	114.37	3	2
4	A	428	PX4	C5-N1-C4	2.59	102.17	108.98	8	6
4	A	307	PX4	C5-N1-C2	2.59	120.20	109.91	7	3
4	A	331	PX4	C29-C28-C27	2.59	101.28	114.37	4	3
4	A	409	PX4	C34-C33-C32	2.59	101.28	114.37	14	3
4	A	415	PX4	C26-C25-C24	2.59	122.64	113.13	18	2
4	A	322	PX4	C20-C19-C18	2.59	101.29	114.37	15	2
4	A	323	PX4	C31-C30-C29	2.59	101.29	114.37	11	1
4	A	339	PX4	C12-C11-C10	2.59	103.62	113.13	11	1
4	A	360	PX4	O4-P1-O2	2.59	119.19	108.94	8	1
4	A	373	PX4	C3-N1-C2	2.59	120.19	109.91	7	3
4	A	307	PX4	C28-C27-C26	2.58	101.30	114.37	5	3
4	A	324	PX4	C33-C32-C31	2.59	101.30	114.37	19	1
4	A	339	PX4	C8-O5-C9	2.59	107.67	117.12	7	3
4	A	352	PX4	O5-C9-C10	2.59	119.72	111.83	3	5
4	A	361	PX4	C8-O5-C9	2.59	107.67	117.12	20	3
4	A	427	PX4	C5-N1-C3	2.59	102.18	108.98	16	4
4	A	430	PX4	C26-C25-C24	2.59	103.62	113.13	5	1
4	A	349	PX4	C30-C29-C28	2.58	101.31	114.37	18	3
4	A	383	PX4	C31-C30-C29	2.58	101.31	114.37	16	5
4	A	406	PX4	C28-C27-C26	2.58	101.31	114.37	5	2
4	A	309	PX4	C16-C15-C14	2.58	101.32	114.37	16	1
4	A	331	PX4	C12-C11-C10	2.58	103.64	113.13	8	4
4	A	331	PX4	C15-C14-C13	2.58	101.31	114.37	12	2
4	A	318	PX4	C32-C31-C30	2.58	101.32	114.37	4	3
4	A	334	PX4	C5-N1-C3	2.58	102.19	108.98	1	2
4	A	362	PX4	C30-C29-C28	2.58	101.32	114.37	7	2
4	A	367	PX4	C13-C12-C11	2.58	101.31	114.37	7	4
4	A	371	PX4	C31-C30-C29	2.58	101.32	114.37	18	3
4	A	390	PX4	C30-C29-C28	2.58	101.32	114.37	2	3
4	A	398	PX4	C12-C11-C10	2.58	103.64	113.13	8	2
4	A	322	PX4	C4-N1-C3	2.58	102.20	108.98	3	7
4	A	310	PX4	C19-C18-C17	2.58	101.33	114.37	13	2
4	A	324	PX4	C28-C27-C26	2.58	101.33	114.37	20	3
4	A	411	PX4	C11-C10-C9	2.58	104.24	113.69	7	2
4	A	429	PX4	C4-N1-C2	2.58	120.17	109.91	16	2
4	A	308	PX4	C19-C18-C17	2.58	101.34	114.37	8	1
4	A	337	PX4	C15-C14-C13	2.58	101.33	114.37	9	1
4	A	337	PX4	C31-C30-C29	2.58	101.33	114.37	20	1
4	A	339	PX4	C27-C26-C25	2.58	101.33	114.37	4	3
4	A	321	PX4	O8-C23-C24	2.58	113.70	123.78	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	347	PX4	C18-C17-C16	2.58	101.34	114.37	11	3
4	A	370	PX4	C4-N1-C2	2.58	120.15	109.91	4	3
4	A	373	PX4	C25-C24-C23	2.58	104.25	113.69	17	3
4	A	385	PX4	C4-N1-C2	2.58	120.16	109.91	15	2
4	A	394	PX4	C15-C14-C13	2.58	101.34	114.37	8	2
4	A	423	PX4	C5-N1-C3	2.58	102.20	108.98	4	5
4	A	306	PX4	O6-C9-C10	2.58	113.71	123.78	13	1
4	A	363	PX4	O1-P1-O3	2.58	95.89	107.57	19	4
4	A	413	PX4	C31-C30-C29	2.58	101.35	114.37	7	1
4	A	310	PX4	C31-C30-C29	2.57	101.36	114.37	10	1
4	A	313	PX4	C16-C15-C14	2.57	101.35	114.37	5	2
4	A	392	PX4	C4-N1-C3	2.58	115.74	108.98	7	4
4	A	403	PX4	O7-C7-C8	2.57	117.58	108.34	16	5
4	A	404	PX4	C8-O5-C9	2.57	107.71	117.12	1	1
4	A	407	PX4	C28-C27-C26	2.57	101.35	114.37	3	2
4	A	427	PX4	C31-C30-C29	2.57	101.36	114.37	18	4
4	A	332	PX4	O6-C9-C10	2.57	113.72	123.78	14	2
4	A	369	PX4	C31-C30-C29	2.57	101.36	114.37	12	1
4	A	395	PX4	C12-C11-C10	2.57	103.67	113.13	9	6
4	A	398	PX4	C11-C10-C9	2.57	104.27	113.69	16	2
4	A	401	PX4	C8-O5-C9	2.57	107.72	117.12	1	3
4	A	331	PX4	C4-N1-C2	2.57	120.12	109.91	19	4
4	A	355	PX4	C15-C14-C13	2.57	101.38	114.37	6	2
4	A	382	PX4	C19-C18-C17	2.57	101.38	114.37	7	4
4	A	421	PX4	C32-C31-C30	2.57	101.38	114.37	11	1
4	A	330	PX4	C4-N1-C2	2.57	120.11	109.91	2	1
4	A	359	PX4	C17-C16-C15	2.57	101.39	114.37	8	2
4	A	373	PX4	C32-C31-C30	2.57	101.38	114.37	4	1
4	A	374	PX4	C34-C33-C32	2.57	101.39	114.37	20	1
4	A	383	PX4	C25-C24-C23	2.57	104.28	113.69	7	2
4	A	385	PX4	C3-N1-C2	2.57	120.12	109.91	13	1
4	A	415	PX4	C27-C26-C25	2.57	101.38	114.37	4	1
4	A	416	PX4	O1-P1-O3	2.57	95.92	107.57	8	3
4	A	401	PX4	C11-C10-C9	2.57	104.29	113.69	3	2
4	A	417	PX4	O8-C23-C24	2.57	113.75	123.78	3	1
4	A	423	PX4	O4-P1-O2	2.57	119.11	108.94	10	5
4	A	312	PX4	C1-C2-N1	2.56	124.05	115.82	11	4
4	A	341	PX4	O4-P1-O2	2.56	119.10	108.94	12	1
4	A	362	PX4	C15-C14-C13	2.56	101.40	114.37	10	3
4	A	406	PX4	C14-C13-C12	2.56	101.41	114.37	20	4
4	A	318	PX4	C3-N1-C2	2.56	120.10	109.91	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	324	PX4	C5-N1-C2	2.56	99.72	109.91	10	3
4	A	341	PX4	C34-C33-C32	2.56	101.42	114.37	13	2
4	A	383	PX4	C15-C14-C13	2.56	101.42	114.37	13	3
4	A	389	PX4	C12-C11-C10	2.56	103.72	113.13	10	5
4	A	408	PX4	C25-C24-C23	2.56	123.08	113.69	10	2
4	A	308	PX4	O4-P1-O2	2.56	98.79	108.94	2	2
4	A	347	PX4	C29-C28-C27	2.56	101.43	114.37	5	2
4	A	361	PX4	O1-P1-O3	2.56	95.97	107.57	20	1
4	A	373	PX4	C5-N1-C4	2.56	102.26	108.98	5	2
4	A	385	PX4	C31-C30-C29	2.56	101.44	114.37	19	4
4	A	408	PX4	C14-C13-C12	2.56	101.43	114.37	6	3
4	A	325	PX4	C14-C13-C12	2.56	101.44	114.37	19	3
4	A	341	PX4	C16-C15-C14	2.56	101.44	114.37	19	2
4	A	373	PX4	C16-C15-C14	2.56	101.45	114.37	13	2
4	A	383	PX4	C4-N1-C3	2.56	102.26	108.98	1	3
4	A	396	PX4	C13-C12-C11	2.56	101.44	114.37	9	1
4	A	400	PX4	O6-C9-C10	2.56	113.78	123.78	4	1
4	A	408	PX4	C17-C16-C15	2.56	101.44	114.37	10	4
4	A	321	PX4	C28-C27-C26	2.56	101.45	114.37	19	2
4	A	331	PX4	C34-C33-C32	2.56	101.45	114.37	13	3
4	A	335	PX4	C32-C31-C30	2.55	101.45	114.37	18	4
4	A	365	PX4	C19-C18-C17	2.56	101.45	114.37	20	2
4	A	352	PX4	O7-C7-C8	2.55	117.51	108.34	6	2
4	A	368	PX4	C4-N1-C3	2.55	102.27	108.98	13	5
4	A	373	PX4	C34-C33-C32	2.55	101.46	114.37	10	1
4	A	374	PX4	O5-C9-O6	2.56	117.24	123.63	2	3
4	A	407	PX4	C3-N1-C2	2.55	120.06	109.91	3	1
4	A	412	PX4	C11-C10-C9	2.55	104.33	113.69	16	1
4	A	422	PX4	O8-C23-C24	2.56	113.79	123.78	9	1
4	A	330	PX4	C11-C10-C9	2.55	123.05	113.69	18	2
4	A	330	PX4	C13-C12-C11	2.55	101.47	114.37	10	2
4	A	352	PX4	C20-C19-C18	2.55	101.47	114.37	8	2
4	A	366	PX4	C14-C13-C12	2.55	101.46	114.37	12	3
4	A	314	PX4	C34-C33-C32	2.55	101.47	114.37	11	3
4	A	362	PX4	C1-C2-N1	2.55	124.01	115.82	11	3
4	A	369	PX4	C30-C29-C28	2.55	101.48	114.37	16	3
4	A	390	PX4	C5-N1-C3	2.55	102.28	108.98	8	4
4	A	394	PX4	C4-N1-C2	2.55	120.05	109.91	7	2
4	A	400	PX4	O1-P1-O4	2.55	119.13	107.57	4	2
4	A	386	PX4	C4-N1-C2	2.55	120.05	109.91	19	4
4	A	392	PX4	C18-C17-C16	2.55	101.48	114.37	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	407	PX4	O3-C1-C2	2.55	121.92	109.65	4	3
4	A	418	PX4	C28-C27-C26	2.55	101.47	114.37	15	2
4	A	322	PX4	C3-N1-C2	2.55	99.78	109.91	13	2
4	A	349	PX4	C11-C10-C9	2.55	104.35	113.69	4	4
4	A	350	PX4	C30-C29-C28	2.55	101.48	114.37	19	2
4	A	396	PX4	C17-C16-C15	2.55	101.48	114.37	14	2
4	A	410	PX4	O1-P1-O3	2.55	119.12	107.57	5	3
4	A	353	PX4	C34-C33-C32	2.55	101.49	114.37	9	4
4	A	391	PX4	C32-C31-C30	2.55	101.49	114.37	18	2
4	A	410	PX4	C13-C12-C11	2.55	101.49	114.37	3	1
4	A	411	PX4	C16-C15-C14	2.55	101.49	114.37	2	4
4	A	397	PX4	C14-C13-C12	2.55	101.49	114.37	15	2
4	A	399	PX4	C14-C13-C12	2.55	101.50	114.37	14	3
4	A	412	PX4	O1-P1-O3	2.55	96.02	107.57	6	2
4	A	413	PX4	C5-N1-C4	2.55	102.29	108.98	17	2
4	A	413	PX4	O4-P1-O2	2.55	119.03	108.94	12	2
4	A	422	PX4	C8-O5-C9	2.55	107.81	117.12	13	1
4	A	312	PX4	C14-C13-C12	2.55	101.50	114.37	2	2
4	A	317	PX4	O3-P1-O2	2.55	119.03	108.94	17	3
4	A	320	PX4	C33-C32-C31	2.54	101.50	114.37	11	1
4	A	339	PX4	O3-P1-O2	2.55	98.85	108.94	4	4
4	A	344	PX4	C3-N1-C2	2.55	120.03	109.91	10	1
4	A	339	PX4	C4-N1-C3	2.54	102.29	108.98	14	3
4	A	349	PX4	C5-N1-C2	2.54	99.80	109.91	1	3
4	A	427	PX4	C25-C24-C23	2.55	104.37	113.69	2	1
4	A	352	PX4	C16-C15-C14	2.54	101.51	114.37	3	1
4	A	373	PX4	C4-N1-C2	2.54	120.02	109.91	19	2
4	A	418	PX4	C27-C26-C25	2.54	101.51	114.37	16	2
4	A	318	PX4	O3-P1-O2	2.54	119.01	108.94	6	3
4	A	387	PX4	O1-P1-O4	2.54	119.09	107.57	9	4
4	A	332	PX4	C32-C31-C30	2.54	101.52	114.37	6	2
4	A	400	PX4	C3-N1-C2	2.54	120.01	109.91	19	1
4	A	325	PX4	C5-N1-C3	2.54	102.30	108.98	1	4
4	A	331	PX4	C5-N1-C3	2.54	102.31	108.98	1	1
4	A	381	PX4	O8-C23-C24	2.54	113.85	123.78	17	2
4	A	372	PX4	C29-C28-C27	2.54	101.53	114.37	14	3
4	A	382	PX4	C28-C27-C26	2.54	101.53	114.37	15	1
4	A	396	PX4	C5-N1-C4	2.54	102.31	108.98	1	6
4	A	408	PX4	C12-C11-C10	2.54	103.80	113.13	3	1
4	A	417	PX4	C34-C33-C32	2.54	101.53	114.37	15	1
4	A	338	PX4	C13-C12-C11	2.54	101.54	114.37	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	340	PX4	C8-O5-C9	2.54	107.84	117.12	4	2
4	A	344	PX4	C4-N1-C2	2.54	120.00	109.91	19	2
4	A	333	PX4	C15-C14-C13	2.54	101.55	114.37	14	1
4	A	350	PX4	O5-C9-O6	2.54	117.28	123.63	8	2
4	A	389	PX4	C31-C30-C29	2.54	101.54	114.37	18	1
4	A	371	PX4	C33-C32-C31	2.54	101.55	114.37	1	1
4	A	390	PX4	O8-C23-C24	2.54	113.87	123.78	17	1
4	A	317	PX4	O3-C1-C2	2.53	121.84	109.65	3	3
4	A	333	PX4	C30-C29-C28	2.53	101.56	114.37	12	4
4	A	390	PX4	C15-C14-C13	2.53	101.56	114.37	5	2
4	A	319	PX4	C29-C28-C27	2.53	101.57	114.37	15	1
4	A	338	PX4	C18-C17-C16	2.53	101.57	114.37	9	1
4	A	418	PX4	C18-C17-C16	2.53	101.56	114.37	1	4
4	A	325	PX4	C19-C18-C17	2.53	101.57	114.37	11	2
4	A	348	PX4	C26-C25-C24	2.53	103.83	113.13	4	2
4	A	349	PX4	C33-C32-C31	2.53	101.57	114.37	20	2
4	A	362	PX4	C32-C31-C30	2.53	101.57	114.37	15	2
4	A	381	PX4	C28-C27-C26	2.53	101.57	114.37	13	2
4	A	351	PX4	C1-C2-N1	2.53	123.94	115.82	8	2
4	A	379	PX4	C13-C12-C11	2.53	101.58	114.37	17	3
4	A	387	PX4	C30-C29-C28	2.53	101.57	114.37	20	3
4	A	404	PX4	C19-C18-C17	2.53	101.58	114.37	10	2
4	A	412	PX4	C15-C14-C13	2.53	101.58	114.37	17	2
4	A	360	PX4	C25-C24-C23	2.53	104.42	113.69	20	3
4	A	419	PX4	C3-N1-C2	2.53	119.97	109.91	20	1
4	A	329	PX4	O3-C1-C2	2.53	121.82	109.65	16	2
4	A	329	PX4	C32-C31-C30	2.53	101.58	114.37	19	1
4	A	317	PX4	C4-N1-C2	2.53	119.96	109.91	15	2
4	A	357	PX4	C3-N1-C2	2.53	99.86	109.91	7	3
4	A	320	PX4	C5-N1-C2	2.53	99.87	109.91	16	3
4	A	385	PX4	C17-C16-C15	2.53	101.59	114.37	11	1
4	A	389	PX4	C29-C28-C27	2.53	101.59	114.37	9	2
4	A	371	PX4	C11-C10-C9	2.53	104.44	113.69	13	5
4	A	408	PX4	C18-C17-C16	2.53	101.59	114.37	12	1
4	A	357	PX4	C12-C11-C10	2.53	103.85	113.13	2	2
4	A	366	PX4	C20-C19-C18	2.53	101.60	114.37	8	2
4	A	396	PX4	O4-P1-O2	2.53	118.94	108.94	8	3
4	A	373	PX4	C13-C12-C11	2.52	101.61	114.37	1	1
4	A	397	PX4	C13-C12-C11	2.52	101.61	114.37	4	3
4	A	413	PX4	C16-C15-C14	2.52	101.61	114.37	17	2
4	A	350	PX4	C4-N1-C2	2.52	119.94	109.91	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	348	PX4	C18-C17-C16	2.52	101.62	114.37	17	1
4	A	354	PX4	C16-C15-C14	2.52	101.62	114.37	15	3
4	A	390	PX4	C19-C18-C17	2.52	101.61	114.37	20	1
4	A	313	PX4	C17-C16-C15	2.52	101.62	114.37	12	1
4	A	338	PX4	C20-C19-C18	2.52	101.62	114.37	18	2
4	A	371	PX4	C20-C19-C18	2.52	101.62	114.37	8	2
4	A	321	PX4	C19-C18-C17	2.52	101.63	114.37	15	2
4	A	332	PX4	C3-N1-C2	2.52	99.89	109.91	19	1
4	A	357	PX4	C17-C16-C15	2.52	101.63	114.37	2	1
4	A	428	PX4	C20-C19-C18	2.52	101.63	114.37	16	2
4	A	378	PX4	O1-P1-O3	2.52	96.15	107.57	19	2
4	A	307	PX4	C11-C10-C9	2.52	104.47	113.69	1	3
4	A	314	PX4	O1-P1-O3	2.52	118.98	107.57	18	2
4	A	362	PX4	C17-C16-C15	2.52	101.64	114.37	3	1
4	A	323	PX4	C15-C14-C13	2.52	101.65	114.37	18	3
4	A	336	PX4	C25-C24-C23	2.52	122.91	113.69	5	2
4	A	363	PX4	O4-P1-O2	2.52	118.91	108.94	11	4
4	A	363	PX4	C4-N1-C2	2.52	99.91	109.91	13	1
4	A	407	PX4	C11-C10-C9	2.52	104.47	113.69	13	3
4	A	430	PX4	O3-P1-O2	2.52	98.96	108.94	1	1
4	A	395	PX4	O8-C23-C24	2.52	133.62	123.78	7	1
4	A	316	PX4	C28-C27-C26	2.51	101.66	114.37	3	1
4	A	318	PX4	C26-C25-C24	2.51	103.89	113.13	18	2
4	A	340	PX4	C16-C15-C14	2.51	101.66	114.37	14	2
4	A	347	PX4	C15-C14-C13	2.51	101.66	114.37	7	1
4	A	429	PX4	C19-C18-C17	2.51	101.66	114.37	15	2
4	A	343	PX4	C3-N1-C2	2.51	119.89	109.91	14	1
4	A	355	PX4	O1-P1-O3	2.51	96.18	107.57	15	3
4	A	411	PX4	O6-C9-C10	2.51	113.96	123.78	1	2
4	A	412	PX4	C20-C19-C18	2.51	101.67	114.37	20	3
4	A	421	PX4	C16-C15-C14	2.51	101.67	114.37	13	2
4	A	312	PX4	C19-C18-C17	2.51	101.68	114.37	5	2
4	A	356	PX4	O5-C9-O6	2.51	117.35	123.63	10	6
4	A	367	PX4	C25-C24-C23	2.51	104.50	113.69	14	2
4	A	380	PX4	C3-N1-C2	2.51	119.89	109.91	6	1
4	A	406	PX4	O3-P1-O2	2.51	98.99	108.94	9	1
4	A	416	PX4	C25-C24-C23	2.51	104.50	113.69	20	4
4	A	424	PX4	C25-C24-C23	2.51	104.50	113.69	3	2
4	A	375	PX4	C32-C31-C30	2.51	101.69	114.37	4	1
4	A	427	PX4	C27-C26-C25	2.51	101.69	114.37	10	1
4	A	305	PX4	O3-C1-C2	2.51	121.71	109.65	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	406	PX4	C4-N1-C2	2.51	99.94	109.91	15	3
4	A	307	PX4	C14-C13-C12	2.51	101.70	114.37	14	2
4	A	324	PX4	C4-N1-C2	2.51	119.87	109.91	10	1
4	A	327	PX4	C5-N1-C3	2.50	102.40	108.98	17	3
4	A	328	PX4	C4-N1-C2	2.51	99.95	109.91	12	3
4	A	332	PX4	O1-P1-O4	2.51	118.92	107.57	16	4
4	A	353	PX4	C27-C26-C25	2.51	101.70	114.37	18	3
4	A	371	PX4	C14-C13-C12	2.51	101.70	114.37	5	4
4	A	394	PX4	C30-C29-C28	2.51	101.70	114.37	12	2
4	A	423	PX4	C31-C30-C29	2.51	101.70	114.37	3	1
4	A	306	PX4	O1-P1-O3	2.50	96.22	107.57	6	1
4	A	339	PX4	O1-P1-O3	2.50	96.22	107.57	17	1
4	A	337	PX4	C14-C13-C12	2.50	101.72	114.37	15	1
4	A	340	PX4	C19-C18-C17	2.50	101.71	114.37	20	2
4	A	342	PX4	C27-C26-C25	2.50	101.71	114.37	6	1
4	A	344	PX4	C28-C27-C26	2.50	101.71	114.37	19	2
4	A	398	PX4	C27-C26-C25	2.50	101.71	114.37	15	1
4	A	426	PX4	C26-C25-C24	2.50	122.33	113.13	15	2
4	A	392	PX4	C16-C15-C14	2.50	101.72	114.37	17	3
4	A	396	PX4	C12-C11-C10	2.50	103.93	113.13	18	3
4	A	406	PX4	O8-C23-C24	2.50	114.00	123.78	9	1
4	A	422	PX4	O1-P1-O3	2.50	96.23	107.57	18	4
4	A	311	PX4	O8-C23-C24	2.50	114.00	123.78	11	2
4	A	412	PX4	C26-C25-C24	2.50	103.94	113.13	18	3
4	A	420	PX4	C34-C33-C32	2.50	101.73	114.37	3	2
4	A	314	PX4	O4-P1-O2	2.50	99.03	108.94	18	4
4	A	423	PX4	C12-C11-C10	2.50	103.94	113.13	5	2
4	A	429	PX4	C16-C15-C14	2.50	101.73	114.37	15	1
4	A	319	PX4	C1-C2-N1	2.50	123.84	115.82	17	4
4	A	345	PX4	C11-C10-C9	2.50	104.54	113.69	5	2
4	A	325	PX4	C3-N1-C2	2.49	119.83	109.91	6	2
4	A	339	PX4	C16-C15-C14	2.50	101.75	114.37	7	1
4	A	356	PX4	C33-C32-C31	2.50	101.75	114.37	13	3
4	A	415	PX4	C13-C12-C11	2.50	101.75	114.37	11	3
4	A	356	PX4	C19-C18-C17	2.49	101.76	114.37	20	1
4	A	383	PX4	C26-C25-C24	2.49	103.96	113.13	7	1
4	A	352	PX4	C28-C27-C26	2.49	101.77	114.37	8	1
4	A	379	PX4	C26-C25-C24	2.49	103.97	113.13	4	1
4	A	329	PX4	C15-C14-C13	2.49	101.78	114.37	19	2
4	A	355	PX4	C32-C31-C30	2.49	101.78	114.37	14	4
4	A	357	PX4	C15-C14-C13	2.49	101.77	114.37	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	O5-C9-C10	2.49	119.44	111.83	1	5
4	A	366	PX4	O1-P1-O3	2.49	96.27	107.57	6	3
4	A	329	PX4	O1-P1-O3	2.49	118.85	107.57	15	3
4	A	353	PX4	C28-C27-C26	2.49	101.78	114.37	16	2
4	A	366	PX4	C13-C12-C11	2.49	101.78	114.37	2	2
4	A	372	PX4	C3-N1-C2	2.49	119.81	109.91	19	2
4	A	374	PX4	O3-P1-O2	2.49	99.06	108.94	11	3
4	A	385	PX4	C25-C24-C23	2.49	104.57	113.69	17	1
4	A	387	PX4	C4-N1-C2	2.49	119.81	109.91	18	2
4	A	311	PX4	C32-C31-C30	2.49	101.80	114.37	10	3
4	A	312	PX4	C15-C14-C13	2.49	101.80	114.37	2	5
4	A	327	PX4	C11-C10-C9	2.49	104.58	113.69	10	1
4	A	389	PX4	O5-C9-C10	2.49	119.42	111.83	11	5
4	A	308	PX4	C30-C29-C28	2.48	101.81	114.37	7	2
4	A	330	PX4	C19-C18-C17	2.49	101.80	114.37	9	3
4	A	348	PX4	C33-C32-C31	2.49	101.80	114.37	7	4
4	A	355	PX4	C4-N1-C2	2.48	119.79	109.91	2	3
4	A	359	PX4	C5-N1-C3	2.49	115.50	108.98	7	2
4	A	427	PX4	C16-C15-C14	2.49	101.80	114.37	7	3
4	A	324	PX4	C16-C15-C14	2.48	101.81	114.37	1	4
4	A	346	PX4	C18-C17-C16	2.48	101.81	114.37	4	2
4	A	405	PX4	C28-C27-C26	2.48	101.81	114.37	9	1
4	A	315	PX4	C28-C27-C26	2.48	101.82	114.37	14	1
4	A	326	PX4	O8-C23-C24	2.48	114.07	123.78	11	2
4	A	408	PX4	C8-O5-C9	2.48	108.04	117.12	1	2
4	A	336	PX4	C28-C27-C26	2.48	101.82	114.37	1	1
4	A	349	PX4	O8-C23-C24	2.48	114.07	123.78	9	1
4	A	408	PX4	O4-P1-O2	2.48	99.10	108.94	19	1
4	A	410	PX4	C8-O5-C9	2.48	126.19	117.12	8	1
4	A	329	PX4	C5-N1-C2	2.48	119.77	109.91	5	1
4	A	406	PX4	O6-C9-C10	2.48	114.08	123.78	17	1
4	A	428	PX4	C4-N1-C2	2.48	100.05	109.91	4	2
4	A	402	PX4	C25-C24-C23	2.48	104.61	113.69	16	3
4	A	307	PX4	C5-N1-C3	2.48	102.47	108.98	4	5
4	A	341	PX4	C14-C13-C12	2.48	101.85	114.37	13	2
4	A	352	PX4	C25-C24-C23	2.48	122.77	113.69	5	3
4	A	363	PX4	C34-C33-C32	2.48	101.84	114.37	12	2
4	A	372	PX4	C15-C14-C13	2.48	101.84	114.37	1	2
4	A	374	PX4	O8-C23-C24	2.48	114.09	123.78	9	1
4	A	376	PX4	C30-C29-C28	2.48	101.85	114.37	20	1
4	A	385	PX4	C8-O5-C9	2.48	108.06	117.12	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	389	PX4	C17-C16-C15	2.48	101.84	114.37	20	2
4	A	398	PX4	C19-C18-C17	2.48	101.85	114.37	2	2
4	A	417	PX4	C15-C14-C13	2.48	101.84	114.37	11	3
4	A	375	PX4	C13-C12-C11	2.48	101.86	114.37	2	3
4	A	400	PX4	C29-C28-C27	2.48	101.85	114.37	14	2
4	A	316	PX4	C11-C10-C9	2.47	104.63	113.69	13	3
4	A	320	PX4	C34-C33-C32	2.47	101.86	114.37	1	1
4	A	322	PX4	C31-C30-C29	2.47	101.86	114.37	15	1
4	A	364	PX4	C12-C11-C10	2.47	104.04	113.13	9	1
4	A	341	PX4	C15-C14-C13	2.47	101.87	114.37	14	2
4	A	369	PX4	O1-P1-O3	2.47	96.35	107.57	7	2
4	A	416	PX4	O3-P1-O2	2.47	99.13	108.94	20	3
4	A	424	PX4	C5-N1-C2	2.47	119.75	109.91	7	3
4	A	329	PX4	C34-C33-C32	2.47	101.87	114.37	15	5
4	A	336	PX4	C20-C19-C18	2.47	101.87	114.37	6	2
5	A	432	C3S	C57-C54-C48	2.47	121.99	115.08	16	2
4	A	337	PX4	O1-P1-O4	2.47	118.77	107.57	18	2
4	A	368	PX4	C18-C17-C16	2.47	101.88	114.37	12	2
4	A	374	PX4	C16-C15-C14	2.47	101.87	114.37	3	2
4	A	378	PX4	C3-N1-C2	2.47	100.09	109.91	8	1
4	A	305	PX4	C4-N1-C2	2.47	119.72	109.91	15	2
4	A	307	PX4	C12-C11-C10	2.47	104.05	113.13	8	2
4	A	384	PX4	C13-C12-C11	2.47	101.88	114.37	7	3
4	A	430	PX4	C33-C32-C31	2.47	101.89	114.37	11	2
4	A	326	PX4	C34-C33-C32	2.47	101.89	114.37	17	1
4	A	351	PX4	C27-C26-C25	2.47	101.89	114.37	5	2
4	A	305	PX4	C31-C30-C29	2.47	101.90	114.37	3	1
4	A	355	PX4	C5-N1-C2	2.47	119.72	109.91	6	2
4	A	362	PX4	C12-C11-C10	2.47	104.06	113.13	17	3
4	A	378	PX4	O3-C1-C2	2.47	121.53	109.65	19	2
4	A	397	PX4	C20-C19-C18	2.47	101.90	114.37	13	2
4	A	404	PX4	C26-C25-C24	2.47	104.06	113.13	20	2
4	A	427	PX4	C15-C14-C13	2.47	101.90	114.37	8	1
4	A	321	PX4	C15-C14-C13	2.47	101.91	114.37	11	4
4	A	339	PX4	C30-C29-C28	2.47	101.91	114.37	8	1
4	A	394	PX4	C32-C31-C30	2.46	101.91	114.37	2	1
4	A	400	PX4	C18-C17-C16	2.47	101.91	114.37	7	1
4	A	407	PX4	C27-C26-C25	2.47	101.91	114.37	14	1
4	A	305	PX4	O4-P1-O2	2.46	118.70	108.94	3	1
4	A	306	PX4	O7-C23-O8	2.46	117.95	123.70	14	1
4	A	309	PX4	C8-O5-C9	2.46	108.11	117.12	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	C4-N1-C2	2.46	119.70	109.91	18	2
4	A	349	PX4	C28-C27-C26	2.46	101.92	114.37	18	2
4	A	355	PX4	C8-O5-C9	2.46	108.11	117.12	15	3
4	A	382	PX4	O3-C1-C2	2.46	121.50	109.65	3	3
4	A	386	PX4	C15-C14-C13	2.46	101.92	114.37	5	2
4	A	392	PX4	C34-C33-C32	2.46	101.93	114.37	7	2
4	A	402	PX4	C17-C16-C15	2.46	101.92	114.37	8	1
5	A	434	C3S	C15-C18-C30	2.46	114.42	110.93	17	4
4	A	315	PX4	C16-C15-C14	2.46	101.93	114.37	11	2
4	A	355	PX4	C33-C32-C31	2.46	101.93	114.37	8	1
4	A	388	PX4	C25-C24-C23	2.46	104.68	113.69	1	1
4	A	423	PX4	C3-N1-C2	2.46	119.69	109.91	14	1
4	A	426	PX4	O8-C23-C24	2.46	114.16	123.78	18	3
4	A	319	PX4	O6-C9-C10	2.46	114.16	123.78	20	1
4	A	322	PX4	O3-C1-C2	2.46	121.48	109.65	15	4
4	A	328	PX4	C28-C27-C26	2.46	101.93	114.37	1	3
4	A	312	PX4	C30-C29-C28	2.46	101.94	114.37	9	2
4	A	347	PX4	C14-C13-C12	2.46	101.94	114.37	16	1
4	A	425	PX4	C20-C19-C18	2.46	101.93	114.37	16	2
4	A	429	PX4	C28-C27-C26	2.46	101.93	114.37	19	1
4	A	327	PX4	C27-C26-C25	2.46	101.94	114.37	12	3
4	A	317	PX4	C16-C15-C14	2.46	101.95	114.37	18	2
4	A	323	PX4	C19-C18-C17	2.46	101.95	114.37	16	2
4	A	343	PX4	C29-C28-C27	2.46	101.95	114.37	9	2
4	A	374	PX4	C28-C27-C26	2.46	101.95	114.37	1	1
4	A	381	PX4	O1-P1-O3	2.46	96.43	107.57	2	3
4	A	390	PX4	C4-N1-C2	2.46	100.14	109.91	9	2
4	A	415	PX4	C19-C18-C17	2.46	101.95	114.37	14	3
4	A	427	PX4	O1-P1-O3	2.46	96.43	107.57	11	3
4	A	315	PX4	C32-C31-C30	2.45	101.96	114.37	20	3
4	A	330	PX4	O6-C9-C10	2.46	114.18	123.78	8	1
4	A	423	PX4	C5-N1-C2	2.46	119.67	109.91	12	2
4	A	423	PX4	C16-C15-C14	2.45	101.96	114.37	19	3
4	A	425	PX4	C4-N1-C2	2.46	119.67	109.91	5	3
4	A	328	PX4	C15-C14-C13	2.45	101.97	114.37	5	2
4	A	342	PX4	C3-N1-C2	2.45	119.66	109.91	16	3
4	A	356	PX4	O3-C1-C2	2.45	121.45	109.65	10	2
4	A	362	PX4	O4-P1-O2	2.45	99.21	108.94	2	3
4	A	362	PX4	C13-C12-C11	2.45	101.97	114.37	10	1
4	A	311	PX4	C20-C19-C18	2.45	101.98	114.37	19	3
4	A	328	PX4	C26-C25-C24	2.45	104.12	113.13	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	332	PX4	C29-C28-C27	2.45	101.98	114.37	20	3
4	A	333	PX4	C33-C32-C31	2.45	101.98	114.37	15	1
4	A	338	PX4	C4-N1-C2	2.45	119.65	109.91	7	3
4	A	362	PX4	C33-C32-C31	2.45	101.98	114.37	9	3
4	A	385	PX4	C14-C13-C12	2.45	126.77	114.37	10	3
4	A	377	PX4	C16-C15-C14	2.45	101.98	114.37	6	1
4	A	406	PX4	C16-C15-C14	2.45	101.97	114.37	4	3
4	A	409	PX4	C19-C18-C17	2.45	101.97	114.37	9	4
4	A	338	PX4	C11-C10-C9	2.45	122.67	113.69	18	2
4	A	310	PX4	C28-C27-C26	2.45	101.99	114.37	10	1
4	A	338	PX4	C28-C27-C26	2.45	101.99	114.37	15	2
4	A	368	PX4	C26-C25-C24	2.45	104.13	113.13	16	3
4	A	323	PX4	C16-C15-C14	2.45	102.00	114.37	19	3
4	A	332	PX4	C5-N1-C2	2.45	119.64	109.91	19	2
4	A	383	PX4	C14-C13-C12	2.45	102.00	114.37	13	1
4	A	411	PX4	C19-C18-C17	2.45	101.99	114.37	8	4
4	A	421	PX4	O1-P1-O3	2.45	96.47	107.57	18	4
4	A	419	PX4	C30-C29-C28	2.45	102.00	114.37	7	4
4	A	309	PX4	C31-C30-C29	2.44	102.01	114.37	8	1
4	A	346	PX4	O1-P1-O4	2.44	118.65	107.57	5	3
4	A	373	PX4	O3-C1-C2	2.44	121.41	109.65	3	2
4	A	378	PX4	C4-N1-C2	2.44	119.63	109.91	9	3
4	A	379	PX4	C19-C18-C17	2.44	102.01	114.37	5	1
4	A	387	PX4	C20-C19-C18	2.44	102.01	114.37	2	2
4	A	306	PX4	O3-P1-O2	2.44	118.62	108.94	13	1
4	A	320	PX4	C29-C28-C27	2.44	102.02	114.37	20	3
4	A	333	PX4	C3-N1-C2	2.44	119.62	109.91	14	1
4	A	377	PX4	C36-C35-C34	2.44	96.87	113.36	12	1
4	A	307	PX4	C13-C12-C11	2.44	102.03	114.37	7	1
4	A	329	PX4	O5-C9-C10	2.44	119.28	111.83	2	3
4	A	340	PX4	O8-C23-C24	2.44	114.23	123.78	16	3
4	A	350	PX4	C27-C26-C25	2.44	102.03	114.37	10	1
4	A	364	PX4	C13-C12-C11	2.44	102.03	114.37	20	3
4	A	364	PX4	C31-C30-C29	2.44	102.03	114.37	5	2
4	A	370	PX4	C29-C28-C27	2.44	102.03	114.37	7	4
4	A	423	PX4	C30-C29-C28	2.44	102.03	114.37	12	2
4	A	427	PX4	C12-C11-C10	2.44	104.16	113.13	18	1
4	A	395	PX4	C5-N1-C2	2.44	119.61	109.91	12	3
4	A	360	PX4	C14-C13-C12	2.44	102.05	114.37	8	1
4	A	389	PX4	C13-C12-C11	2.44	102.05	114.37	17	1
4	A	390	PX4	C20-C19-C18	2.44	102.05	114.37	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	329	PX4	C14-C13-C12	2.44	102.05	114.37	13	2
4	A	334	PX4	C20-C19-C18	2.44	102.05	114.37	7	2
4	A	358	PX4	C4-N1-C2	2.44	119.59	109.91	14	2
4	A	417	PX4	C30-C29-C28	2.44	102.05	114.37	6	4
4	A	316	PX4	O6-C9-C10	2.44	114.26	123.78	1	1
4	A	323	PX4	O5-C9-O6	2.43	117.54	123.63	18	7
4	A	360	PX4	C31-C30-C29	2.44	102.06	114.37	15	2
4	A	383	PX4	C19-C18-C17	2.44	102.06	114.37	10	2
4	A	394	PX4	C19-C18-C17	2.44	102.06	114.37	2	1
4	A	353	PX4	O6-C9-C10	2.43	114.26	123.78	18	2
4	A	310	PX4	C13-C12-C11	2.43	102.07	114.37	3	3
4	A	337	PX4	C16-C15-C14	2.43	102.07	114.37	18	1
4	A	357	PX4	C19-C18-C17	2.43	102.07	114.37	6	3
4	A	370	PX4	C14-C13-C12	2.43	102.06	114.37	11	1
4	A	371	PX4	C12-C11-C10	2.43	104.18	113.13	14	1
4	A	411	PX4	O4-P1-O2	2.43	118.58	108.94	11	2
4	A	414	PX4	C14-C13-C12	2.43	102.06	114.37	18	2
4	A	428	PX4	C18-C17-C16	2.43	102.07	114.37	20	1
4	A	309	PX4	C29-C28-C27	2.43	102.08	114.37	7	2
4	A	315	PX4	C33-C32-C31	2.43	102.08	114.37	15	2
4	A	326	PX4	C4-N1-C2	2.43	119.58	109.91	2	2
4	A	358	PX4	C20-C19-C18	2.43	102.08	114.37	12	2
4	A	388	PX4	C8-O5-C9	2.43	108.23	117.12	7	4
4	A	396	PX4	O1-P1-O4	2.43	118.59	107.57	1	1
4	A	323	PX4	C5-N1-C2	2.43	119.57	109.91	14	2
4	A	330	PX4	C27-C26-C25	2.43	102.08	114.37	13	1
4	A	425	PX4	C32-C31-C30	2.43	102.08	114.37	2	2
4	A	354	PX4	O5-C9-O6	2.43	117.55	123.63	8	5
4	A	359	PX4	C16-C15-C14	2.43	102.09	114.37	9	2
4	A	380	PX4	C17-C16-C15	2.43	102.09	114.37	6	2
4	A	381	PX4	C17-C16-C15	2.43	102.09	114.37	12	2
4	A	393	PX4	C32-C31-C30	2.43	102.09	114.37	8	4
4	A	402	PX4	C28-C27-C26	2.43	102.09	114.37	20	2
4	A	414	PX4	C27-C26-C25	2.43	102.09	114.37	9	2
4	A	337	PX4	C4-N1-C2	2.43	119.56	109.91	11	1
4	A	368	PX4	C8-O5-C9	2.43	108.24	117.12	18	1
4	A	427	PX4	C26-C25-C24	2.43	104.20	113.13	18	2
4	A	316	PX4	C31-C30-C29	2.43	102.11	114.37	19	1
4	A	317	PX4	C5-N1-C3	2.43	102.60	108.98	18	4
4	A	330	PX4	O3-C1-C2	2.43	121.32	109.65	17	1
4	A	356	PX4	C15-C14-C13	2.43	102.11	114.37	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	357	PX4	C20-C19-C18	2.43	102.11	114.37	18	3
4	A	404	PX4	O3-C1-C2	2.43	121.33	109.65	4	3
4	A	410	PX4	C27-C26-C25	2.43	102.10	114.37	5	2
4	A	414	PX4	C29-C28-C27	2.43	102.10	114.37	11	1
4	A	421	PX4	C33-C32-C31	2.43	102.10	114.37	17	2
4	A	422	PX4	C13-C12-C11	2.43	102.11	114.37	12	1
4	A	328	PX4	O6-C9-C10	2.42	114.30	123.78	1	1
4	A	396	PX4	C31-C30-C29	2.42	102.11	114.37	1	3
4	A	318	PX4	O8-C23-C24	2.42	114.31	123.78	2	2
4	A	400	PX4	C27-C26-C25	2.42	102.12	114.37	9	1
4	A	356	PX4	C4-N1-C2	2.42	119.54	109.91	5	2
4	A	405	PX4	O6-C9-C10	2.42	114.31	123.78	11	2
4	A	405	PX4	C18-C17-C16	2.42	102.13	114.37	7	2
4	A	409	PX4	C30-C29-C28	2.42	102.14	114.37	11	2
4	A	413	PX4	C17-C16-C15	2.42	102.13	114.37	17	4
4	A	345	PX4	C4-N1-C2	2.42	119.53	109.91	6	2
4	A	314	PX4	C18-C17-C16	2.42	102.14	114.37	20	3
4	A	324	PX4	C8-O5-C9	2.42	108.28	117.12	17	4
4	A	336	PX4	C31-C30-C29	2.42	102.14	114.37	12	2
4	A	337	PX4	C27-C26-C25	2.42	102.14	114.37	1	2
4	A	352	PX4	O3-C1-C2	2.42	121.29	109.65	17	2
4	A	418	PX4	C34-C33-C32	2.42	102.14	114.37	4	1
4	A	419	PX4	O4-P1-O2	2.42	118.53	108.94	10	4
4	A	356	PX4	C27-C26-C25	2.42	102.15	114.37	15	1
4	A	357	PX4	O3-C1-C2	2.42	121.28	109.65	14	3
4	A	390	PX4	C13-C12-C11	2.42	102.14	114.37	16	1
4	A	328	PX4	C13-C12-C11	2.42	102.16	114.37	10	2
4	A	338	PX4	O1-P1-O4	2.42	118.52	107.57	6	1
4	A	340	PX4	C15-C14-C13	2.42	102.15	114.37	17	3
4	A	355	PX4	C16-C15-C14	2.42	102.16	114.37	11	3
4	A	355	PX4	C14-C13-C12	2.42	102.16	114.37	4	1
4	A	377	PX4	O3-C1-C2	2.42	121.28	109.65	17	2
4	A	405	PX4	O8-C23-C24	2.41	114.35	123.78	17	1
4	A	424	PX4	C28-C27-C26	2.41	102.17	114.37	4	1
4	A	419	PX4	C18-C17-C16	2.41	102.18	114.37	13	3
4	A	430	PX4	C25-C24-C23	2.41	104.86	113.69	18	2
4	A	320	PX4	C31-C30-C29	2.41	102.19	114.37	9	1
4	A	388	PX4	C11-C10-C9	2.41	104.86	113.69	15	3
4	A	417	PX4	C17-C16-C15	2.41	102.19	114.37	17	2
4	A	321	PX4	C13-C12-C11	2.41	102.20	114.37	16	3
4	A	356	PX4	C17-C16-C15	2.41	102.19	114.37	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	383	PX4	C12-C11-C10	2.41	104.28	113.13	18	2
4	A	396	PX4	C32-C31-C30	2.41	102.19	114.37	12	1
4	A	423	PX4	C13-C12-C11	2.41	102.20	114.37	6	4
4	A	313	PX4	C18-C17-C16	2.41	102.21	114.37	8	1
4	A	329	PX4	C30-C29-C28	2.41	102.21	114.37	11	2
4	A	331	PX4	O1-P1-O4	2.41	118.47	107.57	12	1
4	A	354	PX4	C4-N1-C2	2.41	119.47	109.91	13	1
4	A	363	PX4	C18-C17-C16	2.41	102.20	114.37	19	1
4	A	369	PX4	C28-C27-C26	2.41	102.20	114.37	15	1
4	A	378	PX4	O8-C23-C24	2.41	114.37	123.78	10	2
4	A	411	PX4	C15-C14-C13	2.41	102.20	114.37	9	2
4	A	407	PX4	C20-C19-C18	2.40	102.21	114.37	7	1
4	A	413	PX4	O1-P1-O3	2.41	96.67	107.57	14	3
4	A	430	PX4	O1-P1-O4	2.41	118.47	107.57	2	3
4	A	344	PX4	C5-N1-C2	2.40	119.47	109.91	12	3
4	A	349	PX4	C34-C33-C32	2.40	102.22	114.37	14	1
4	A	309	PX4	O3-C1-C2	2.40	121.21	109.65	6	3
4	A	315	PX4	C27-C26-C25	2.40	102.22	114.37	14	2
4	A	327	PX4	C5-N1-C2	2.40	119.46	109.91	7	1
4	A	353	PX4	C3-N1-C2	2.40	100.36	109.91	4	1
4	A	356	PX4	C16-C15-C14	2.40	102.22	114.37	2	4
4	A	344	PX4	C12-C11-C10	2.40	104.31	113.13	2	2
4	A	312	PX4	C27-C26-C25	2.40	102.24	114.37	15	2
4	A	327	PX4	O1-P1-O4	2.40	118.44	107.57	7	2
4	A	328	PX4	O4-P1-O2	2.40	118.45	108.94	10	1
4	A	394	PX4	C8-O5-C9	2.40	108.34	117.12	13	4
4	A	403	PX4	C4-N1-C2	2.40	100.37	109.91	14	2
4	A	405	PX4	C4-N1-C2	2.40	100.37	109.91	2	2
4	A	414	PX4	O6-C9-C10	2.40	114.39	123.78	2	1
4	A	330	PX4	C14-C13-C12	2.40	102.25	114.37	6	2
4	A	337	PX4	C17-C16-C15	2.40	102.24	114.37	20	1
4	A	405	PX4	C32-C31-C30	2.40	102.24	114.37	9	1
4	A	412	PX4	C16-C15-C14	2.40	102.24	114.37	8	1
4	A	422	PX4	C31-C30-C29	2.40	102.24	114.37	20	4
4	A	338	PX4	C5-N1-C2	2.40	100.38	109.91	9	1
4	A	344	PX4	C25-C24-C23	2.40	104.91	113.69	18	3
4	A	346	PX4	C15-C14-C13	2.40	102.25	114.37	5	2
4	A	327	PX4	C26-C25-C24	2.40	104.33	113.13	15	3
4	A	355	PX4	C19-C18-C17	2.40	102.26	114.37	7	3
4	A	360	PX4	C8-O5-C9	2.40	108.36	117.12	3	3
4	A	377	PX4	C34-C33-C32	2.40	102.25	114.37	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PX4	C3-N1-C2	2.40	119.44	109.91	20	1
4	A	351	PX4	C33-C32-C31	2.39	102.26	114.37	13	1
4	A	358	PX4	O6-C9-C10	2.40	114.41	123.78	19	1
4	A	412	PX4	C25-C24-C23	2.40	104.92	113.69	19	4
4	A	418	PX4	O1-P1-O3	2.39	96.71	107.57	2	3
4	A	418	PX4	C3-N1-C2	2.40	100.39	109.91	11	4
4	A	419	PX4	C31-C30-C29	2.40	102.26	114.37	1	2
4	A	311	PX4	O3-C1-C2	2.39	121.17	109.65	13	3
4	A	332	PX4	C20-C19-C18	2.39	102.27	114.37	13	3
4	A	357	PX4	C18-C17-C16	2.39	102.27	114.37	19	1
4	A	320	PX4	C13-C12-C11	2.39	102.27	114.37	10	3
4	A	328	PX4	C22-C21-C20	2.39	97.20	113.36	4	1
4	A	360	PX4	O8-C23-C24	2.39	114.42	123.78	11	2
4	A	365	PX4	C4-N1-C2	2.39	119.42	109.91	20	1
4	A	328	PX4	C29-C28-C27	2.39	102.28	114.37	19	2
4	A	331	PX4	C18-C17-C16	2.39	102.27	114.37	5	2
4	A	373	PX4	C14-C13-C12	2.39	102.27	114.37	1	2
4	A	378	PX4	C33-C32-C31	2.39	102.27	114.37	5	3
4	A	415	PX4	C4-N1-C2	2.39	119.42	109.91	18	1
4	A	378	PX4	C17-C16-C15	2.39	102.28	114.37	2	1
4	A	396	PX4	C11-C10-C9	2.39	122.46	113.69	2	3
4	A	322	PX4	C13-C12-C11	2.39	102.29	114.37	5	2
4	A	350	PX4	C13-C12-C11	2.39	102.29	114.37	18	2
4	A	356	PX4	C28-C27-C26	2.39	102.29	114.37	3	2
4	A	357	PX4	C13-C12-C11	2.39	102.29	114.37	9	1
4	A	381	PX4	C36-C35-C34	2.39	97.22	113.36	1	1
4	A	394	PX4	C4-N1-C3	2.39	102.70	108.98	19	3
4	A	402	PX4	O8-C23-C24	2.39	114.44	123.78	17	2
4	A	403	PX4	C34-C33-C32	2.39	102.29	114.37	13	2
4	A	425	PX4	C27-C26-C25	2.39	102.29	114.37	8	2
4	A	426	PX4	O6-C9-C10	2.39	114.43	123.78	7	1
4	A	316	PX4	C30-C29-C28	2.39	102.31	114.37	10	2
4	A	342	PX4	O4-P1-O2	2.39	118.39	108.94	1	2
4	A	344	PX4	O3-C1-C2	2.39	121.14	109.65	19	1
4	A	417	PX4	C5-N1-C2	2.39	119.40	109.91	10	2
4	A	383	PX4	C3-N1-C2	2.39	119.40	109.91	16	2
4	A	426	PX4	C15-C14-C13	2.39	102.30	114.37	18	1
4	A	329	PX4	C26-C25-C24	2.39	104.36	113.13	1	1
4	A	365	PX4	C15-C14-C13	2.39	102.31	114.37	7	2
4	A	384	PX4	C8-O5-C9	2.39	108.40	117.12	11	4
4	A	430	PX4	C19-C18-C17	2.39	102.30	114.37	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	343	PX4	C27-C26-C25	2.39	102.31	114.37	8	3
4	A	346	PX4	C30-C29-C28	2.38	102.31	114.37	7	4
4	A	348	PX4	C19-C18-C17	2.38	102.31	114.37	11	1
4	A	356	PX4	C5-N1-C2	2.39	119.39	109.91	11	2
4	A	361	PX4	C20-C19-C18	2.38	102.31	114.37	14	2
4	A	397	PX4	C31-C30-C29	2.38	102.31	114.37	16	1
4	A	407	PX4	C31-C30-C29	2.39	102.31	114.37	1	1
4	A	411	PX4	C5-N1-C2	2.38	100.43	109.91	19	2
4	A	412	PX4	C33-C32-C31	2.38	102.31	114.37	12	1
4	A	335	PX4	C27-C26-C25	2.38	102.32	114.37	14	2
4	A	345	PX4	C14-C13-C12	2.38	102.32	114.37	18	2
4	A	347	PX4	C30-C29-C28	2.38	102.32	114.37	15	2
4	A	413	PX4	O1-P1-O4	2.38	118.37	107.57	6	1
4	A	396	PX4	C27-C26-C25	2.38	102.33	114.37	16	1
4	A	423	PX4	C4-N1-C2	2.38	100.44	109.91	8	1
4	A	316	PX4	C14-C13-C12	2.38	102.33	114.37	6	1
4	A	324	PX4	O1-P1-O3	2.38	118.36	107.57	1	3
4	A	312	PX4	O6-C9-C10	2.38	114.47	123.78	4	2
4	A	340	PX4	C33-C32-C31	2.38	102.33	114.37	16	3
4	A	348	PX4	C4-N1-C2	2.38	100.44	109.91	19	1
4	A	361	PX4	C28-C27-C26	2.38	102.33	114.37	10	2
4	A	367	PX4	C28-C27-C26	2.38	102.33	114.37	17	1
4	A	375	PX4	C27-C26-C25	2.38	102.34	114.37	9	1
4	A	392	PX4	O3-C1-C2	2.38	121.10	109.65	5	2
4	A	401	PX4	C28-C27-C26	2.38	102.34	114.37	8	1
4	A	413	PX4	C3-N1-C2	2.38	100.45	109.91	6	2
4	A	316	PX4	C12-C11-C10	2.38	121.87	113.13	2	2
4	A	321	PX4	O6-C9-C10	2.38	114.48	123.78	19	2
4	A	339	PX4	C5-N1-C3	2.38	102.73	108.98	1	3
4	A	364	PX4	C4-N1-C3	2.38	102.73	108.98	16	2
4	A	309	PX4	C19-C18-C17	2.38	102.35	114.37	6	4
4	A	328	PX4	C5-N1-C2	2.38	119.36	109.91	9	2
4	A	334	PX4	C11-C10-C9	2.38	104.98	113.69	6	2
4	A	357	PX4	C25-C24-C23	2.38	104.98	113.69	19	1
4	A	360	PX4	C15-C14-C13	2.38	102.35	114.37	12	1
4	A	384	PX4	C32-C31-C30	2.38	102.35	114.37	6	3
4	A	400	PX4	C5-N1-C2	2.38	119.36	109.91	1	1
4	A	368	PX4	C11-C10-C9	2.38	122.40	113.69	5	2
4	A	376	PX4	C31-C30-C29	2.38	102.36	114.37	14	4
4	A	386	PX4	C18-C17-C16	2.38	102.36	114.37	13	2
4	A	407	PX4	C12-C11-C10	2.38	104.40	113.13	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	410	PX4	C19-C18-C17	2.37	102.37	114.37	13	1
4	A	415	PX4	C32-C31-C30	2.37	102.37	114.37	12	2
4	A	419	PX4	C4-N1-C2	2.37	119.35	109.91	7	3
4	A	430	PX4	C12-C11-C10	2.37	104.40	113.13	11	2
4	A	307	PX4	O1-P1-O4	2.37	118.32	107.57	12	2
4	A	330	PX4	C20-C19-C18	2.37	102.38	114.37	20	2
4	A	376	PX4	C8-O5-C9	2.37	125.79	117.12	3	1
4	A	379	PX4	C29-C28-C27	2.37	102.38	114.37	12	1
4	A	393	PX4	C30-C29-C28	2.37	102.37	114.37	16	2
4	A	398	PX4	C29-C28-C27	2.37	102.38	114.37	18	2
4	A	365	PX4	C28-C27-C26	2.37	102.38	114.37	9	2
4	A	379	PX4	O1-P1-O3	2.37	118.31	107.57	4	4
4	A	370	PX4	C34-C33-C32	2.37	102.39	114.37	15	1
4	A	360	PX4	C22-C21-C20	2.37	97.37	113.36	4	1
4	A	365	PX4	C13-C12-C11	2.37	102.40	114.37	12	1
4	A	374	PX4	C29-C28-C27	2.37	102.40	114.37	16	2
4	A	393	PX4	C29-C28-C27	2.37	102.40	114.37	13	2
4	A	344	PX4	C8-O5-C9	2.37	108.47	117.12	12	1
4	A	401	PX4	C4-N1-C2	2.37	119.32	109.91	6	2
4	A	405	PX4	C29-C28-C27	2.37	102.40	114.37	11	1
4	A	405	PX4	C34-C33-C32	2.37	102.40	114.37	15	2
4	A	406	PX4	C29-C28-C27	2.37	102.41	114.37	6	2
4	A	413	PX4	C13-C12-C11	2.37	102.41	114.37	6	3
4	A	333	PX4	C28-C27-C26	2.37	102.41	114.37	16	1
4	A	349	PX4	C15-C14-C13	2.37	102.41	114.37	13	1
4	A	382	PX4	C31-C30-C29	2.36	102.42	114.37	19	1
4	A	390	PX4	C18-C17-C16	2.37	102.41	114.37	16	1
4	A	413	PX4	C15-C14-C13	2.37	102.41	114.37	5	1
4	A	393	PX4	C15-C14-C13	2.36	102.42	114.37	7	1
4	A	415	PX4	C18-C17-C16	2.37	102.41	114.37	13	1
4	A	321	PX4	C20-C19-C18	2.36	102.42	114.37	9	1
4	A	352	PX4	C34-C33-C32	2.36	102.42	114.37	5	3
4	A	358	PX4	C33-C32-C31	2.36	102.42	114.37	20	1
4	A	421	PX4	C17-C16-C15	2.36	102.42	114.37	1	1
4	A	340	PX4	C5-N1-C4	2.36	102.77	108.98	14	1
4	A	359	PX4	C20-C19-C18	2.36	102.42	114.37	5	1
4	A	409	PX4	C32-C31-C30	2.36	102.43	114.37	2	1
4	A	420	PX4	C31-C30-C29	2.36	102.42	114.37	10	2
4	A	421	PX4	C31-C30-C29	2.36	102.42	114.37	17	2
4	A	336	PX4	C21-C20-C19	2.36	94.54	115.25	14	1
4	A	399	PX4	O6-C9-C10	2.36	114.54	123.78	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	416	PX4	C18-C17-C16	2.36	102.43	114.37	4	2
4	A	420	PX4	C15-C14-C13	2.36	102.44	114.37	12	1
4	A	353	PX4	O1-P1-O4	2.36	118.26	107.57	4	1
4	A	363	PX4	C11-C10-C9	2.36	105.05	113.69	2	3
4	A	378	PX4	C25-C24-C23	2.36	105.05	113.69	9	2
4	A	403	PX4	O1-P1-O3	2.36	96.88	107.57	15	3
4	A	405	PX4	C16-C15-C14	2.36	102.44	114.37	20	1
4	A	414	PX4	C15-C14-C13	2.36	102.44	114.37	20	3
4	A	417	PX4	O4-P1-O2	2.36	118.28	108.94	5	1
4	A	365	PX4	C32-C31-C30	2.36	102.45	114.37	13	3
4	A	422	PX4	C5-N1-C2	2.36	100.54	109.91	16	1
4	A	387	PX4	C33-C32-C31	2.36	102.45	114.37	5	1
4	A	402	PX4	C11-C10-C9	2.36	105.06	113.69	4	1
4	A	354	PX4	O3-P1-O2	2.36	99.60	108.94	2	3
4	A	331	PX4	C27-C26-C25	2.35	102.47	114.37	8	3
4	A	336	PX4	C29-C28-C27	2.36	102.46	114.37	2	5
4	A	376	PX4	C29-C28-C27	2.36	102.46	114.37	10	3
4	A	388	PX4	C13-C12-C11	2.35	102.47	114.37	20	1
4	A	399	PX4	C20-C19-C18	2.36	102.46	114.37	8	2
4	A	400	PX4	C31-C30-C29	2.36	102.46	114.37	8	1
4	A	362	PX4	C26-C25-C24	2.35	104.48	113.13	5	1
4	A	382	PX4	C5-N1-C2	2.35	100.55	109.91	14	3
4	A	384	PX4	C18-C17-C16	2.35	102.47	114.37	8	1
4	A	403	PX4	C31-C30-C29	2.35	102.46	114.37	13	3
4	A	422	PX4	C3-N1-C2	2.35	100.55	109.91	13	2
4	A	307	PX4	C15-C14-C13	2.35	102.48	114.37	5	1
4	A	381	PX4	C25-C24-C23	2.35	105.07	113.69	5	2
4	A	377	PX4	C28-C27-C26	2.35	102.48	114.37	14	1
4	A	379	PX4	C33-C32-C31	2.35	102.47	114.37	17	2
4	A	386	PX4	C20-C19-C18	2.35	102.47	114.37	6	2
4	A	407	PX4	C30-C29-C28	2.35	102.47	114.37	7	2
4	A	323	PX4	C11-C10-C9	2.35	105.08	113.69	11	2
4	A	377	PX4	C4-N1-C2	2.35	100.56	109.91	17	1
4	A	428	PX4	C30-C29-C28	2.35	102.48	114.37	7	1
4	A	305	PX4	C14-C13-C12	2.35	102.49	114.37	8	2
4	A	308	PX4	C14-C13-C12	2.35	102.50	114.37	2	1
4	A	339	PX4	C5-N1-C2	2.35	100.57	109.91	10	1
4	A	341	PX4	C29-C28-C27	2.35	102.49	114.37	13	4
4	A	384	PX4	C3-N1-C2	2.35	100.57	109.91	16	1
4	A	419	PX4	O3-C1-C2	2.35	120.96	109.65	15	2
4	A	352	PX4	C5-N1-C3	2.35	115.14	108.98	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	359	PX4	C13-C12-C11	2.35	102.50	114.37	1	1
4	A	373	PX4	C27-C26-C25	2.35	102.50	114.37	4	2
4	A	376	PX4	C34-C33-C32	2.35	102.50	114.37	15	1
4	A	388	PX4	O6-C9-C10	2.35	114.59	123.78	6	1
4	A	371	PX4	C28-C27-C26	2.35	102.51	114.37	10	1
4	A	372	PX4	C11-C10-C9	2.35	105.09	113.69	1	1
4	A	396	PX4	C14-C13-C12	2.35	102.51	114.37	17	2
4	A	411	PX4	C5-N1-C4	2.35	115.14	108.98	16	3
4	A	350	PX4	O8-C23-C24	2.35	114.61	123.78	8	1
4	A	429	PX4	O3-P1-O2	2.35	99.63	108.94	2	2
4	A	354	PX4	O4-P1-O2	2.35	118.23	108.94	18	3
4	A	366	PX4	C25-C24-C23	2.35	105.10	113.69	12	3
4	A	336	PX4	C27-C26-C25	2.34	102.52	114.37	2	2
4	A	373	PX4	C29-C28-C27	2.34	102.52	114.37	12	2
4	A	385	PX4	C15-C14-C13	2.34	126.22	114.37	7	2
4	A	386	PX4	C17-C16-C15	2.34	102.52	114.37	18	1
4	A	427	PX4	C30-C29-C28	2.35	102.51	114.37	9	1
4	A	345	PX4	C32-C31-C30	2.34	102.52	114.37	8	2
4	A	407	PX4	C5-N1-C2	2.34	119.23	109.91	5	1
4	A	306	PX4	O3-C1-C2	2.34	120.92	109.65	7	3
4	A	338	PX4	C8-O5-C9	2.34	108.56	117.12	9	3
4	A	413	PX4	C5-N1-C2	2.34	119.23	109.91	6	3
4	A	310	PX4	C5-N1-C2	2.34	119.22	109.91	19	1
4	A	317	PX4	C15-C14-C13	2.34	102.53	114.37	10	3
4	A	320	PX4	C27-C26-C25	2.34	102.53	114.37	18	3
4	A	324	PX4	C19-C18-C17	2.34	102.53	114.37	3	3
4	A	336	PX4	C3-N1-C2	2.34	119.22	109.91	11	1
4	A	341	PX4	C33-C32-C31	2.34	102.53	114.37	17	2
4	A	344	PX4	C20-C19-C18	2.34	102.53	114.37	6	2
4	A	346	PX4	C33-C32-C31	2.34	102.53	114.37	9	4
4	A	361	PX4	C26-C25-C24	2.34	104.52	113.13	16	1
4	A	350	PX4	O3-C1-C2	2.34	120.91	109.65	16	1
4	A	371	PX4	O8-C23-C24	2.34	114.63	123.78	16	2
4	A	379	PX4	C11-C10-C9	2.34	105.12	113.69	20	2
4	A	311	PX4	C4-N1-C2	2.34	100.61	109.91	5	2
4	A	410	PX4	C28-C27-C26	2.34	102.54	114.37	13	1
4	A	412	PX4	C30-C29-C28	2.34	102.54	114.37	4	2
4	A	416	PX4	O6-C9-C10	2.34	114.63	123.78	7	1
4	A	424	PX4	C5-N1-C4	2.34	102.83	108.98	20	4
4	A	310	PX4	C32-C31-C30	2.34	102.55	114.37	8	1
4	A	344	PX4	C17-C16-C15	2.34	102.55	114.37	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	375	PX4	C3-N1-C2	2.34	119.21	109.91	7	3
4	A	395	PX4	O6-C9-C10	2.34	114.64	123.78	14	2
4	A	308	PX4	C31-C30-C29	2.34	102.56	114.37	10	2
4	A	333	PX4	C13-C12-C11	2.34	102.56	114.37	16	3
4	A	358	PX4	C14-C13-C12	2.34	102.56	114.37	3	1
4	A	394	PX4	C28-C27-C26	2.34	102.56	114.37	5	3
4	A	397	PX4	C29-C28-C27	2.34	102.56	114.37	2	2
4	A	426	PX4	C29-C28-C27	2.34	102.56	114.37	14	3
4	A	427	PX4	C8-O5-C9	2.34	108.58	117.12	19	4
4	A	340	PX4	C34-C33-C32	2.33	102.57	114.37	18	2
4	A	327	PX4	C4-N1-C2	2.33	119.18	109.91	2	2
4	A	342	PX4	O3-C1-C2	2.33	120.88	109.65	9	2
4	A	351	PX4	C4-N1-C2	2.33	100.64	109.91	9	4
4	A	345	PX4	O3-C1-C2	2.33	120.87	109.65	14	4
4	A	351	PX4	C8-O5-C9	2.33	108.59	117.12	10	1
4	A	384	PX4	C5-N1-C2	2.33	119.18	109.91	10	2
4	A	391	PX4	C19-C18-C17	2.33	102.58	114.37	9	4
4	A	415	PX4	C33-C32-C31	2.33	102.58	114.37	6	1
4	A	360	PX4	C4-N1-C3	2.33	102.85	108.98	16	2
4	A	405	PX4	C30-C29-C28	2.33	102.59	114.37	7	3
4	A	410	PX4	O6-C9-C10	2.33	114.67	123.78	11	2
4	A	323	PX4	C34-C33-C32	2.33	102.60	114.37	15	2
4	A	325	PX4	C13-C12-C11	2.33	102.60	114.37	9	1
4	A	348	PX4	C17-C16-C15	2.33	102.60	114.37	3	1
4	A	377	PX4	C20-C19-C18	2.33	102.59	114.37	16	3
4	A	389	PX4	C16-C15-C14	2.33	102.60	114.37	11	1
4	A	393	PX4	C28-C27-C26	2.33	102.60	114.37	14	1
4	A	325	PX4	C20-C19-C18	2.33	102.60	114.37	13	3
4	A	362	PX4	C14-C13-C12	2.33	102.61	114.37	16	1
4	A	399	PX4	C26-C25-C24	2.33	104.58	113.13	20	4
4	A	404	PX4	C20-C19-C18	2.33	102.61	114.37	9	2
4	A	417	PX4	C26-C25-C24	2.33	104.58	113.13	14	1
4	A	319	PX4	C12-C11-C10	2.33	104.58	113.13	19	2
4	A	318	PX4	C33-C32-C31	2.32	102.62	114.37	20	2
4	A	348	PX4	C15-C14-C13	2.33	102.61	114.37	11	1
4	A	319	PX4	C30-C29-C28	2.32	102.62	114.37	9	1
4	A	351	PX4	C31-C30-C29	2.33	102.61	114.37	18	1
4	A	366	PX4	O3-C1-C2	2.33	120.84	109.65	6	1
4	A	414	PX4	C12-C11-C10	2.33	104.58	113.13	5	1
4	A	417	PX4	C16-C15-C14	2.33	102.61	114.37	4	2
4	A	313	PX4	C13-C12-C11	2.32	102.63	114.37	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	316	PX4	C26-C25-C24	2.32	104.59	113.13	15	4
4	A	327	PX4	C28-C27-C26	2.32	102.62	114.37	17	1
4	A	374	PX4	C31-C30-C29	2.32	102.63	114.37	5	1
4	A	395	PX4	C11-C10-C9	2.32	105.18	113.69	1	2
4	A	411	PX4	C13-C12-C11	2.32	102.62	114.37	4	2
4	A	424	PX4	C5-N1-C3	2.32	102.87	108.98	15	4
4	A	310	PX4	C29-C28-C27	2.32	102.63	114.37	18	1
4	A	322	PX4	C16-C15-C14	2.32	102.63	114.37	7	1
4	A	329	PX4	C17-C16-C15	2.32	102.64	114.37	19	1
4	A	339	PX4	C18-C17-C16	2.32	102.64	114.37	8	2
4	A	340	PX4	C30-C29-C28	2.32	102.63	114.37	16	3
4	A	353	PX4	C13-C12-C11	2.32	102.63	114.37	7	1
4	A	385	PX4	O1-P1-O4	2.32	97.05	107.57	12	1
4	A	389	PX4	C30-C29-C28	2.32	102.64	114.37	9	1
4	A	400	PX4	C14-C13-C12	2.32	102.63	114.37	4	4
4	A	315	PX4	C11-C10-C9	2.32	105.19	113.69	16	1
4	A	406	PX4	C32-C31-C30	2.32	102.64	114.37	2	1
4	A	409	PX4	O3-C1-C2	2.32	120.81	109.65	5	3
4	A	417	PX4	O1-P1-O3	2.32	97.05	107.57	20	2
4	A	339	PX4	C28-C27-C26	2.32	102.65	114.37	20	1
4	A	311	PX4	C26-C25-C24	2.32	104.61	113.13	9	2
4	A	327	PX4	O3-C1-C2	2.32	120.80	109.65	3	4
4	A	392	PX4	O3-P1-O2	2.32	99.75	108.94	20	1
4	A	402	PX4	C13-C12-C11	2.32	102.65	114.37	3	1
4	A	411	PX4	C3-N1-C2	2.32	119.13	109.91	3	2
4	A	341	PX4	O3-P1-O2	2.32	99.75	108.94	13	4
4	A	364	PX4	C8-O5-C9	2.32	108.65	117.12	18	3
4	A	368	PX4	C31-C30-C29	2.32	102.65	114.37	14	3
4	A	403	PX4	C3-N1-C2	2.32	119.12	109.91	10	1
4	A	425	PX4	C29-C28-C27	2.32	102.65	114.37	10	4
4	A	315	PX4	O4-P1-O2	2.32	118.11	108.94	10	1
4	A	368	PX4	C28-C27-C26	2.32	102.66	114.37	12	1
4	A	428	PX4	O4-P1-O2	2.32	118.11	108.94	3	2
5	A	433	C3S	C54-C57-C60	2.32	123.66	113.28	20	1
4	A	324	PX4	O1-P1-O4	2.31	118.06	107.57	14	3
4	A	414	PX4	C4-N1-C2	2.31	119.11	109.91	1	1
4	A	428	PX4	C33-C32-C31	2.32	102.67	114.37	16	1
4	A	307	PX4	C32-C31-C30	2.31	102.68	114.37	4	1
4	A	370	PX4	C15-C14-C13	2.31	102.67	114.37	1	1
4	A	374	PX4	C11-C10-C9	2.31	105.22	113.69	19	1
4	A	384	PX4	C29-C28-C27	2.31	102.68	114.37	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	394	PX4	C34-C33-C32	2.31	102.67	114.37	6	2
5	A	434	C3S	C57-C54-C48	2.31	108.60	115.08	13	1
4	A	398	PX4	C3-N1-C2	2.31	119.11	109.91	4	2
4	A	422	PX4	C15-C14-C13	2.31	102.67	114.37	18	2
4	A	312	PX4	C34-C33-C32	2.31	102.68	114.37	5	2
4	A	307	PX4	O1-P1-O3	2.31	118.04	107.57	15	2
4	A	329	PX4	C25-C24-C23	2.31	122.16	113.69	11	2
4	A	313	PX4	C28-C27-C26	2.31	102.69	114.37	12	2
4	A	361	PX4	C15-C14-C13	2.31	102.69	114.37	4	1
4	A	376	PX4	C15-C14-C13	2.31	102.69	114.37	8	1
4	A	395	PX4	C28-C27-C26	2.31	102.68	114.37	1	1
4	A	430	PX4	C18-C17-C16	2.31	126.05	114.37	17	1
4	A	314	PX4	C15-C14-C13	2.31	102.69	114.37	11	1
4	A	322	PX4	C11-C10-C9	2.31	105.23	113.69	17	2
4	A	322	PX4	C5-N1-C4	2.31	102.91	108.98	8	4
4	A	326	PX4	C31-C30-C29	2.31	102.70	114.37	16	1
4	A	343	PX4	C30-C29-C28	2.31	102.69	114.37	2	2
4	A	416	PX4	C29-C28-C27	2.31	102.69	114.37	2	1
4	A	362	PX4	O8-C23-C24	2.31	114.75	123.78	13	2
4	A	402	PX4	O3-C1-C2	2.31	120.76	109.65	11	3
4	A	333	PX4	C17-C16-C15	2.31	102.70	114.37	2	1
4	A	344	PX4	C27-C26-C25	2.31	102.70	114.37	6	1
4	A	418	PX4	C32-C31-C30	2.31	102.70	114.37	11	2
4	A	333	PX4	C16-C15-C14	2.31	102.71	114.37	10	2
4	A	351	PX4	C29-C28-C27	2.31	102.70	114.37	11	1
4	A	389	PX4	O4-P1-O2	2.31	99.79	108.94	8	2
4	A	403	PX4	C32-C31-C30	2.31	102.71	114.37	8	1
4	A	305	PX4	C13-C12-C11	2.30	102.72	114.37	11	2
4	A	315	PX4	C19-C18-C17	2.31	102.72	114.37	16	1
4	A	373	PX4	C15-C14-C13	2.31	102.72	114.37	12	1
4	A	425	PX4	O4-P1-O2	2.31	118.07	108.94	10	2
4	A	425	PX4	O6-C9-C10	2.31	114.76	123.78	20	1
4	A	408	PX4	C19-C18-C17	2.30	102.72	114.37	9	2
4	A	413	PX4	O6-C9-C10	2.30	132.80	123.78	19	1
4	A	426	PX4	C32-C31-C30	2.31	102.71	114.37	9	1
4	A	331	PX4	O1-P1-O3	2.30	97.12	107.57	1	1
4	A	335	PX4	C33-C32-C31	2.30	102.72	114.37	14	1
4	A	365	PX4	C20-C19-C18	2.30	102.72	114.37	6	2
4	A	368	PX4	C30-C29-C28	2.30	102.73	114.37	16	1
4	A	377	PX4	C18-C17-C16	2.30	102.73	114.37	18	2
4	A	402	PX4	O1-P1-O4	2.30	118.00	107.57	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	402	PX4	C20-C19-C18	2.30	102.73	114.37	11	3
4	A	415	PX4	O8-C23-C24	2.30	114.78	123.78	2	1
4	A	430	PX4	C29-C28-C27	2.30	102.72	114.37	3	2
4	A	312	PX4	C18-C17-C16	2.30	102.73	114.37	15	2
4	A	314	PX4	C3-N1-C2	2.30	119.06	109.91	12	3
4	A	327	PX4	C8-O5-C9	2.30	108.70	117.12	11	1
4	A	333	PX4	O3-C1-C2	2.30	120.71	109.65	5	3
4	A	346	PX4	C31-C30-C29	2.30	102.74	114.37	3	1
4	A	362	PX4	C5-N1-C4	2.30	102.93	108.98	2	2
4	A	364	PX4	C15-C14-C13	2.30	102.73	114.37	3	4
4	A	389	PX4	O6-C9-C10	2.30	132.78	123.78	1	2
4	A	406	PX4	C31-C30-C29	2.30	102.73	114.37	9	1
4	A	408	PX4	C26-C25-C24	2.30	104.67	113.13	9	1
4	A	413	PX4	C18-C17-C16	2.30	102.73	114.37	3	1
4	A	383	PX4	C18-C17-C16	2.30	102.74	114.37	4	1
4	A	320	PX4	O3-C1-C2	2.30	120.71	109.65	3	3
4	A	355	PX4	C29-C28-C27	2.30	102.75	114.37	6	1
4	A	420	PX4	C12-C11-C10	2.30	104.68	113.13	20	1
4	A	368	PX4	O3-C1-C2	2.30	120.71	109.65	4	1
4	A	376	PX4	O8-C23-C24	2.30	114.80	123.78	3	1
4	A	385	PX4	C16-C15-C14	2.30	102.76	114.37	11	2
4	A	396	PX4	O6-C9-C10	2.30	114.80	123.78	1	1
4	A	403	PX4	C28-C27-C26	2.30	102.75	114.37	11	2
4	A	422	PX4	C16-C15-C14	2.30	102.75	114.37	6	1
4	A	308	PX4	O8-C23-C24	2.30	114.81	123.78	13	2
4	A	356	PX4	C18-C17-C16	2.29	102.77	114.37	13	2
4	A	358	PX4	C5-N1-C2	2.29	119.03	109.91	20	1
4	A	359	PX4	O6-C9-C10	2.29	132.76	123.78	7	1
4	A	409	PX4	C33-C32-C31	2.30	102.76	114.37	19	1
4	A	424	PX4	C13-C12-C11	2.30	102.76	114.37	20	1
4	A	367	PX4	C26-C25-C24	2.29	121.56	113.13	6	2
4	A	370	PX4	C3-N1-C2	2.29	119.03	109.91	8	1
4	A	305	PX4	C18-C17-C16	2.29	102.78	114.37	17	1
4	A	323	PX4	O3-C1-C2	2.29	120.68	109.65	19	3
4	A	329	PX4	C19-C18-C17	2.29	102.78	114.37	6	1
4	A	389	PX4	C3-N1-C2	2.29	119.03	109.91	3	2
4	A	392	PX4	C3-N1-C2	2.29	119.03	109.91	2	1
4	A	343	PX4	O1-P1-O3	2.29	117.95	107.57	7	1
4	A	365	PX4	C3-N1-C2	2.29	119.02	109.91	17	2
4	A	388	PX4	C14-C13-C12	2.29	102.78	114.37	10	1
4	A	396	PX4	C3-N1-C2	2.29	119.02	109.91	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	348	PX4	C12-C11-C10	2.29	104.71	113.13	15	1
4	A	306	PX4	C34-C33-C32	2.29	102.80	114.37	19	1
4	A	314	PX4	C13-C12-C11	2.29	102.79	114.37	8	1
4	A	317	PX4	C33-C32-C31	2.29	102.80	114.37	14	1
4	A	325	PX4	C29-C28-C27	2.29	102.80	114.37	8	1
4	A	396	PX4	O8-C23-C24	2.29	114.83	123.78	6	2
4	A	404	PX4	C33-C32-C31	2.29	102.80	114.37	8	2
4	A	404	PX4	O1-P1-O4	2.29	117.94	107.57	15	1
4	A	424	PX4	C34-C33-C32	2.29	102.80	114.37	5	2
4	A	369	PX4	C16-C15-C14	2.29	102.80	114.37	18	2
4	A	403	PX4	O6-C9-C10	2.29	114.83	123.78	19	1
5	A	436	C3S	C26-C23-C20	2.29	117.03	113.14	15	2
4	A	315	PX4	C5-N1-C3	2.29	114.98	108.98	9	2
4	A	322	PX4	O8-C23-C24	2.29	114.84	123.78	11	1
4	A	331	PX4	C11-C10-C9	2.29	105.32	113.69	8	1
4	A	332	PX4	C14-C13-C12	2.29	102.81	114.37	11	2
4	A	342	PX4	C19-C18-C17	2.29	102.81	114.37	1	1
4	A	310	PX4	O8-C23-C24	2.28	114.85	123.78	19	1
4	A	333	PX4	C20-C19-C18	2.29	102.81	114.37	10	3
4	A	376	PX4	C17-C16-C15	2.29	102.81	114.37	16	1
4	A	401	PX4	C14-C13-C12	2.29	102.81	114.37	3	2
4	A	410	PX4	C29-C28-C27	2.29	102.82	114.37	12	1
4	A	325	PX4	C31-C30-C29	2.28	102.83	114.37	7	2
4	A	328	PX4	C5-N1-C3	2.28	102.98	108.98	16	4
4	A	335	PX4	O3-C1-C2	2.28	120.64	109.65	3	1
4	A	347	PX4	C26-C25-C24	2.28	104.74	113.13	16	1
4	A	369	PX4	C26-C25-C24	2.28	104.74	113.13	14	4
4	A	386	PX4	C29-C28-C27	2.28	102.83	114.37	5	1
4	A	418	PX4	C31-C30-C29	2.28	102.83	114.37	3	1
4	A	316	PX4	C16-C15-C14	2.28	102.83	114.37	10	1
4	A	340	PX4	C29-C28-C27	2.28	102.83	114.37	15	3
4	A	366	PX4	O1-P1-O4	2.28	117.91	107.57	7	2
4	A	414	PX4	O7-C23-O8	2.28	118.37	123.70	20	5
4	A	388	PX4	O1-P1-O4	2.28	117.91	107.57	20	3
4	A	429	PX4	O6-C9-C10	2.28	114.86	123.78	20	2
4	A	385	PX4	C13-C12-C11	2.28	102.85	114.37	17	1
4	A	423	PX4	C19-C18-C17	2.28	102.85	114.37	2	1
4	A	429	PX4	C18-C17-C16	2.28	102.84	114.37	17	3
4	A	325	PX4	C34-C33-C32	2.28	102.85	114.37	16	3
4	A	362	PX4	C18-C17-C16	2.28	102.85	114.37	2	1
4	A	393	PX4	C13-C12-C11	2.28	102.85	114.37	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	405	PX4	C5-N1-C2	2.28	118.97	109.91	8	2
4	A	424	PX4	O3-C1-C2	2.28	120.61	109.65	14	1
4	A	429	PX4	C20-C19-C18	2.28	102.85	114.37	16	1
4	A	317	PX4	C30-C29-C28	2.28	102.86	114.37	17	3
4	A	330	PX4	C31-C30-C29	2.28	102.87	114.37	20	2
4	A	339	PX4	C31-C30-C29	2.28	102.86	114.37	7	2
4	A	376	PX4	C33-C32-C31	2.28	102.86	114.37	5	2
4	A	380	PX4	C28-C27-C26	2.28	102.87	114.37	16	1
4	A	385	PX4	C34-C33-C32	2.28	102.86	114.37	5	1
4	A	333	PX4	O8-C23-C24	2.27	114.89	123.78	14	2
4	A	363	PX4	C31-C30-C29	2.27	102.87	114.37	2	1
4	A	369	PX4	C29-C28-C27	2.27	102.87	114.37	8	1
4	A	371	PX4	C25-C24-C23	2.27	122.03	113.69	12	2
4	A	372	PX4	C18-C17-C16	2.27	125.86	114.37	10	1
4	A	381	PX4	C15-C14-C13	2.27	102.87	114.37	1	1
4	A	384	PX4	C14-C13-C12	2.27	102.88	114.37	16	2
4	A	429	PX4	O1-P1-O3	2.27	97.26	107.57	19	3
4	A	430	PX4	O3-C1-C2	2.27	120.59	109.65	20	2
4	A	341	PX4	C26-C25-C24	2.27	104.78	113.13	2	1
4	A	326	PX4	C25-C24-C23	2.27	105.37	113.69	18	1
4	A	402	PX4	O6-C9-C10	2.27	114.90	123.78	20	1
4	A	408	PX4	C30-C29-C28	2.27	102.88	114.37	17	1
4	A	314	PX4	C14-C13-C12	2.27	102.90	114.37	10	2
4	A	316	PX4	C5-N1-C4	2.27	114.94	108.98	11	1
4	A	319	PX4	C5-N1-C2	2.27	118.93	109.91	20	2
4	A	363	PX4	C3-N1-C2	2.27	118.93	109.91	13	1
4	A	376	PX4	C26-C25-C24	2.27	104.79	113.13	10	2
4	A	383	PX4	O4-P1-O2	2.27	99.94	108.94	7	3
4	A	378	PX4	O4-P1-O2	2.27	99.94	108.94	2	2
4	A	383	PX4	C11-C10-C9	2.27	105.38	113.69	11	1
4	A	422	PX4	C20-C19-C18	2.27	102.90	114.37	20	1
4	A	308	PX4	O1-P1-O3	2.27	117.85	107.57	14	1
4	A	313	PX4	O1-P1-O3	2.27	97.29	107.57	2	1
4	A	345	PX4	C27-C26-C25	2.27	102.90	114.37	19	2
4	A	391	PX4	C25-C24-C23	2.27	105.39	113.69	16	1
4	A	430	PX4	C11-C10-C9	2.27	105.39	113.69	10	2
4	A	315	PX4	C12-C11-C10	2.27	104.80	113.13	11	2
4	A	324	PX4	C31-C30-C29	2.26	102.92	114.37	5	2
4	A	361	PX4	C31-C30-C29	2.27	102.92	114.37	17	1
4	A	369	PX4	O4-P1-O2	2.27	117.91	108.94	10	2
4	A	391	PX4	C5-N1-C4	2.27	103.03	108.98	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	393	PX4	C8-O5-C9	2.27	108.84	117.12	5	1
4	A	425	PX4	C3-N1-C2	2.27	118.92	109.91	19	1
4	A	319	PX4	C27-C26-C25	2.26	102.93	114.37	3	1
4	A	342	PX4	O8-C23-C24	2.26	132.63	123.78	16	1
4	A	353	PX4	C29-C28-C27	2.26	102.93	114.37	7	2
4	A	358	PX4	C8-O5-C9	2.26	125.39	117.12	5	4
4	A	404	PX4	C14-C13-C12	2.26	102.92	114.37	15	2
4	A	430	PX4	O5-C9-O6	2.26	117.97	123.63	18	3
4	A	374	PX4	C8-O5-C9	2.26	108.85	117.12	5	2
4	A	383	PX4	O6-C9-C10	2.26	114.94	123.78	9	1
4	A	384	PX4	C16-C15-C14	2.26	102.93	114.37	19	2
4	A	343	PX4	C28-C27-C26	2.26	102.94	114.37	13	1
4	A	345	PX4	C30-C29-C28	2.26	102.95	114.37	13	2
4	A	363	PX4	O3-C1-C2	2.26	120.53	109.65	3	1
4	A	405	PX4	C14-C13-C12	2.26	102.94	114.37	10	2
4	A	371	PX4	C5-N1-C2	2.26	118.89	109.91	7	2
4	A	307	PX4	C3-N1-C2	2.26	100.94	109.91	8	4
4	A	343	PX4	O6-C9-C10	2.26	114.95	123.78	15	2
4	A	362	PX4	O3-C1-C2	2.26	120.52	109.65	14	1
4	A	375	PX4	C5-N1-C2	2.26	118.89	109.91	4	1
4	A	374	PX4	C35-C34-C33	2.26	95.45	115.25	10	1
4	A	386	PX4	C16-C15-C14	2.26	102.95	114.37	8	1
4	A	396	PX4	C5-N1-C2	2.26	118.89	109.91	2	2
4	A	389	PX4	O8-C23-C24	2.26	114.96	123.78	3	2
4	A	391	PX4	C20-C19-C18	2.26	102.96	114.37	10	2
4	A	427	PX4	C33-C32-C31	2.26	102.96	114.37	17	1
4	A	334	PX4	C33-C32-C31	2.26	102.96	114.37	9	1
4	A	309	PX4	C17-C16-C15	2.25	102.97	114.37	3	1
4	A	351	PX4	C18-C17-C16	2.26	102.97	114.37	19	2
4	A	356	PX4	C34-C33-C32	2.26	102.97	114.37	9	1
4	A	390	PX4	C14-C13-C12	2.25	102.97	114.37	3	2
4	A	391	PX4	O3-C1-C2	2.26	120.50	109.65	15	1
4	A	403	PX4	C25-C24-C23	2.26	105.43	113.69	12	1
4	A	370	PX4	O1-P1-O4	2.25	117.79	107.57	3	3
4	A	364	PX4	C14-C13-C12	2.25	102.98	114.37	7	1
4	A	313	PX4	C34-C33-C32	2.25	102.98	114.37	10	1
4	A	393	PX4	C4-N1-C2	2.25	100.96	109.91	17	3
4	A	325	PX4	C28-C27-C26	2.25	103.00	114.37	17	1
4	A	367	PX4	C16-C15-C14	2.25	102.99	114.37	3	1
4	A	410	PX4	C31-C30-C29	2.25	102.99	114.37	14	1
4	A	424	PX4	C22-C21-C20	2.25	98.16	113.36	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	338	PX4	C30-C29-C28	2.25	103.00	114.37	7	4
4	A	343	PX4	C25-C24-C23	2.25	105.45	113.69	7	1
4	A	350	PX4	C19-C18-C17	2.25	103.00	114.37	6	2
4	A	355	PX4	O3-C1-C2	2.25	120.47	109.65	1	1
4	A	423	PX4	C29-C28-C27	2.25	103.00	114.37	19	1
4	A	358	PX4	C34-C33-C32	2.25	103.01	114.37	4	1
4	A	314	PX4	C33-C32-C31	2.25	103.02	114.37	20	1
4	A	354	PX4	C33-C32-C31	2.25	103.02	114.37	15	1
4	A	361	PX4	C14-C13-C12	2.25	103.01	114.37	7	3
4	A	372	PX4	C14-C13-C12	2.25	103.01	114.37	13	2
4	A	376	PX4	C27-C26-C25	2.25	103.01	114.37	12	3
4	A	408	PX4	O8-C23-C24	2.25	114.99	123.78	5	2
4	A	385	PX4	C29-C28-C27	2.25	103.02	114.37	16	2
4	A	395	PX4	C17-C16-C15	2.25	103.01	114.37	16	2
4	A	305	PX4	C16-C15-C14	2.24	103.03	114.37	2	1
4	A	308	PX4	C29-C28-C27	2.24	103.02	114.37	5	1
4	A	314	PX4	C17-C16-C15	2.24	103.03	114.37	1	1
4	A	317	PX4	C32-C31-C30	2.24	103.02	114.37	9	1
4	A	326	PX4	C16-C15-C14	2.25	103.02	114.37	15	1
4	A	327	PX4	C31-C30-C29	2.24	103.03	114.37	18	1
4	A	363	PX4	C30-C29-C28	2.24	103.02	114.37	12	3
4	A	401	PX4	C26-C25-C24	2.25	104.88	113.13	5	3
4	A	342	PX4	O1-P1-O4	2.24	117.74	107.57	16	3
4	A	391	PX4	O8-C23-C24	2.24	115.00	123.78	4	1
4	A	394	PX4	O1-P1-O4	2.24	117.73	107.57	2	2
4	A	428	PX4	O1-P1-O4	2.24	117.73	107.57	5	2
4	A	320	PX4	C32-C31-C30	2.24	103.04	114.37	10	1
4	A	350	PX4	C18-C17-C16	2.24	103.04	114.37	19	1
4	A	319	PX4	C28-C27-C26	2.24	103.05	114.37	15	2
4	A	358	PX4	C30-C29-C28	2.24	103.05	114.37	18	1
4	A	372	PX4	O8-C23-C24	2.24	115.02	123.78	9	1
4	A	385	PX4	C33-C32-C31	2.24	103.04	114.37	19	1
4	A	393	PX4	C36-C35-C34	2.24	98.23	113.36	19	1
4	A	413	PX4	C12-C11-C10	2.24	104.90	113.13	12	1
4	A	425	PX4	C31-C30-C29	2.24	103.05	114.37	12	1
4	A	381	PX4	C5-N1-C2	2.24	118.81	109.91	10	1
4	A	312	PX4	C12-C11-C10	2.24	104.91	113.13	19	1
4	A	334	PX4	C12-C11-C10	2.24	104.91	113.13	4	1
4	A	336	PX4	C11-C10-C9	2.24	105.50	113.69	18	2
4	A	404	PX4	C16-C15-C14	2.24	103.06	114.37	1	1
4	A	414	PX4	C20-C19-C18	2.24	103.06	114.37	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	368	PX4	O1-P1-O3	2.24	117.70	107.57	16	1
4	A	311	PX4	C5-N1-C2	2.23	101.03	109.91	2	4
4	A	376	PX4	C25-C24-C23	2.23	105.51	113.69	6	1
4	A	369	PX4	C34-C33-C32	2.23	103.08	114.37	11	3
4	A	399	PX4	O3-C1-C2	2.23	120.40	109.65	19	2
4	A	383	PX4	C30-C29-C28	2.23	103.08	114.37	14	1
4	A	415	PX4	C30-C29-C28	2.23	103.08	114.37	13	1
4	A	425	PX4	C5-N1-C2	2.23	118.78	109.91	6	1
4	A	308	PX4	C13-C12-C11	2.23	103.10	114.37	4	2
4	A	309	PX4	C28-C27-C26	2.23	103.10	114.37	5	2
4	A	311	PX4	C27-C26-C25	2.23	103.10	114.37	9	1
4	A	332	PX4	C12-C11-C10	2.23	104.93	113.13	5	2
4	A	345	PX4	C15-C14-C13	2.23	103.09	114.37	4	1
4	A	380	PX4	C12-C11-C10	2.23	104.93	113.13	19	2
4	A	345	PX4	C22-C21-C20	2.23	98.30	113.36	8	1
4	A	381	PX4	C16-C15-C14	2.23	103.09	114.37	7	2
4	A	373	PX4	O1-P1-O3	2.23	97.46	107.57	8	3
4	A	385	PX4	C20-C19-C18	2.23	103.10	114.37	15	2
4	A	408	PX4	C33-C32-C31	2.23	103.09	114.37	3	1
4	A	413	PX4	C26-C25-C24	2.23	104.93	113.13	9	1
4	A	417	PX4	C4-N1-C2	2.23	118.78	109.91	15	1
4	A	419	PX4	C13-C12-C11	2.23	103.09	114.37	20	3
4	A	362	PX4	O1-P1-O3	2.23	97.46	107.57	11	4
4	A	335	PX4	C20-C19-C18	2.23	103.10	114.37	8	1
4	A	323	PX4	C5-N1-C3	2.23	103.13	108.98	6	1
4	A	354	PX4	C19-C18-C17	2.23	103.11	114.37	14	1
4	A	404	PX4	O1-P1-O3	2.23	97.47	107.57	5	1
4	A	310	PX4	C16-C15-C14	2.23	103.12	114.37	18	3
4	A	332	PX4	C27-C26-C25	2.23	103.12	114.37	6	1
4	A	341	PX4	C28-C27-C26	2.23	103.12	114.37	16	1
4	A	343	PX4	C33-C32-C31	2.23	103.11	114.37	14	4
4	A	361	PX4	C16-C15-C14	2.23	103.11	114.37	1	1
4	A	361	PX4	C32-C31-C30	2.23	103.11	114.37	12	1
4	A	418	PX4	C29-C28-C27	2.23	103.11	114.37	15	2
4	A	423	PX4	O3-C1-C2	2.23	120.37	109.65	15	1
4	A	307	PX4	C27-C26-C25	2.22	103.13	114.37	15	2
4	A	340	PX4	C17-C16-C15	2.22	103.12	114.37	12	2
4	A	346	PX4	C12-C11-C10	2.22	104.95	113.13	5	2
4	A	361	PX4	C3-N1-C2	2.23	118.76	109.91	7	4
4	A	359	PX4	C14-C13-C12	2.22	103.12	114.37	8	1
4	A	379	PX4	C3-N1-C2	2.22	118.75	109.91	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	386	PX4	C19-C18-C17	2.23	103.12	114.37	10	1
4	A	388	PX4	O1-P1-O3	2.22	97.48	107.57	5	2
4	A	314	PX4	C11-C10-C9	2.22	105.55	113.69	2	3
4	A	327	PX4	C12-C11-C10	2.22	104.96	113.13	5	2
4	A	326	PX4	C30-C29-C28	2.22	103.14	114.37	4	3
4	A	353	PX4	C17-C16-C15	2.22	103.13	114.37	15	2
4	A	378	PX4	C19-C18-C17	2.22	103.13	114.37	4	1
4	A	426	PX4	C34-C33-C32	2.22	103.13	114.37	5	1
4	A	310	PX4	C25-C24-C23	2.22	121.83	113.69	14	2
4	A	343	PX4	C17-C16-C15	2.22	103.14	114.37	1	1
4	A	397	PX4	C33-C32-C31	2.22	103.14	114.37	5	2
4	A	313	PX4	C20-C19-C18	2.22	103.16	114.37	9	1
4	A	339	PX4	C15-C14-C13	2.22	103.16	114.37	2	1
4	A	357	PX4	C29-C28-C27	2.22	103.15	114.37	14	1
4	A	390	PX4	C27-C26-C25	2.22	103.15	114.37	1	3
4	A	411	PX4	C17-C16-C15	2.22	103.15	114.37	14	3
4	A	319	PX4	C18-C17-C16	2.22	103.17	114.37	16	1
4	A	362	PX4	C5-N1-C3	2.22	103.15	108.98	1	1
4	A	364	PX4	C28-C27-C26	2.22	103.16	114.37	10	1
4	A	374	PX4	C17-C16-C15	2.22	103.16	114.37	18	1
4	A	407	PX4	C16-C15-C14	2.22	103.16	114.37	7	2
4	A	383	PX4	C20-C19-C18	2.21	103.17	114.37	10	2
4	A	384	PX4	C17-C16-C15	2.22	103.17	114.37	18	3
4	A	386	PX4	O8-C23-C24	2.22	115.12	123.78	15	2
4	A	397	PX4	C5-N1-C2	2.22	101.10	109.91	15	1
4	A	424	PX4	C33-C32-C31	2.22	103.17	114.37	6	2
4	A	426	PX4	C18-C17-C16	2.22	103.17	114.37	1	1
4	A	426	PX4	O1-P1-O3	2.22	97.52	107.57	14	2
4	A	311	PX4	C13-C12-C11	2.22	103.17	114.37	19	5
4	A	330	PX4	C29-C28-C27	2.21	103.17	114.37	7	1
4	A	334	PX4	O3-C1-C2	2.21	120.31	109.65	15	1
4	A	339	PX4	C29-C28-C27	2.22	103.17	114.37	7	1
4	A	371	PX4	C30-C29-C28	2.22	103.17	114.37	3	4
4	A	430	PX4	C8-O5-C9	2.21	109.02	117.12	7	1
4	A	311	PX4	C16-C15-C14	2.21	103.18	114.37	15	3
4	A	330	PX4	C28-C27-C26	2.21	103.18	114.37	18	1
4	A	371	PX4	C18-C17-C16	2.21	103.18	114.37	20	1
4	A	388	PX4	C32-C31-C30	2.21	103.18	114.37	10	1
4	A	327	PX4	O4-P1-O2	2.21	117.70	108.94	13	1
4	A	331	PX4	C30-C29-C28	2.21	103.19	114.37	1	2
4	A	328	PX4	C3-N1-C2	2.21	118.70	109.91	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	381	PX4	O3-C1-C2	2.21	120.28	109.65	12	1
4	A	391	PX4	C34-C33-C32	2.21	103.19	114.37	1	1
4	A	363	PX4	C12-C11-C10	2.21	105.01	113.13	14	1
4	A	306	PX4	C13-C12-C11	2.21	103.21	114.37	16	1
4	A	324	PX4	C13-C12-C11	2.21	103.21	114.37	18	2
4	A	352	PX4	C19-C18-C17	2.21	103.21	114.37	15	2
4	A	403	PX4	C17-C16-C15	2.21	103.20	114.37	13	1
4	A	347	PX4	C34-C33-C32	2.21	103.22	114.37	7	1
4	A	372	PX4	C34-C33-C32	2.21	103.22	114.37	8	1
4	A	403	PX4	C19-C18-C17	2.21	103.21	114.37	9	3
4	A	373	PX4	C30-C29-C28	2.21	103.22	114.37	4	2
4	A	371	PX4	O3-C1-C2	2.20	120.26	109.65	6	1
4	A	314	PX4	C22-C21-C20	2.20	98.49	113.36	4	1
4	A	366	PX4	C33-C32-C31	2.20	103.23	114.37	14	2
4	A	377	PX4	C15-C14-C13	2.20	103.23	114.37	12	1
4	A	425	PX4	C16-C15-C14	2.20	103.23	114.37	13	2
4	A	321	PX4	C25-C24-C23	2.20	105.62	113.69	11	1
4	A	324	PX4	C20-C19-C18	2.20	103.24	114.37	15	1
4	A	368	PX4	C15-C14-C13	2.20	103.23	114.37	6	1
4	A	359	PX4	O8-C23-C24	2.20	115.17	123.78	20	2
4	A	359	PX4	C18-C17-C16	2.20	103.23	114.37	18	1
4	A	377	PX4	C32-C31-C30	2.20	103.23	114.37	13	1
4	A	397	PX4	O8-C23-C24	2.20	115.17	123.78	11	1
4	A	411	PX4	C31-C30-C29	2.20	103.24	114.37	20	1
4	A	353	PX4	C30-C29-C28	2.20	103.24	114.37	17	2
4	A	370	PX4	C32-C31-C30	2.20	103.24	114.37	1	1
4	A	315	PX4	C20-C19-C18	2.20	103.25	114.37	16	1
4	A	337	PX4	C28-C27-C26	2.20	103.25	114.37	11	2
4	A	344	PX4	O1-P1-O4	2.20	117.54	107.57	19	1
4	A	358	PX4	O1-P1-O3	2.20	97.60	107.57	2	3
4	A	363	PX4	C28-C27-C26	2.20	103.25	114.37	3	2
4	A	402	PX4	C19-C18-C17	2.20	103.25	114.37	19	1
4	A	392	PX4	C15-C14-C13	2.20	103.26	114.37	12	1
4	A	387	PX4	C8-O5-C9	2.20	109.09	117.12	7	1
4	A	409	PX4	O8-C23-C24	2.20	115.19	123.78	9	3
4	A	409	PX4	C29-C28-C27	2.20	103.26	114.37	14	1
4	A	426	PX4	C17-C16-C15	2.20	103.26	114.37	3	1
4	A	351	PX4	C5-N1-C2	2.20	118.64	109.91	9	1
4	A	317	PX4	C25-C24-C23	2.20	105.65	113.69	11	1
4	A	338	PX4	C14-C13-C12	2.20	103.27	114.37	15	1
4	A	364	PX4	C5-N1-C2	2.20	101.18	109.91	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	343	PX4	O8-C23-C24	2.19	115.20	123.78	6	1
4	A	366	PX4	C12-C11-C10	2.19	105.06	113.13	5	2
4	A	378	PX4	C28-C27-C26	2.20	103.27	114.37	9	1
4	A	422	PX4	C4-N1-C2	2.20	118.64	109.91	5	1
4	A	430	PX4	C17-C16-C15	2.20	103.27	114.37	17	1
4	A	345	PX4	C29-C28-C27	2.19	103.28	114.37	10	1
4	A	379	PX4	C16-C15-C14	2.19	103.28	114.37	14	2
4	A	411	PX4	O3-C1-C2	2.19	120.21	109.65	18	1
4	A	305	PX4	C32-C31-C30	2.19	103.29	114.37	8	2
4	A	310	PX4	C12-C11-C10	2.19	121.18	113.13	11	1
4	A	319	PX4	C11-C10-C9	2.19	105.66	113.69	16	2
4	A	355	PX4	O8-C23-C24	2.19	115.21	123.78	6	1
4	A	320	PX4	C4-N1-C2	2.19	118.62	109.91	18	1
4	A	306	PX4	C8-O5-C9	2.19	109.11	117.12	17	2
4	A	318	PX4	C17-C16-C15	2.19	103.30	114.37	12	3
4	A	322	PX4	C19-C18-C17	2.19	103.30	114.37	17	1
4	A	327	PX4	C33-C32-C31	2.19	103.30	114.37	19	2
4	A	384	PX4	C34-C33-C32	2.19	103.29	114.37	17	2
4	A	357	PX4	C30-C29-C28	2.19	103.30	114.37	1	2
4	A	408	PX4	C29-C28-C27	2.19	103.30	114.37	19	2
4	A	374	PX4	C33-C32-C31	2.19	103.30	114.37	16	1
4	A	401	PX4	C32-C31-C30	2.19	103.30	114.37	20	1
4	A	430	PX4	C28-C27-C26	2.19	103.30	114.37	8	2
4	A	321	PX4	C27-C26-C25	2.19	103.31	114.37	6	1
4	A	322	PX4	C34-C33-C32	2.19	103.31	114.37	3	1
4	A	343	PX4	C18-C17-C16	2.19	103.31	114.37	17	1
4	A	363	PX4	C19-C18-C17	2.19	103.31	114.37	14	1
4	A	340	PX4	O6-C9-C10	2.19	115.23	123.78	14	2
4	A	398	PX4	C33-C32-C31	2.19	103.32	114.37	13	1
4	A	408	PX4	C13-C12-C11	2.19	103.31	114.37	2	1
4	A	430	PX4	C16-C15-C14	2.19	103.31	114.37	6	1
4	A	342	PX4	C33-C32-C31	2.19	103.32	114.37	11	1
4	A	344	PX4	C29-C28-C27	2.18	103.33	114.37	6	2
4	A	383	PX4	C13-C12-C11	2.18	103.33	114.37	6	1
4	A	397	PX4	C28-C27-C26	2.18	103.33	114.37	10	1
4	A	321	PX4	O5-C9-O6	2.18	118.17	123.63	16	2
4	A	339	PX4	C17-C16-C15	2.18	103.34	114.37	11	2
4	A	325	PX4	C16-C15-C14	2.18	103.34	114.37	19	1
4	A	350	PX4	C33-C32-C31	2.18	103.34	114.37	5	2
4	A	398	PX4	C17-C16-C15	2.18	125.40	114.37	10	1
4	A	408	PX4	C34-C33-C32	2.18	103.34	114.37	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	C8-O5-C9	2.18	109.15	117.12	1	1
4	A	349	PX4	C3-N1-C2	2.18	118.57	109.91	1	1
4	A	420	PX4	C11-C10-C9	2.18	105.70	113.69	14	1
4	A	331	PX4	C33-C32-C31	2.18	103.36	114.37	2	2
4	A	336	PX4	C14-C13-C12	2.18	103.35	114.37	3	1
4	A	340	PX4	C32-C31-C30	2.18	103.36	114.37	1	1
4	A	352	PX4	C4-N1-C2	2.18	118.57	109.91	6	3
4	A	370	PX4	O1-P1-O3	2.18	97.69	107.57	2	1
4	A	372	PX4	C31-C30-C29	2.18	103.35	114.37	13	2
4	A	403	PX4	C8-O5-C9	2.18	109.15	117.12	10	1
4	A	370	PX4	C26-C25-C24	2.18	105.12	113.13	16	1
4	A	414	PX4	C11-C10-C9	2.18	105.71	113.69	3	1
4	A	351	PX4	C30-C29-C28	2.18	103.36	114.37	8	2
4	A	377	PX4	C8-O5-C9	2.18	109.16	117.12	7	2
4	A	430	PX4	C20-C19-C18	2.18	103.36	114.37	15	1
4	A	410	PX4	C26-C25-C24	2.18	105.13	113.13	4	1
4	A	424	PX4	C30-C29-C28	2.18	103.37	114.37	16	2
4	A	306	PX4	C25-C24-C23	2.18	105.72	113.69	9	3
4	A	321	PX4	O3-C1-C2	2.17	120.11	109.65	8	1
4	A	322	PX4	O6-C9-C10	2.17	115.28	123.78	17	1
4	A	339	PX4	C13-C12-C11	2.17	103.38	114.37	10	2
4	A	356	PX4	C8-O5-C9	2.18	109.17	117.12	16	1
4	A	357	PX4	C27-C26-C25	2.17	103.37	114.37	13	2
4	A	383	PX4	C16-C15-C14	2.17	103.38	114.37	17	3
4	A	412	PX4	C13-C12-C11	2.17	103.38	114.37	6	2
4	A	354	PX4	C20-C19-C18	2.17	103.39	114.37	20	1
4	A	358	PX4	C25-C24-C23	2.17	105.73	113.69	19	1
4	A	382	PX4	C26-C25-C24	2.17	105.14	113.13	7	2
4	A	383	PX4	O8-C23-C24	2.17	115.28	123.78	18	1
4	A	306	PX4	C19-C18-C17	2.17	103.39	114.37	7	1
4	A	376	PX4	C14-C13-C12	2.17	103.39	114.37	18	2
4	A	395	PX4	C16-C15-C14	2.17	103.39	114.37	2	1
4	A	420	PX4	C30-C29-C28	2.17	103.39	114.37	12	2
4	A	322	PX4	C17-C16-C15	2.17	103.40	114.37	11	3
4	A	330	PX4	O1-P1-O4	2.17	117.40	107.57	5	3
4	A	370	PX4	C25-C24-C23	2.17	105.74	113.69	18	1
4	A	416	PX4	C3-N1-C2	2.17	118.54	109.91	20	2
4	A	312	PX4	C4-N1-C2	2.17	118.53	109.91	3	1
4	A	315	PX4	C17-C16-C15	2.17	103.41	114.37	17	2
4	A	351	PX4	O6-C9-C10	2.17	115.30	123.78	18	1
4	A	417	PX4	C18-C17-C16	2.17	103.41	114.37	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	369	PX4	C5-N1-C2	2.17	118.53	109.91	5	3
4	A	375	PX4	O3-C1-C2	2.17	120.08	109.65	8	1
4	A	403	PX4	O1-P1-O4	2.17	117.39	107.57	15	1
4	A	417	PX4	C28-C27-C26	2.17	103.41	114.37	8	2
4	A	421	PX4	C11-C10-C9	2.17	105.75	113.69	14	3
4	A	424	PX4	C20-C19-C18	2.17	103.41	114.37	8	1
4	A	306	PX4	C12-C11-C10	2.17	105.17	113.13	1	2
4	A	315	PX4	O8-C23-C24	2.17	115.31	123.78	12	1
4	A	364	PX4	C20-C19-C18	2.17	103.42	114.37	19	2
4	A	318	PX4	C16-C15-C14	2.17	103.42	114.37	17	2
4	A	369	PX4	C17-C16-C15	2.17	103.42	114.37	14	1
4	A	382	PX4	C14-C13-C12	2.17	103.42	114.37	10	3
4	A	380	PX4	C30-C29-C28	2.16	103.42	114.37	2	1
4	A	397	PX4	C32-C31-C30	2.17	103.42	114.37	4	2
4	A	404	PX4	O6-C9-C10	2.17	115.31	123.78	18	1
4	A	412	PX4	C32-C31-C30	2.17	103.42	114.37	20	2
4	A	413	PX4	C8-O5-C9	2.17	109.20	117.12	5	1
4	A	430	PX4	O5-C9-C10	2.17	118.44	111.83	12	2
4	A	320	PX4	C17-C16-C15	2.16	103.43	114.37	18	1
4	A	352	PX4	O8-C23-C24	2.16	115.32	123.78	2	1
4	A	356	PX4	C32-C31-C30	2.16	103.43	114.37	8	1
4	A	369	PX4	O6-C9-C10	2.16	115.32	123.78	14	1
4	A	328	PX4	C19-C18-C17	2.16	103.44	114.37	6	3
4	A	362	PX4	O5-C9-C10	2.16	118.43	111.83	12	1
4	A	367	PX4	C17-C16-C15	2.16	103.44	114.37	18	1
4	A	368	PX4	C19-C18-C17	2.16	103.43	114.37	15	1
4	A	388	PX4	C4-N1-C2	2.16	118.51	109.91	12	1
4	A	347	PX4	C5-N1-C2	2.16	118.50	109.91	1	2
4	A	410	PX4	O3-C1-C2	2.16	120.05	109.65	9	1
4	A	356	PX4	O5-C9-C10	2.16	118.42	111.83	7	3
4	A	374	PX4	O1-P1-O4	2.16	117.36	107.57	8	1
4	A	385	PX4	O3-C1-C2	2.16	120.05	109.65	6	1
4	A	390	PX4	C36-C35-C34	2.16	98.77	113.36	5	1
4	A	409	PX4	O1-P1-O3	2.16	97.77	107.57	7	2
4	A	323	PX4	C30-C29-C28	2.16	103.45	114.37	1	1
4	A	399	PX4	C4-N1-C2	2.16	118.49	109.91	3	1
4	A	331	PX4	C3-N1-C2	2.16	118.48	109.91	11	1
4	A	407	PX4	C19-C18-C17	2.16	103.47	114.37	17	1
4	A	336	PX4	C17-C16-C15	2.15	103.48	114.37	14	1
4	A	376	PX4	O3-P1-O2	2.15	100.40	108.94	6	2
4	A	382	PX4	C3-N1-C2	2.15	118.47	109.91	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	416	PX4	C15-C14-C13	2.15	103.47	114.37	2	2
4	A	423	PX4	C17-C16-C15	2.15	125.25	114.37	13	1
4	A	351	PX4	O1-P1-O3	2.15	117.32	107.57	9	1
4	A	312	PX4	C8-O5-C9	2.15	109.26	117.12	6	5
4	A	321	PX4	C31-C30-C29	2.15	125.24	114.37	19	2
4	A	391	PX4	C8-O5-C9	2.15	109.25	117.12	18	1
4	A	337	PX4	O1-P1-O3	2.15	97.82	107.57	18	1
4	A	308	PX4	C11-C10-C9	2.15	121.56	113.69	14	1
4	A	345	PX4	O8-C23-C24	2.15	132.18	123.78	19	2
4	A	347	PX4	C20-C19-C18	2.15	103.50	114.37	6	1
4	A	358	PX4	O3-C1-C2	2.15	119.99	109.65	9	2
4	A	371	PX4	C4-N1-C2	2.15	118.45	109.91	13	1
4	A	375	PX4	C31-C30-C29	2.15	103.50	114.37	12	2
4	A	377	PX4	C3-N1-C2	2.15	118.45	109.91	19	4
4	A	388	PX4	C34-C33-C32	2.15	103.50	114.37	12	1
4	A	409	PX4	C28-C27-C26	2.15	103.50	114.37	16	2
4	A	426	PX4	C25-C24-C23	2.15	105.82	113.69	14	1
4	A	342	PX4	C8-O5-C9	2.15	109.27	117.12	5	1
4	A	353	PX4	C19-C18-C17	2.15	103.52	114.37	1	2
4	A	388	PX4	C18-C17-C16	2.15	103.52	114.37	1	1
4	A	425	PX4	C15-C14-C13	2.15	103.52	114.37	10	2
4	A	368	PX4	O8-C23-C24	2.15	115.39	123.78	5	2
4	A	306	PX4	C14-C13-C12	2.14	103.53	114.37	14	1
4	A	308	PX4	C3-N1-C2	2.14	118.43	109.91	7	2
4	A	314	PX4	O3-C1-C2	2.14	119.97	109.65	10	1
4	A	322	PX4	C26-C25-C24	2.14	121.01	113.13	18	1
4	A	339	PX4	C36-C35-C34	2.14	98.89	113.36	6	1
4	A	369	PX4	O3-C1-C2	2.14	119.97	109.65	18	1
4	A	378	PX4	C32-C31-C30	2.14	103.53	114.37	15	2
4	A	381	PX4	C4-N1-C2	2.14	118.43	109.91	18	1
4	A	430	PX4	C31-C30-C29	2.14	103.53	114.37	6	2
4	A	317	PX4	O1-P1-O4	2.14	117.28	107.57	7	3
4	A	344	PX4	O6-C9-C10	2.14	115.40	123.78	4	1
4	A	350	PX4	C5-N1-C2	2.14	118.43	109.91	16	1
4	A	401	PX4	C36-C35-C34	2.14	98.89	113.36	6	1
4	A	414	PX4	C17-C16-C15	2.14	103.53	114.37	16	2
4	A	418	PX4	C30-C29-C28	2.14	103.53	114.37	12	1
4	A	314	PX4	C28-C27-C26	2.14	103.55	114.37	5	2
4	A	327	PX4	C16-C15-C14	2.14	103.54	114.37	8	1
4	A	362	PX4	C28-C27-C26	2.14	103.54	114.37	1	1
4	A	305	PX4	C27-C26-C25	2.14	103.55	114.37	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	321	PX4	C16-C15-C14	2.14	103.55	114.37	5	1
4	A	328	PX4	C35-C34-C33	2.14	96.48	115.25	1	1
4	A	347	PX4	C8-O5-C9	2.14	109.30	117.12	9	1
4	A	374	PX4	C3-N1-C2	2.14	118.42	109.91	10	2
4	A	425	PX4	C17-C16-C15	2.14	103.55	114.37	14	1
4	A	428	PX4	C3-N1-C2	2.14	118.42	109.91	7	1
4	A	348	PX4	O4-P1-O2	2.14	117.41	108.94	13	1
4	A	363	PX4	C14-C13-C12	2.14	103.56	114.37	11	1
4	A	379	PX4	O6-C9-C10	2.14	115.42	123.78	16	1
4	A	343	PX4	C34-C33-C32	2.14	103.56	114.37	17	1
4	A	337	PX4	C33-C32-C31	2.14	103.57	114.37	9	1
4	A	354	PX4	C15-C14-C13	2.14	103.57	114.37	6	1
4	A	354	PX4	C3-N1-C2	2.14	118.41	109.91	7	1
4	A	359	PX4	C28-C27-C26	2.14	103.56	114.37	9	1
4	A	387	PX4	C19-C18-C17	2.14	103.56	114.37	5	1
4	A	378	PX4	C16-C15-C14	2.14	103.57	114.37	9	1
4	A	382	PX4	O1-P1-O4	2.14	117.25	107.57	15	2
4	A	390	PX4	C29-C28-C27	2.14	103.56	114.37	5	1
4	A	413	PX4	C28-C27-C26	2.14	103.57	114.37	12	1
4	A	417	PX4	C31-C30-C29	2.14	103.57	114.37	4	1
4	A	428	PX4	C16-C15-C14	2.14	103.56	114.37	15	1
4	A	348	PX4	C29-C28-C27	2.13	103.58	114.37	8	2
4	A	350	PX4	C26-C25-C24	2.13	105.28	113.13	11	2
4	A	380	PX4	C32-C31-C30	2.14	103.57	114.37	6	1
4	A	342	PX4	C18-C17-C16	2.13	125.15	114.37	5	1
4	A	356	PX4	C30-C29-C28	2.13	103.58	114.37	9	1
4	A	335	PX4	C13-C12-C11	2.13	103.59	114.37	5	1
4	A	364	PX4	C19-C18-C17	2.13	103.59	114.37	4	1
4	A	383	PX4	C32-C31-C30	2.13	103.59	114.37	20	1
4	A	410	PX4	C17-C16-C15	2.13	103.59	114.37	9	2
4	A	351	PX4	O3-C1-C2	2.13	119.90	109.65	15	1
4	A	353	PX4	C4-N1-C2	2.13	118.38	109.91	20	1
4	A	359	PX4	C4-N1-C2	2.13	118.38	109.91	9	1
4	A	400	PX4	C32-C31-C30	2.13	103.59	114.37	2	1
4	A	379	PX4	C5-N1-C2	2.13	118.38	109.91	13	2
4	A	329	PX4	C27-C26-C25	2.13	103.61	114.37	18	2
4	A	366	PX4	C29-C28-C27	2.13	103.61	114.37	10	1
4	A	315	PX4	C26-C25-C24	2.13	105.31	113.13	14	1
4	A	332	PX4	O3-C1-C2	2.13	119.89	109.65	6	2
4	A	375	PX4	O8-C23-C24	2.13	115.46	123.78	9	2
4	A	387	PX4	O6-C9-C10	2.13	132.10	123.78	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	419	PX4	C15-C14-C13	2.13	103.61	114.37	3	1
4	A	317	PX4	C11-C10-C9	2.13	121.48	113.69	18	1
4	A	412	PX4	C8-O5-C9	2.13	109.35	117.12	2	1
4	A	429	PX4	C14-C13-C12	2.13	103.62	114.37	4	3
4	A	319	PX4	C19-C18-C17	2.12	103.63	114.37	13	1
4	A	350	PX4	C3-N1-C2	2.13	118.36	109.91	10	2
4	A	309	PX4	C36-C35-C34	2.12	99.02	113.36	11	2
4	A	366	PX4	C26-C25-C24	2.12	105.32	113.13	12	1
4	A	374	PX4	C27-C26-C25	2.13	103.62	114.37	12	1
4	A	391	PX4	C13-C12-C11	2.13	103.63	114.37	14	1
4	A	403	PX4	C29-C28-C27	2.13	103.62	114.37	2	1
4	A	308	PX4	O6-C9-C10	2.12	115.48	123.78	15	1
4	A	310	PX4	O3-C1-C2	2.12	119.86	109.65	8	1
4	A	317	PX4	C8-O5-C9	2.12	109.36	117.12	13	1
4	A	338	PX4	O5-C9-O6	2.12	118.32	123.63	9	1
4	A	351	PX4	C19-C18-C17	2.12	103.64	114.37	5	1
4	A	355	PX4	C31-C30-C29	2.12	103.64	114.37	19	1
4	A	412	PX4	C18-C17-C16	2.12	103.64	114.37	9	1
4	A	423	PX4	C27-C26-C25	2.12	103.63	114.37	20	1
4	A	310	PX4	C22-C21-C20	2.12	99.04	113.36	13	1
4	A	328	PX4	C16-C15-C14	2.12	103.64	114.37	4	1
4	A	363	PX4	C17-C16-C15	2.12	103.64	114.37	19	1
4	A	366	PX4	O8-C23-C24	2.12	115.48	123.78	10	1
4	A	406	PX4	C19-C18-C17	2.12	103.64	114.37	2	1
4	A	345	PX4	C18-C17-C16	2.12	103.65	114.37	18	1
4	A	356	PX4	C29-C28-C27	2.12	103.65	114.37	14	3
4	A	417	PX4	C25-C24-C23	2.12	105.92	113.69	1	2
4	A	369	PX4	C33-C32-C31	2.12	125.08	114.37	19	1
4	A	306	PX4	C29-C28-C27	2.12	103.66	114.37	3	1
4	A	370	PX4	O6-C9-C10	2.12	115.49	123.78	17	1
4	A	308	PX4	C27-C26-C25	2.12	103.67	114.37	6	1
4	A	334	PX4	C34-C33-C32	2.12	103.67	114.37	1	2
4	A	363	PX4	C15-C14-C13	2.12	103.67	114.37	15	2
4	A	375	PX4	C30-C29-C28	2.12	103.67	114.37	13	2
4	A	382	PX4	O4-P1-O2	2.12	117.32	108.94	4	2
4	A	403	PX4	O4-P1-O2	2.12	117.32	108.94	17	1
4	A	351	PX4	C16-C15-C14	2.11	103.68	114.37	13	1
4	A	389	PX4	C5-N1-C2	2.12	118.32	109.91	12	2
4	A	421	PX4	C25-C24-C23	2.12	121.45	113.69	11	1
4	A	364	PX4	O6-C9-C10	2.11	115.51	123.78	9	2
4	A	348	PX4	O6-C9-C10	2.11	115.52	123.78	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	373	PX4	C12-C11-C10	2.11	105.36	113.13	2	1
4	A	381	PX4	C20-C19-C18	2.11	103.69	114.37	19	2
4	A	305	PX4	C29-C28-C27	2.11	103.70	114.37	11	1
4	A	333	PX4	C18-C17-C16	2.11	103.69	114.37	11	1
4	A	429	PX4	O8-C23-C24	2.11	132.04	123.78	7	1
4	A	410	PX4	C14-C13-C12	2.11	103.70	114.37	2	1
4	A	313	PX4	C19-C18-C17	2.11	103.71	114.37	7	2
4	A	313	PX4	C14-C13-C12	2.11	103.71	114.37	11	1
4	A	335	PX4	C18-C17-C16	2.11	103.70	114.37	9	1
4	A	413	PX4	C4-N1-C2	2.11	118.30	109.91	9	1
4	A	415	PX4	C17-C16-C15	2.11	103.70	114.37	10	1
4	A	327	PX4	C20-C19-C18	2.11	103.72	114.37	13	1
4	A	345	PX4	C5-N1-C4	2.11	103.44	108.98	5	1
4	A	346	PX4	C5-N1-C2	2.11	118.28	109.91	9	1
4	A	351	PX4	O1-P1-O4	2.11	98.02	107.57	6	2
4	A	388	PX4	C5-N1-C4	2.11	114.51	108.98	1	1
4	A	349	PX4	C27-C26-C25	2.10	125.01	114.37	1	1
4	A	353	PX4	C5-N1-C2	2.11	101.54	109.91	9	1
4	A	360	PX4	C34-C33-C32	2.11	103.72	114.37	19	1
4	A	362	PX4	C31-C30-C29	2.11	103.73	114.37	12	3
4	A	367	PX4	C3-N1-C2	2.11	118.28	109.91	8	1
4	A	372	PX4	C16-C15-C14	2.11	103.72	114.37	11	1
4	A	378	PX4	C27-C26-C25	2.11	103.73	114.37	7	2
4	A	403	PX4	C13-C12-C11	2.10	103.73	114.37	10	1
4	A	410	PX4	C16-C15-C14	2.10	103.73	114.37	9	1
4	A	417	PX4	C19-C18-C17	2.11	103.72	114.37	9	1
4	A	313	PX4	C5-N1-C2	2.10	118.27	109.91	13	1
4	A	336	PX4	C5-N1-C4	2.10	103.45	108.98	13	1
4	A	371	PX4	C13-C12-C11	2.10	103.73	114.37	11	1
4	A	419	PX4	C28-C27-C26	2.10	103.73	114.37	1	2
4	A	342	PX4	C20-C19-C18	2.10	103.74	114.37	6	2
4	A	358	PX4	C3-N1-C2	2.10	101.55	109.91	16	1
4	A	376	PX4	C4-N1-C2	2.10	118.27	109.91	14	1
4	A	409	PX4	C8-O5-C9	2.10	109.44	117.12	7	1
4	A	418	PX4	C36-C35-C34	2.10	99.17	113.36	8	1
4	A	427	PX4	C14-C13-C12	2.10	103.74	114.37	13	1
4	A	335	PX4	C4-N1-C2	2.10	101.56	109.91	2	1
4	A	360	PX4	C13-C12-C11	2.10	103.75	114.37	16	2
4	A	390	PX4	C22-C21-C20	2.10	99.17	113.36	19	1
4	A	395	PX4	C20-C19-C18	2.10	103.75	114.37	12	1
4	A	407	PX4	C15-C14-C13	2.10	103.75	114.37	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	417	PX4	C29-C28-C27	2.10	103.75	114.37	15	2
4	A	430	PX4	C34-C33-C32	2.10	103.75	114.37	4	1
4	A	371	PX4	C17-C16-C15	2.10	103.76	114.37	16	2
4	A	410	PX4	C32-C31-C30	2.10	103.76	114.37	15	1
4	A	415	PX4	C5-N1-C2	2.10	101.57	109.91	2	1
4	A	384	PX4	C20-C19-C18	2.10	103.77	114.37	8	1
4	A	416	PX4	C27-C26-C25	2.10	103.76	114.37	13	1
4	A	347	PX4	C32-C31-C30	2.10	103.77	114.37	7	1
4	A	417	PX4	C20-C19-C18	2.10	103.77	114.37	7	1
4	A	333	PX4	O1-P1-O4	2.10	117.06	107.57	16	1
4	A	376	PX4	C19-C18-C17	2.09	103.78	114.37	8	1
4	A	379	PX4	O7-C7-C6	2.10	115.86	108.34	9	3
4	A	382	PX4	C12-C11-C10	2.10	105.43	113.13	13	1
4	A	309	PX4	C22-C21-C20	2.09	99.22	113.36	18	1
4	A	333	PX4	O1-P1-O3	2.09	117.06	107.57	2	1
4	A	349	PX4	O4-P1-O2	2.09	117.23	108.94	3	1
4	A	367	PX4	C5-N1-C2	2.09	118.23	109.91	2	3
4	A	392	PX4	C22-C21-C20	2.09	99.22	113.36	1	1
4	A	405	PX4	C11-C10-C9	2.09	106.02	113.69	3	2
4	A	414	PX4	C34-C33-C32	2.10	103.78	114.37	14	2
4	A	429	PX4	C15-C14-C13	2.09	103.78	114.37	19	1
5	A	432	C3S	C54-C57-C60	2.09	122.66	113.28	16	1
4	A	386	PX4	C31-C30-C29	2.09	103.79	114.37	10	1
4	A	333	PX4	C26-C25-C24	2.09	120.81	113.13	10	1
4	A	340	PX4	O3-C1-C2	2.09	119.70	109.65	4	1
4	A	346	PX4	C35-C34-C33	2.09	96.91	115.25	5	1
4	A	313	PX4	C27-C26-C25	2.09	103.81	114.37	15	1
4	A	324	PX4	O3-C1-C2	2.09	119.70	109.65	16	1
4	A	339	PX4	C26-C25-C24	2.09	105.45	113.13	20	1
4	A	349	PX4	C25-C24-C23	2.09	106.04	113.69	15	1
4	A	393	PX4	C19-C18-C17	2.09	103.81	114.37	12	1
4	A	314	PX4	C27-C26-C25	2.09	103.82	114.37	1	1
4	A	323	PX4	C8-O5-C9	2.09	109.49	117.12	17	1
4	A	375	PX4	C14-C13-C12	2.09	103.81	114.37	16	1
4	A	388	PX4	O8-C23-C24	2.09	115.62	123.78	2	1
4	A	399	PX4	C29-C28-C27	2.09	103.81	114.37	13	1
4	A	320	PX4	O4-P1-O2	2.09	117.20	108.94	15	1
4	A	327	PX4	C30-C29-C28	2.09	103.82	114.37	11	2
4	A	355	PX4	C28-C27-C26	2.09	103.82	114.37	2	2
4	A	373	PX4	O6-C9-C10	2.09	115.62	123.78	20	1
4	A	382	PX4	C32-C31-C30	2.09	103.82	114.37	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	399	PX4	C19-C18-C17	2.09	103.83	114.37	12	1
4	A	401	PX4	C33-C32-C31	2.09	103.82	114.37	11	2
4	A	409	PX4	C3-N1-C2	2.09	118.21	109.91	5	1
4	A	360	PX4	C11-C10-C9	2.09	106.05	113.69	8	1
4	A	312	PX4	C17-C16-C15	2.08	103.83	114.37	7	1
4	A	354	PX4	C34-C33-C32	2.08	103.83	114.37	2	1
4	A	410	PX4	O8-C23-C24	2.09	115.63	123.78	15	1
4	A	364	PX4	O3-C1-C2	2.08	119.67	109.65	3	1
4	A	377	PX4	C27-C26-C25	2.08	103.83	114.37	2	1
4	A	398	PX4	C14-C13-C12	2.08	103.83	114.37	1	2
4	A	408	PX4	C5-N1-C2	2.08	118.19	109.91	12	1
4	A	422	PX4	C14-C13-C12	2.08	103.83	114.37	20	1
4	A	326	PX4	C13-C12-C11	2.08	103.85	114.37	16	1
4	A	366	PX4	C5-N1-C2	2.08	101.63	109.91	20	1
4	A	377	PX4	C4-N1-C3	2.08	103.51	108.98	13	2
4	A	411	PX4	C27-C26-C25	2.08	103.84	114.37	2	1
4	A	335	PX4	C19-C18-C17	2.08	103.85	114.37	3	1
4	A	359	PX4	C5-N1-C2	2.08	101.64	109.91	5	2
4	A	365	PX4	C30-C29-C28	2.08	103.85	114.37	6	1
4	A	368	PX4	C13-C12-C11	2.08	103.85	114.37	6	1
4	A	379	PX4	C20-C19-C18	2.08	103.86	114.37	9	1
4	A	402	PX4	C18-C17-C16	2.08	103.85	114.37	5	1
4	A	331	PX4	C17-C16-C15	2.08	103.86	114.37	11	1
4	A	333	PX4	C21-C20-C19	2.08	97.02	115.25	13	1
4	A	338	PX4	O3-C1-C2	2.08	119.65	109.65	16	1
4	A	348	PX4	C32-C31-C30	2.08	103.86	114.37	10	1
4	A	341	PX4	C17-C16-C15	2.08	103.87	114.37	8	1
4	A	409	PX4	C12-C11-C10	2.08	105.49	113.13	1	1
4	A	429	PX4	C27-C26-C25	2.08	103.86	114.37	8	1
4	A	317	PX4	C31-C30-C29	2.08	103.88	114.37	14	1
4	A	360	PX4	C4-N1-C2	2.08	101.66	109.91	2	2
4	A	320	PX4	C28-C27-C26	2.08	103.88	114.37	9	1
4	A	366	PX4	C19-C18-C17	2.08	103.87	114.37	11	1
4	A	398	PX4	O1-P1-O3	2.08	98.15	107.57	5	1
4	A	413	PX4	C29-C28-C27	2.08	103.87	114.37	2	2
4	A	352	PX4	C30-C29-C28	2.07	103.88	114.37	13	1
4	A	396	PX4	C29-C28-C27	2.07	103.88	114.37	8	1
4	A	397	PX4	C34-C33-C32	2.07	103.89	114.37	3	1
4	A	413	PX4	C33-C32-C31	2.07	103.88	114.37	7	1
4	A	320	PX4	C18-C17-C16	2.07	103.89	114.37	6	1
4	A	404	PX4	C30-C29-C28	2.07	103.89	114.37	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	313	PX4	C30-C29-C28	2.07	103.90	114.37	1	1
4	A	313	PX4	C32-C31-C30	2.07	103.90	114.37	5	1
4	A	364	PX4	C36-C35-C34	2.07	99.38	113.36	20	1
4	A	368	PX4	C27-C26-C25	2.07	103.90	114.37	14	1
4	A	370	PX4	O8-C23-C24	2.07	115.68	123.78	2	1
4	A	387	PX4	C14-C13-C12	2.07	103.89	114.37	1	1
4	A	381	PX4	C14-C13-C12	2.07	103.90	114.37	6	1
4	A	425	PX4	C26-C25-C24	2.07	105.52	113.13	11	2
4	A	318	PX4	C22-C21-C20	2.07	99.39	113.36	11	1
4	A	326	PX4	C32-C31-C30	2.07	103.91	114.37	7	2
4	A	345	PX4	C13-C12-C11	2.07	103.91	114.37	17	1
4	A	324	PX4	C14-C13-C12	2.07	103.91	114.37	12	1
4	A	412	PX4	C29-C28-C27	2.07	103.91	114.37	12	2
4	A	306	PX4	C17-C16-C15	2.07	124.81	114.37	1	1
4	A	322	PX4	C28-C27-C26	2.07	103.92	114.37	9	1
4	A	382	PX4	C25-C24-C23	2.07	106.12	113.69	10	1
4	A	392	PX4	C26-C25-C24	2.07	105.53	113.13	15	1
4	A	401	PX4	O3-C1-C2	2.07	119.59	109.65	15	2
4	A	324	PX4	C18-C17-C16	2.07	103.93	114.37	18	1
4	A	328	PX4	C27-C26-C25	2.06	103.93	114.37	12	1
4	A	354	PX4	C27-C26-C25	2.07	103.92	114.37	8	1
4	A	418	PX4	O1-P1-O4	2.07	116.93	107.57	12	1
4	A	428	PX4	C27-C26-C25	2.07	103.92	114.37	16	1
4	A	318	PX4	O1-P1-O4	2.06	116.92	107.57	7	1
4	A	324	PX4	C15-C14-C13	2.06	103.94	114.37	20	1
4	A	332	PX4	C34-C33-C32	2.06	103.93	114.37	6	1
4	A	381	PX4	C19-C18-C17	2.06	103.93	114.37	15	2
4	A	406	PX4	C12-C11-C10	2.06	105.54	113.13	9	1
4	A	374	PX4	C15-C14-C13	2.06	103.94	114.37	8	1
4	A	406	PX4	C30-C29-C28	2.06	103.94	114.37	2	1
4	A	415	PX4	C22-C21-C20	2.06	99.44	113.36	16	1
4	A	318	PX4	C29-C28-C27	2.06	103.95	114.37	7	1
4	A	330	PX4	C12-C11-C10	2.06	120.70	113.13	18	2
4	A	341	PX4	C3-N1-C2	2.06	101.72	109.91	15	1
4	A	423	PX4	C20-C19-C18	2.06	103.96	114.37	2	1
4	A	430	PX4	C4-N1-C2	2.06	118.10	109.91	16	2
4	A	334	PX4	C4-N1-C2	2.06	118.09	109.91	14	1
4	A	344	PX4	C26-C25-C24	2.06	105.56	113.13	20	2
4	A	376	PX4	C3-N1-C2	2.06	101.73	109.91	20	1
4	A	399	PX4	C12-C11-C10	2.06	105.56	113.13	17	2
5	A	436	C3S	C65-C63-C60	2.06	123.74	111.55	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	344	PX4	O1-P1-O3	2.06	98.24	107.57	16	1
4	A	399	PX4	C8-O5-C9	2.06	109.60	117.12	12	1
4	A	316	PX4	C27-C26-C25	2.06	103.98	114.37	12	1
4	A	316	PX4	C5-N1-C2	2.06	101.74	109.91	18	1
4	A	329	PX4	C18-C17-C16	2.06	103.98	114.37	20	1
4	A	311	PX4	C33-C32-C31	2.05	103.98	114.37	19	1
4	A	359	PX4	C29-C28-C27	2.05	103.98	114.37	8	1
4	A	382	PX4	C33-C32-C31	2.06	103.98	114.37	12	1
4	A	406	PX4	C3-N1-C2	2.06	118.08	109.91	5	1
4	A	339	PX4	C4-N1-C2	2.05	118.07	109.91	10	1
4	A	318	PX4	C30-C29-C28	2.05	103.99	114.37	9	1
4	A	329	PX4	C28-C27-C26	2.05	103.99	114.37	6	2
4	A	379	PX4	C27-C26-C25	2.05	103.99	114.37	4	1
4	A	384	PX4	C25-C24-C23	2.05	106.17	113.69	18	1
4	A	341	PX4	C25-C24-C23	2.05	121.21	113.69	19	1
4	A	406	PX4	C5-N1-C2	2.05	118.07	109.91	16	1
4	A	384	PX4	O6-C9-C10	2.05	115.76	123.78	12	1
4	A	406	PX4	C20-C19-C18	2.05	104.00	114.37	8	2
4	A	409	PX4	O6-C9-C10	2.05	115.76	123.78	15	1
4	A	424	PX4	C18-C17-C16	2.05	104.00	114.37	9	2
4	A	333	PX4	C19-C18-C17	2.05	104.01	114.37	3	1
4	A	393	PX4	C21-C20-C19	2.05	97.27	115.25	6	1
4	A	426	PX4	C14-C13-C12	2.05	104.00	114.37	8	1
4	A	350	PX4	C15-C14-C13	2.05	104.01	114.37	14	1
4	A	367	PX4	C30-C29-C28	2.05	104.01	114.37	18	1
4	A	318	PX4	C20-C19-C18	2.05	104.02	114.37	2	1
4	A	319	PX4	C36-C35-C34	2.05	99.53	113.36	16	1
4	A	375	PX4	O6-C9-C10	2.05	131.79	123.78	14	1
4	A	391	PX4	C28-C27-C26	2.05	104.02	114.37	15	1
5	A	431	C3S	O4-S1-O2	2.05	120.14	112.24	18	2
4	A	306	PX4	C27-C26-C25	2.05	104.02	114.37	9	1
4	A	342	PX4	O6-C9-C10	2.05	115.78	123.78	14	1
4	A	402	PX4	C29-C28-C27	2.05	104.03	114.37	9	2
4	A	403	PX4	C15-C14-C13	2.05	104.03	114.37	4	2
4	A	427	PX4	O8-C23-C24	2.05	115.78	123.78	10	1
4	A	414	PX4	C13-C12-C11	2.05	104.03	114.37	18	1
4	A	416	PX4	C28-C27-C26	2.05	104.03	114.37	6	1
4	A	318	PX4	C34-C33-C32	2.04	104.04	114.37	11	1
4	A	325	PX4	C25-C24-C23	2.04	106.20	113.69	9	1
4	A	333	PX4	C29-C28-C27	2.04	104.03	114.37	10	1
4	A	360	PX4	C16-C15-C14	2.04	104.03	114.37	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	362	PX4	C29-C28-C27	2.04	104.04	114.37	4	2
4	A	375	PX4	C34-C33-C32	2.04	104.04	114.37	12	2
4	A	380	PX4	C29-C28-C27	2.04	104.04	114.37	10	1
4	A	315	PX4	C15-C14-C13	2.04	104.05	114.37	8	1
4	A	386	PX4	C33-C32-C31	2.04	104.05	114.37	10	1
4	A	401	PX4	C25-C24-C23	2.04	106.21	113.69	10	1
4	A	429	PX4	C29-C28-C27	2.04	104.04	114.37	10	1
4	A	351	PX4	C17-C16-C15	2.04	104.05	114.37	1	1
4	A	312	PX4	C16-C15-C14	2.04	104.06	114.37	3	2
4	A	323	PX4	C27-C26-C25	2.04	104.06	114.37	14	1
4	A	342	PX4	C11-C10-C9	2.04	106.22	113.69	16	1
4	A	423	PX4	C34-C33-C32	2.04	104.05	114.37	8	1
4	A	428	PX4	C25-C24-C23	2.04	106.22	113.69	16	1
4	A	314	PX4	C29-C28-C27	2.04	104.07	114.37	9	1
4	A	326	PX4	O1-P1-O3	2.04	98.33	107.57	17	1
4	A	345	PX4	C8-O5-C9	2.04	109.67	117.12	17	1
4	A	401	PX4	C12-C11-C10	2.04	105.64	113.13	6	1
4	A	381	PX4	C29-C28-C27	2.04	104.07	114.37	13	1
4	A	412	PX4	O4-P1-O2	2.04	100.86	108.94	7	1
4	A	419	PX4	C17-C16-C15	2.04	104.07	114.37	7	2
4	A	421	PX4	C27-C26-C25	2.04	104.07	114.37	18	1
4	A	330	PX4	C17-C16-C15	2.04	104.08	114.37	10	1
4	A	351	PX4	O8-C23-C24	2.03	115.82	123.78	11	1
4	A	370	PX4	C13-C12-C11	2.04	104.08	114.37	15	1
4	A	311	PX4	C8-O5-C9	2.03	109.68	117.12	11	1
4	A	337	PX4	C12-C11-C10	2.03	105.65	113.13	1	1
4	A	378	PX4	C18-C17-C16	2.03	104.09	114.37	10	1
4	A	411	PX4	C34-C33-C32	2.04	104.08	114.37	5	1
4	A	421	PX4	C29-C28-C27	2.03	104.08	114.37	17	1
4	A	318	PX4	C12-C11-C10	2.03	105.66	113.13	13	1
4	A	324	PX4	C17-C16-C15	2.03	104.09	114.37	17	1
4	A	342	PX4	C14-C13-C12	2.03	104.10	114.37	5	1
4	A	343	PX4	C12-C11-C10	2.03	105.66	113.13	3	1
4	A	385	PX4	C22-C21-C20	2.03	99.64	113.36	20	1
4	A	392	PX4	C20-C19-C18	2.03	104.10	114.37	12	1
4	A	403	PX4	C33-C32-C31	2.03	104.09	114.37	3	1
5	A	436	C3S	C57-C54-C48	2.03	120.76	115.08	12	1
4	A	346	PX4	C13-C12-C11	2.03	104.10	114.37	15	1
4	A	314	PX4	C31-C30-C29	2.03	104.11	114.37	1	1
4	A	420	PX4	O6-C9-C10	2.03	115.84	123.78	6	1
4	A	305	PX4	C19-C18-C17	2.03	104.11	114.37	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	344	PX4	O8-C23-C24	2.03	115.84	123.78	2	1
4	A	362	PX4	C34-C33-C32	2.03	104.11	114.37	5	1
4	A	398	PX4	C28-C27-C26	2.03	104.11	114.37	16	1
4	A	424	PX4	C8-O5-C9	2.03	109.70	117.12	2	1
4	A	349	PX4	C32-C31-C30	2.03	104.12	114.37	4	1
4	A	308	PX4	C28-C27-C26	2.03	104.13	114.37	3	1
4	A	420	PX4	C28-C27-C26	2.03	104.13	114.37	5	1
4	A	428	PX4	C34-C33-C32	2.03	104.13	114.37	19	1
4	A	313	PX4	O6-C9-C10	2.02	115.86	123.78	8	1
4	A	315	PX4	C18-C17-C16	2.02	104.14	114.37	20	1
4	A	321	PX4	C34-C33-C32	2.02	104.14	114.37	7	1
4	A	343	PX4	C15-C14-C13	2.02	104.14	114.37	14	1
4	A	343	PX4	C14-C13-C12	2.02	104.14	114.37	20	1
4	A	352	PX4	C32-C31-C30	2.02	104.14	114.37	19	1
4	A	348	PX4	C16-C15-C14	2.02	104.14	114.37	5	1
4	A	354	PX4	C17-C16-C15	2.02	104.14	114.37	9	1
4	A	375	PX4	C17-C16-C15	2.02	104.14	114.37	8	1
4	A	390	PX4	C16-C15-C14	2.02	104.14	114.37	6	1
4	A	401	PX4	O4-P1-O2	2.02	116.95	108.94	18	1
4	A	415	PX4	C3-N1-C2	2.02	117.95	109.91	2	1
4	A	374	PX4	C19-C18-C17	2.02	104.15	114.37	19	1
4	A	377	PX4	C25-C24-C23	2.02	121.10	113.69	12	1
4	A	411	PX4	C20-C19-C18	2.02	104.16	114.37	15	2
4	A	415	PX4	O5-C9-C10	2.02	118.00	111.83	6	1
4	A	356	PX4	C31-C30-C29	2.02	104.16	114.37	8	1
4	A	306	PX4	C16-C15-C14	2.02	104.17	114.37	6	1
4	A	307	PX4	C18-C17-C16	2.02	104.17	114.37	12	1
4	A	316	PX4	C33-C32-C31	2.02	104.16	114.37	18	1
4	A	397	PX4	C36-C35-C34	2.02	99.73	113.36	4	1
4	A	341	PX4	O1-P1-O3	2.02	98.42	107.57	18	1
4	A	382	PX4	C27-C26-C25	2.02	104.17	114.37	12	1
4	A	386	PX4	C27-C26-C25	2.02	104.17	114.37	1	1
4	A	388	PX4	C20-C19-C18	2.02	104.17	114.37	20	1
4	A	318	PX4	C27-C26-C25	2.02	104.17	114.37	11	1
4	A	322	PX4	C15-C14-C13	2.02	104.17	114.37	13	2
4	A	346	PX4	C16-C15-C14	2.02	104.17	114.37	4	1
4	A	357	PX4	C33-C32-C31	2.02	104.17	114.37	4	1
4	A	402	PX4	C27-C26-C25	2.02	104.17	114.37	15	1
4	A	410	PX4	C34-C33-C32	2.02	104.17	114.37	19	1
4	A	412	PX4	C36-C35-C34	2.02	99.74	113.36	17	2
4	A	427	PX4	C4-N1-C2	2.02	117.93	109.91	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	365	PX4	C4-N1-C3	2.02	103.68	108.98	17	1
4	A	307	PX4	C33-C32-C31	2.02	104.18	114.37	9	1
4	A	329	PX4	C16-C15-C14	2.02	104.18	114.37	9	1
4	A	332	PX4	C15-C14-C13	2.02	104.18	114.37	9	1
4	A	368	PX4	C17-C16-C15	2.02	104.18	114.37	2	1
4	A	427	PX4	C5-N1-C2	2.02	101.90	109.91	20	1
5	A	431	C3S	C54-C57-C60	2.02	104.24	113.28	7	1
4	A	308	PX4	C8-O5-C9	2.01	109.76	117.12	5	1
4	A	319	PX4	O3-C1-C2	2.01	119.34	109.65	20	1
4	A	404	PX4	C25-C24-C23	2.01	106.31	113.69	13	1
4	A	400	PX4	C11-C10-C9	2.01	106.32	113.69	9	1
4	A	374	PX4	C20-C19-C18	2.01	104.20	114.37	13	1
4	A	380	PX4	C22-C21-C20	2.01	99.78	113.36	10	1
4	A	386	PX4	O1-P1-O3	2.01	98.45	107.57	16	1
4	A	395	PX4	O4-P1-O2	2.01	116.90	108.94	8	2
4	A	398	PX4	C16-C15-C14	2.01	104.21	114.37	17	1
4	A	407	PX4	O6-C9-C10	2.01	115.92	123.78	13	1
4	A	338	PX4	C16-C15-C14	2.01	104.21	114.37	20	1
4	A	309	PX4	C13-C12-C11	2.01	104.22	114.37	14	1
4	A	315	PX4	O1-P1-O3	2.01	98.47	107.57	12	1
4	A	333	PX4	O6-C9-C10	2.01	115.93	123.78	4	1
4	A	345	PX4	C12-C11-C10	2.01	105.75	113.13	7	1
4	A	367	PX4	C36-C35-C34	2.01	99.80	113.36	11	1
4	A	398	PX4	C26-C25-C24	2.01	120.51	113.13	12	1
4	A	400	PX4	C5-N1-C3	2.01	114.25	108.98	12	1
4	A	308	PX4	C15-C14-C13	2.01	104.23	114.37	13	1
4	A	341	PX4	O6-C9-C10	2.01	115.93	123.78	14	1
4	A	345	PX4	C16-C15-C14	2.01	104.22	114.37	17	1
4	A	313	PX4	O3-C1-C2	2.01	119.30	109.65	2	1
4	A	313	PX4	O8-C23-C24	2.01	115.94	123.78	9	1
4	A	315	PX4	C4-N1-C3	2.01	103.71	108.98	8	1
4	A	332	PX4	C28-C27-C26	2.01	104.23	114.37	19	1
4	A	354	PX4	C28-C27-C26	2.01	104.23	114.37	16	1
4	A	363	PX4	C27-C26-C25	2.01	104.23	114.37	20	1
4	A	380	PX4	C18-C17-C16	2.01	104.22	114.37	1	1
4	A	377	PX4	C29-C28-C27	2.01	104.23	114.37	10	1
4	A	385	PX4	C32-C31-C30	2.01	104.22	114.37	3	1
4	A	392	PX4	C31-C30-C29	2.01	104.23	114.37	5	1
4	A	321	PX4	C22-C21-C20	2.00	99.83	113.36	4	1
4	A	329	PX4	O8-C23-C24	2.00	115.95	123.78	18	1
4	A	330	PX4	C36-C35-C34	2.00	99.83	113.36	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
4	A	349	PX4	C18-C17-C16	2.00	104.24	114.37	15	1
4	A	364	PX4	O1-P1-O4	2.00	116.65	107.57	4	1
4	A	361	PX4	C30-C29-C28	2.00	104.24	114.37	3	1
4	A	391	PX4	C3-N1-C2	2.00	101.95	109.91	4	1
4	A	391	PX4	C29-C28-C27	2.00	104.24	114.37	14	1
4	A	398	PX4	C34-C33-C32	2.00	104.24	114.37	19	1
4	A	335	PX4	C25-C24-C23	2.00	121.03	113.69	14	1
4	A	331	PX4	C32-C31-C30	2.00	104.25	114.37	17	1
4	A	355	PX4	C20-C19-C18	2.00	104.25	114.37	16	1
4	A	409	PX4	C25-C24-C23	2.00	106.36	113.69	17	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
5	A	431	C3S	C7	20
5	A	431	C3S	C48	20
5	A	432	C3S	C48	20
5	A	433	C3S	C48	20
5	A	434	C3S	C48	20
5	A	435	C3S	C7	20
5	A	435	C3S	C48	20
5	A	436	C3S	C7	20
5	A	436	C3S	C48	20

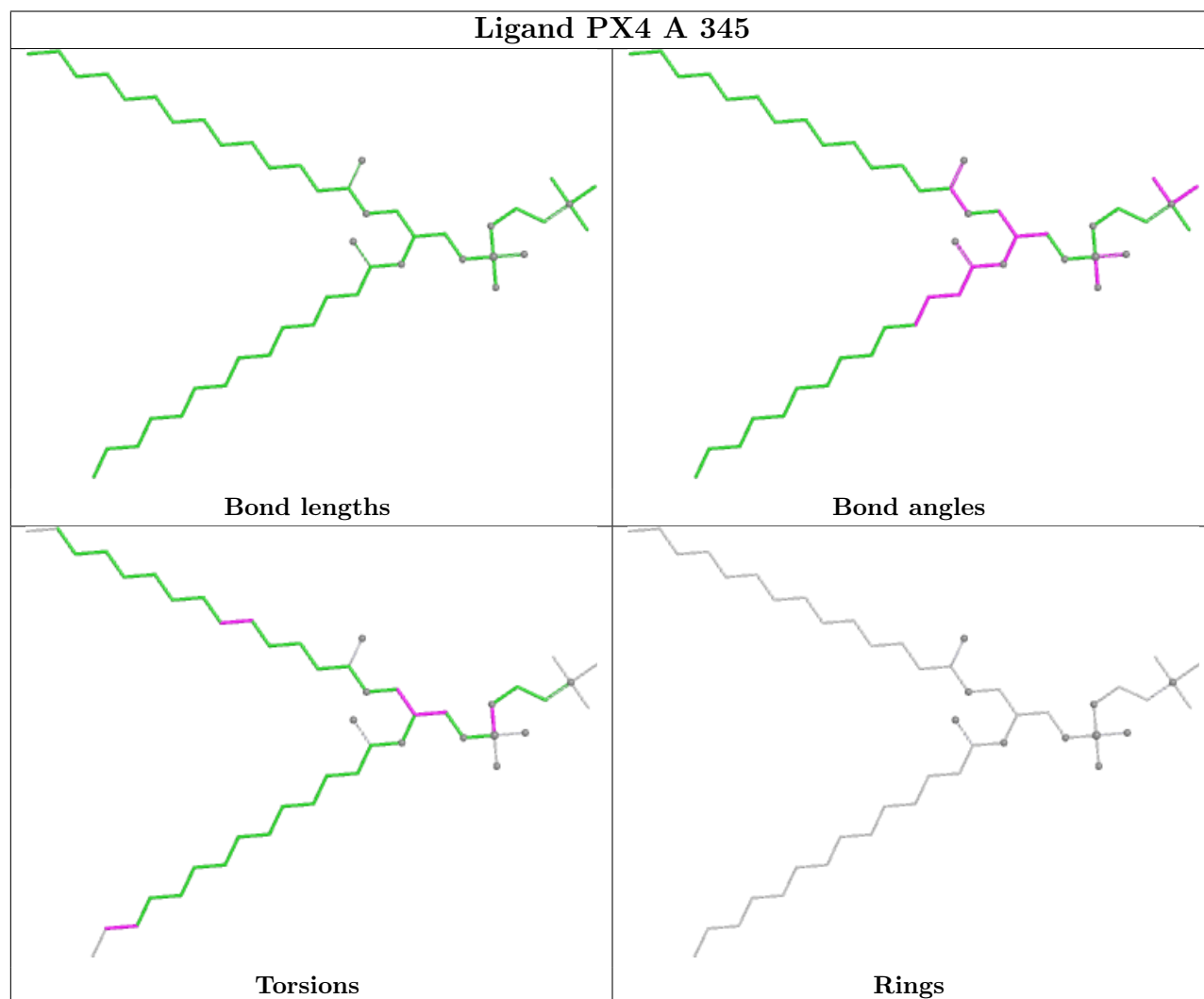
All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

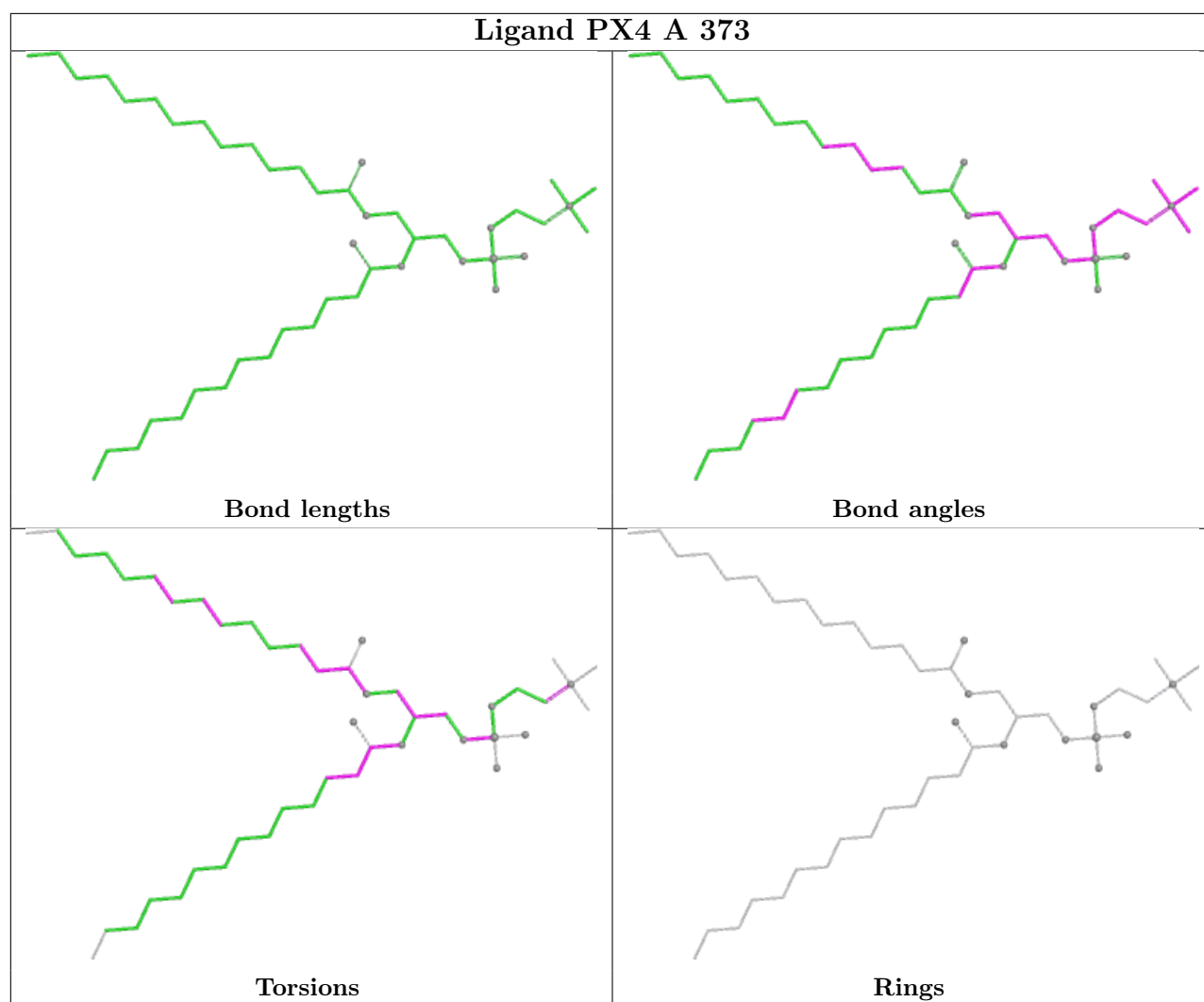
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	377	PX4	O8-C23-O7-C7	12
4	A	376	PX4	O8-C23-O7-C7	5
4	A	356	PX4	O8-C23-O7-C7	3
4	A	372	PX4	O8-C23-O7-C7	1
4	A	376	PX4	C24-C23-O7-C7	1
4	A	424	PX4	O8-C23-O7-C7	1

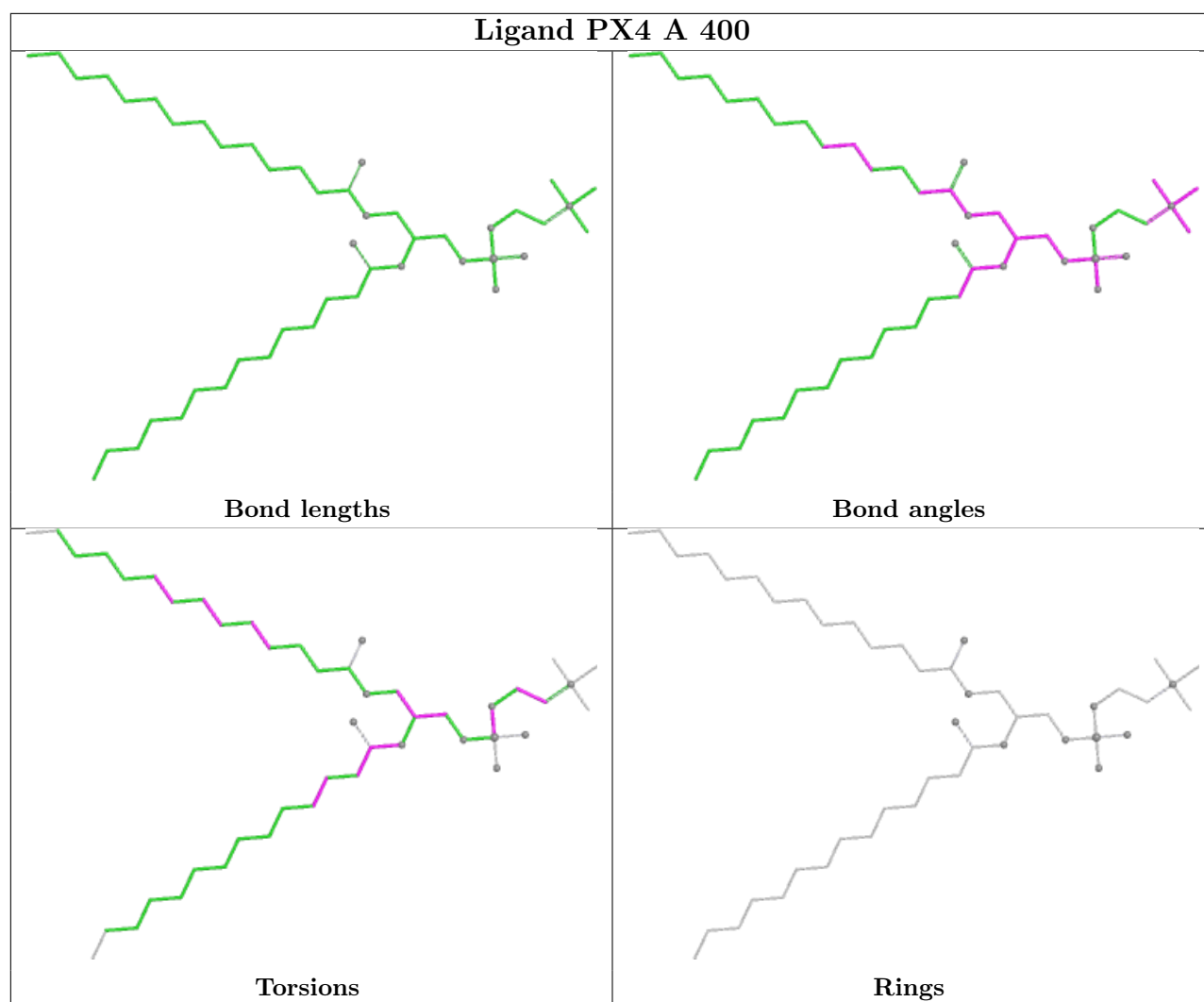
There are no ring outliers.

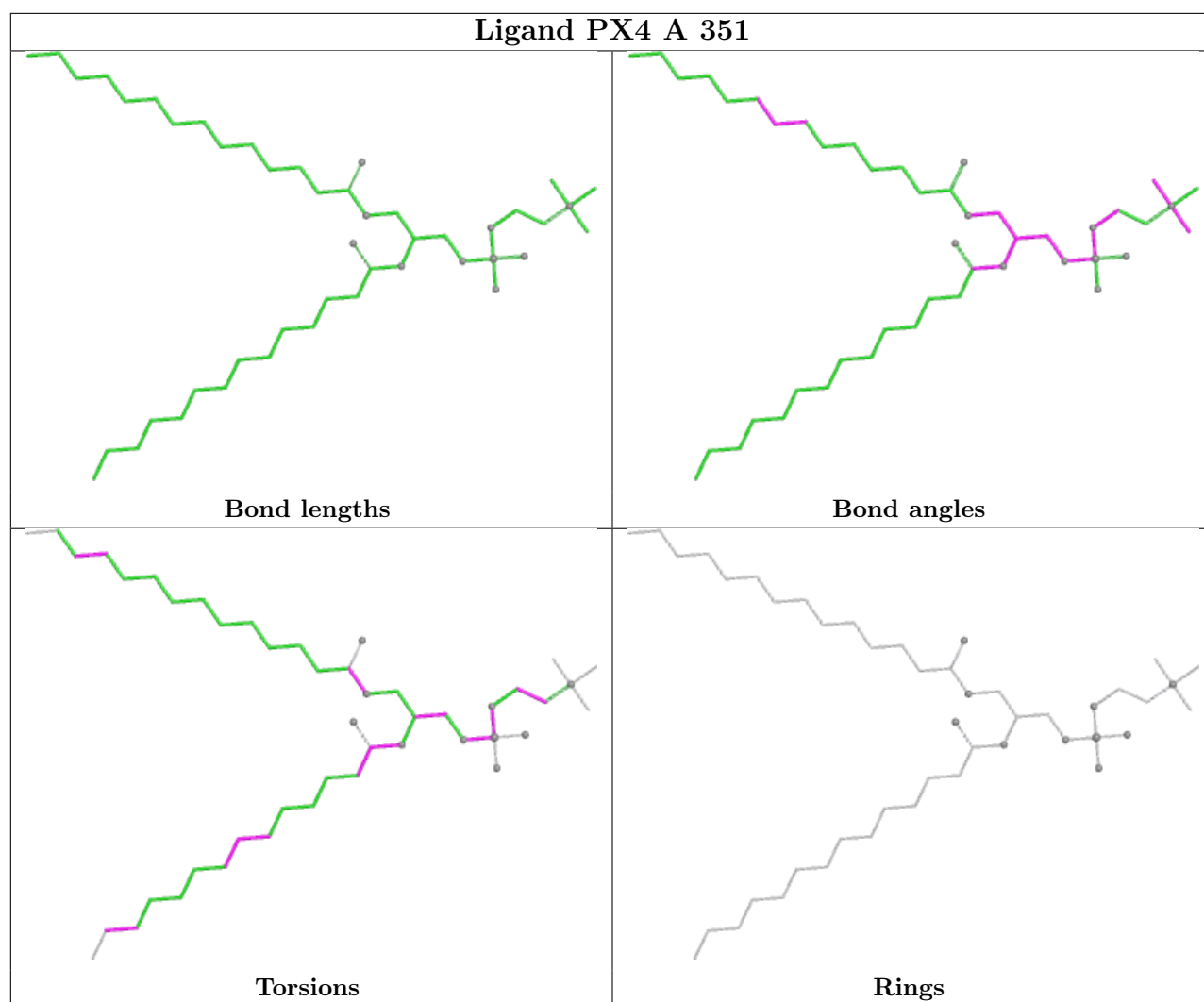
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

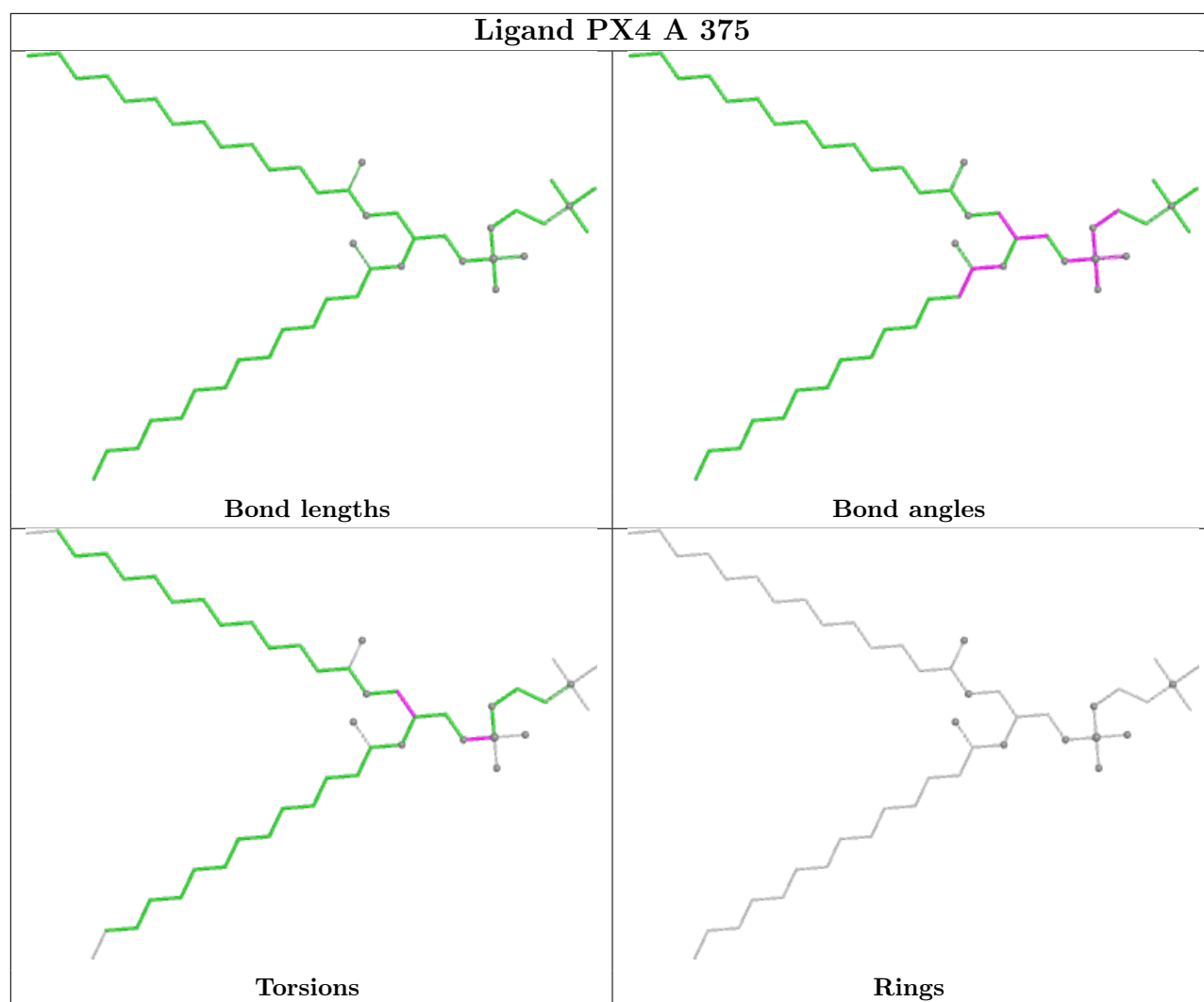
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

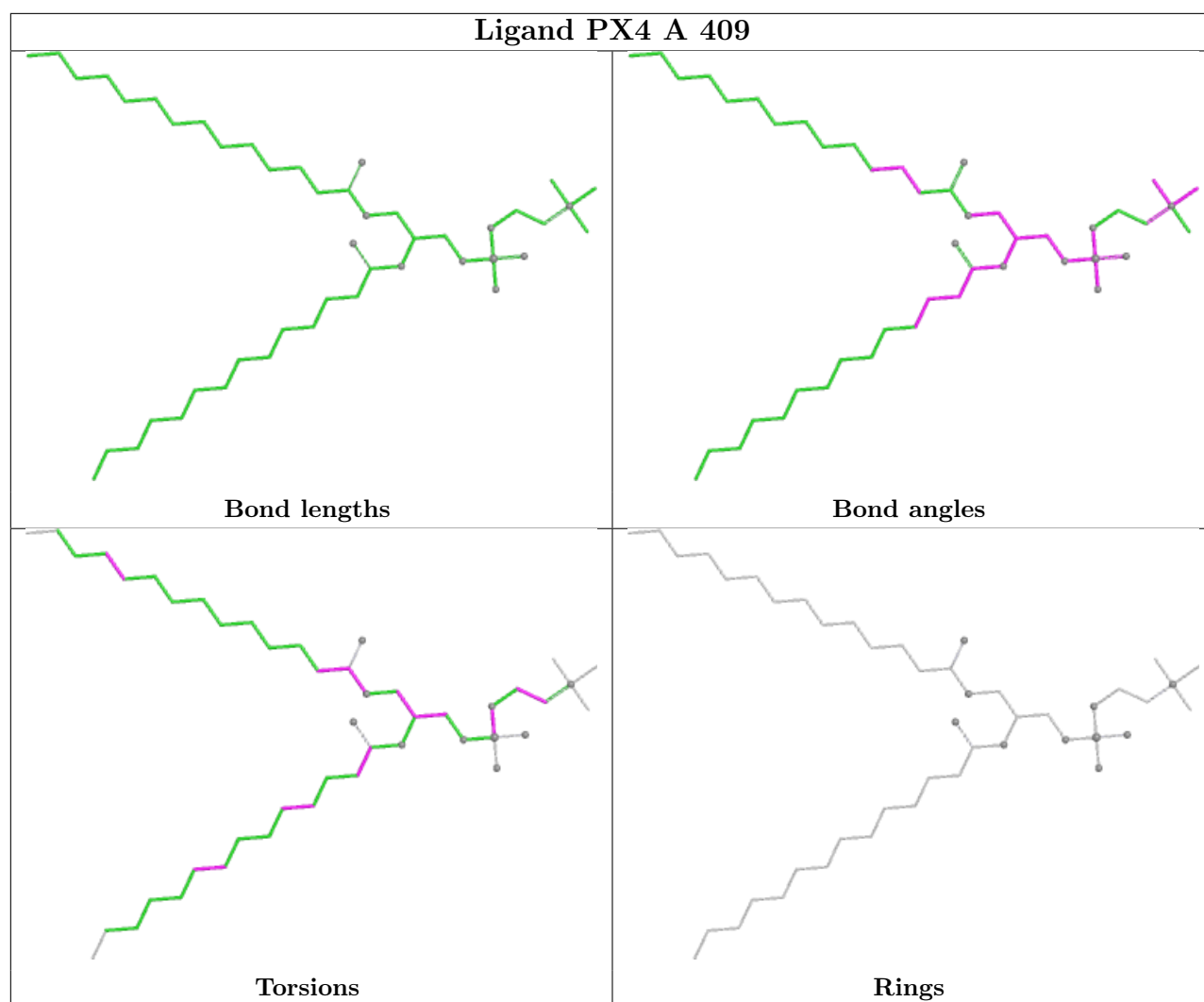


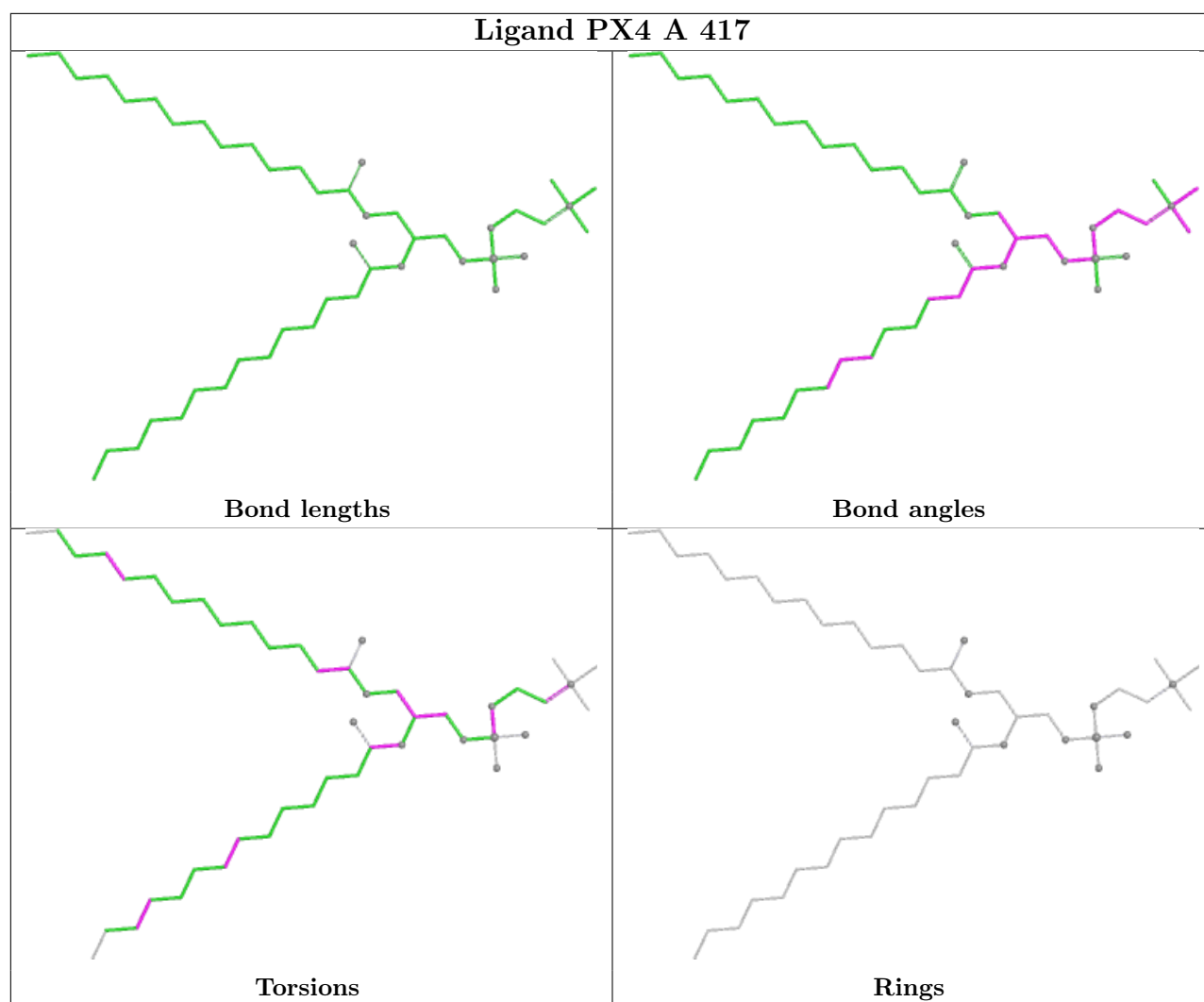


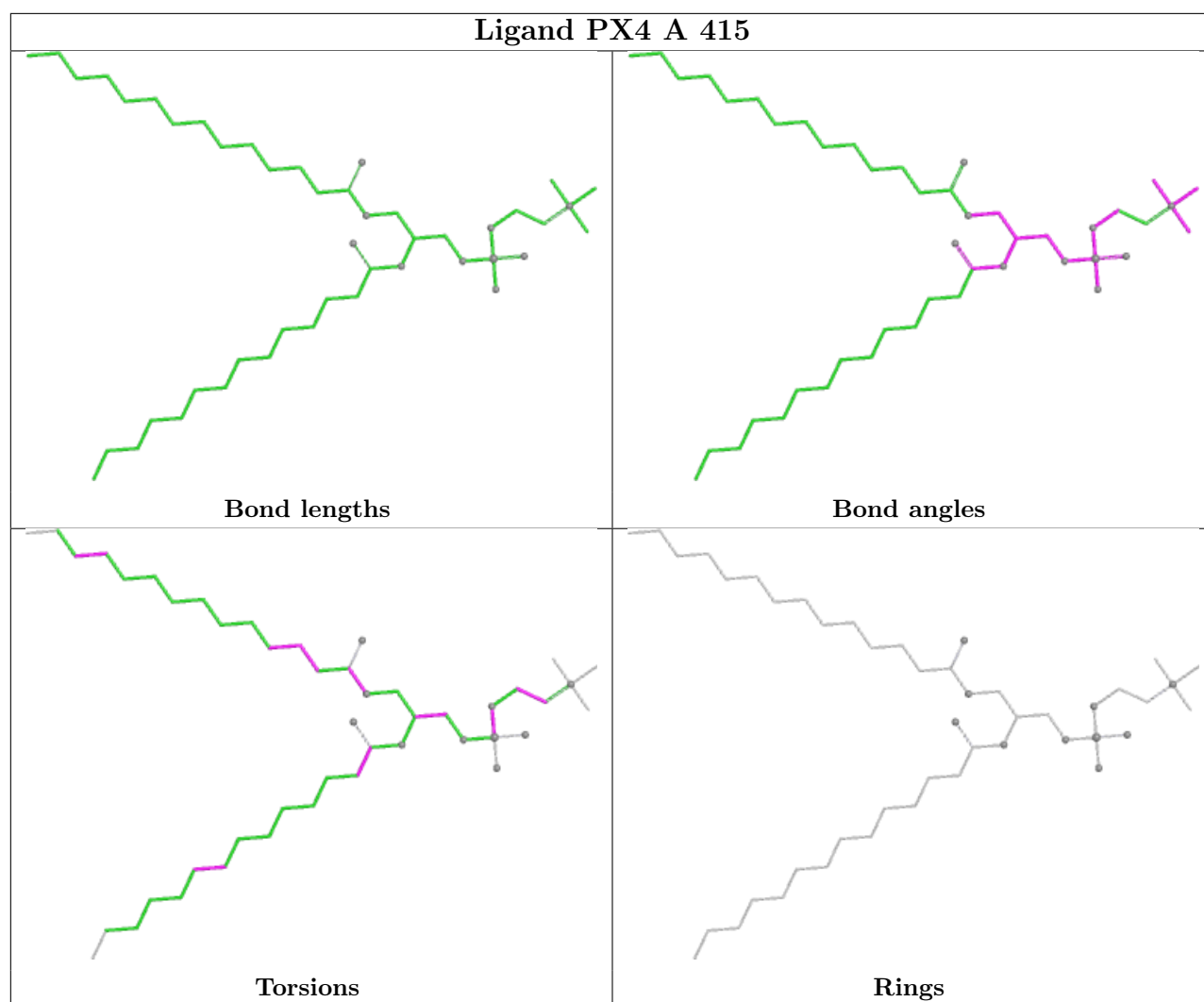


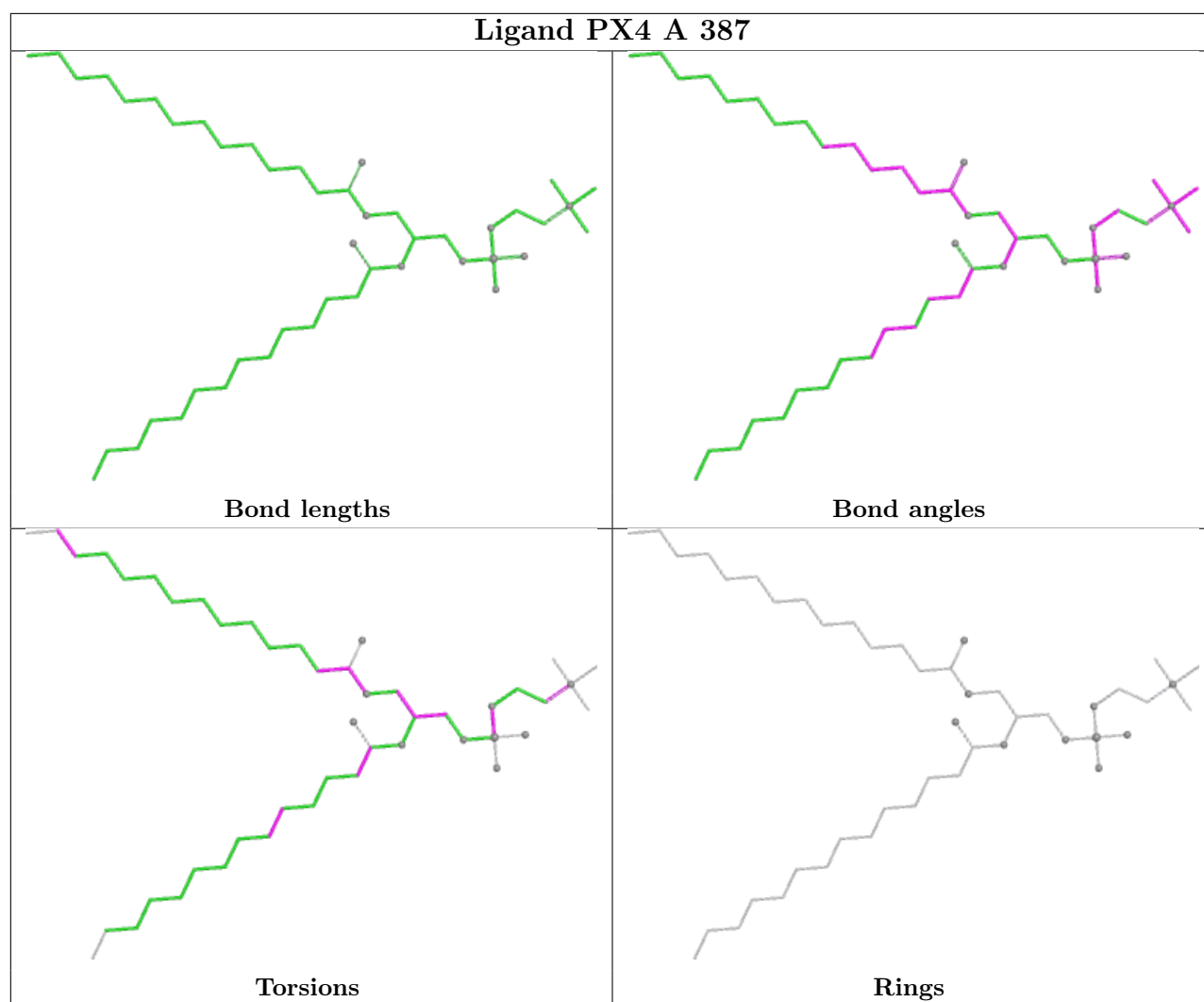


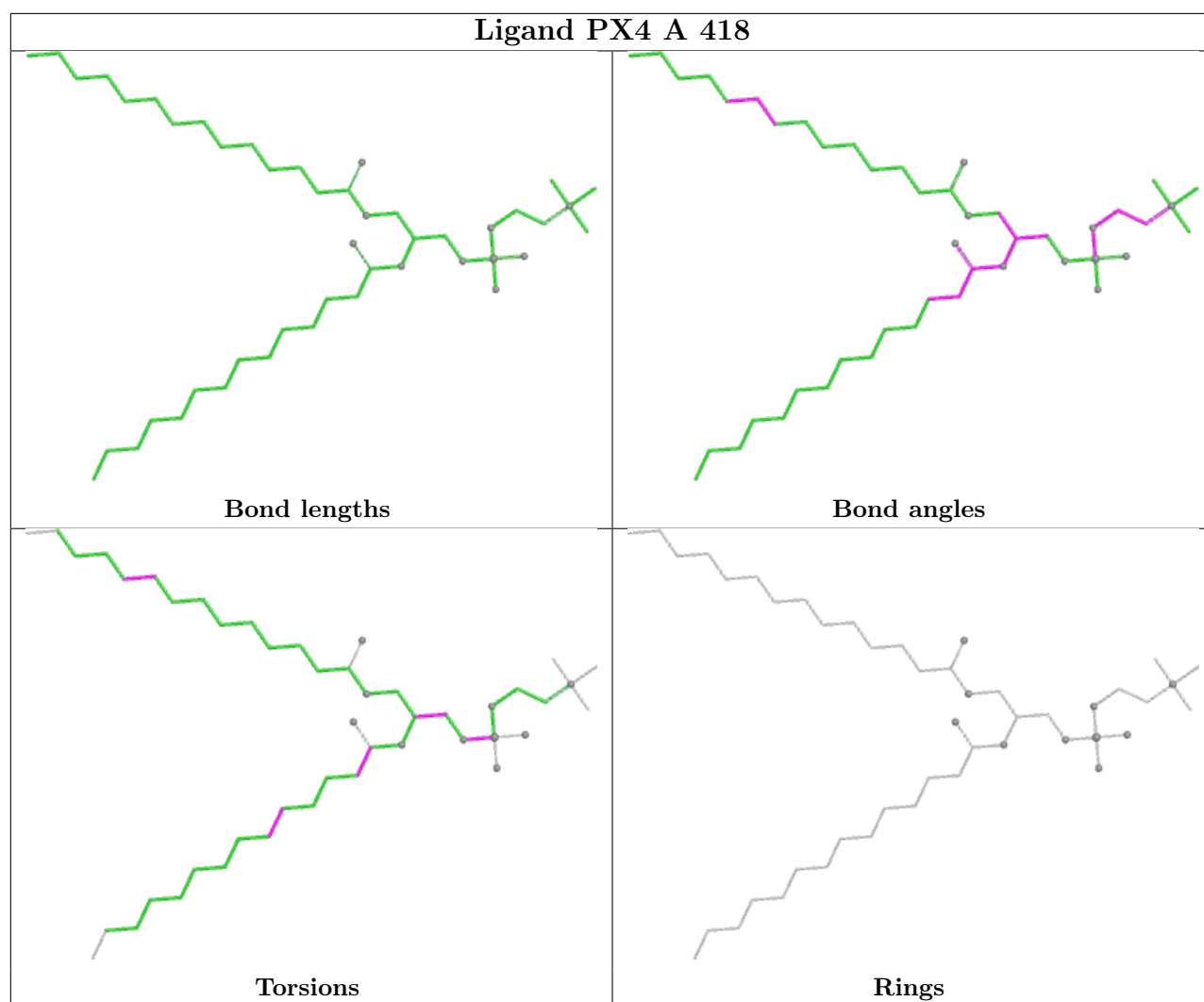


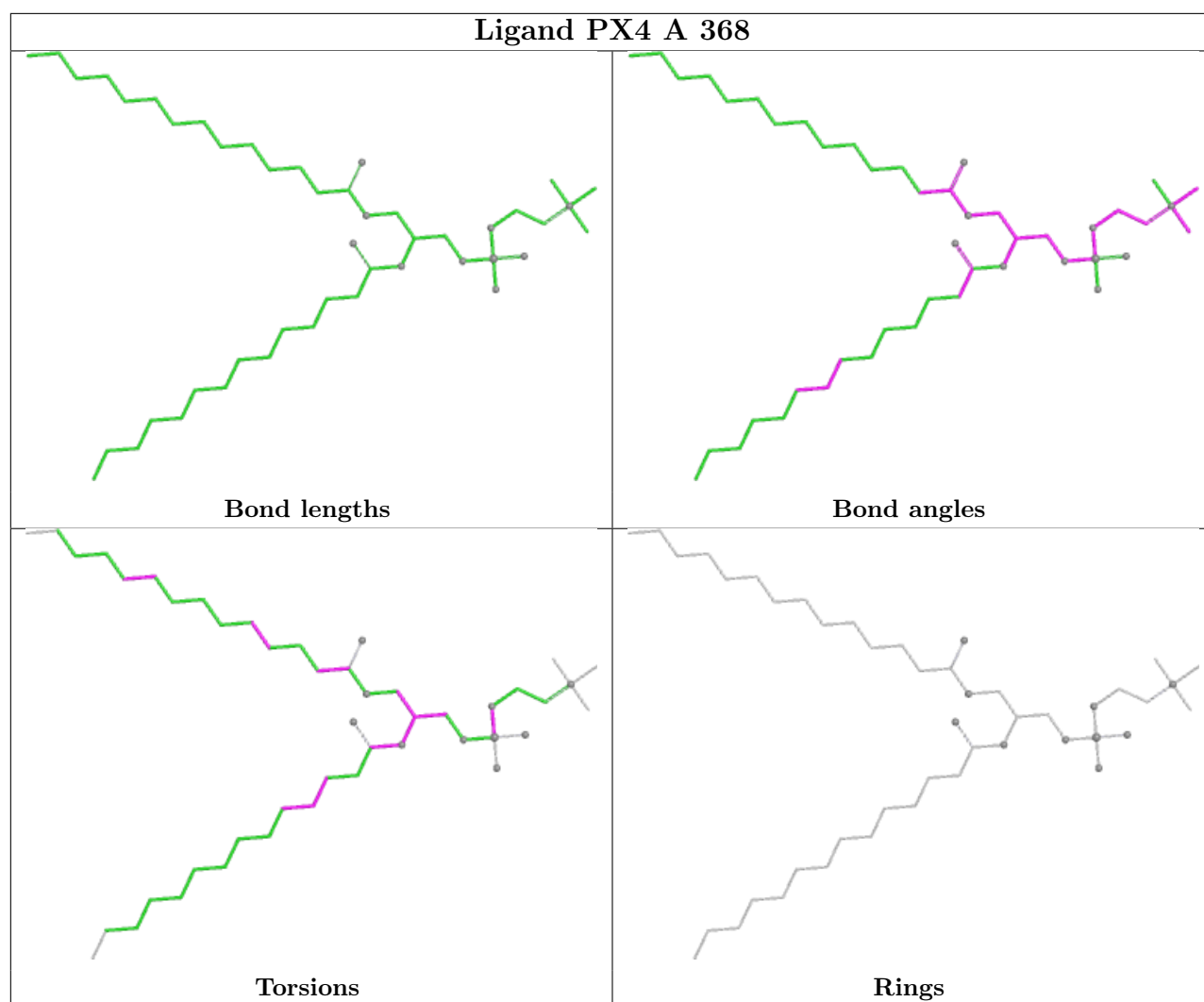


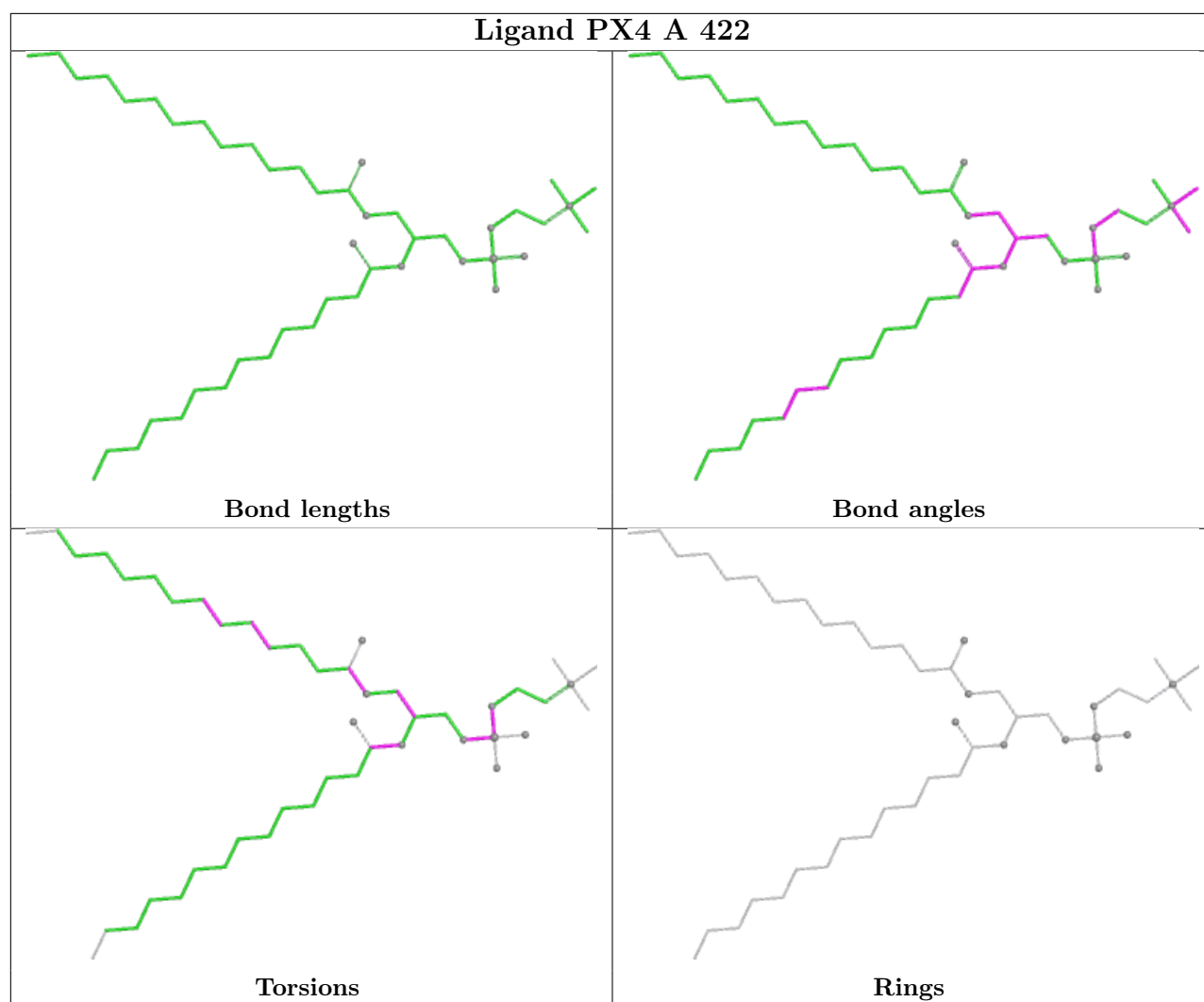


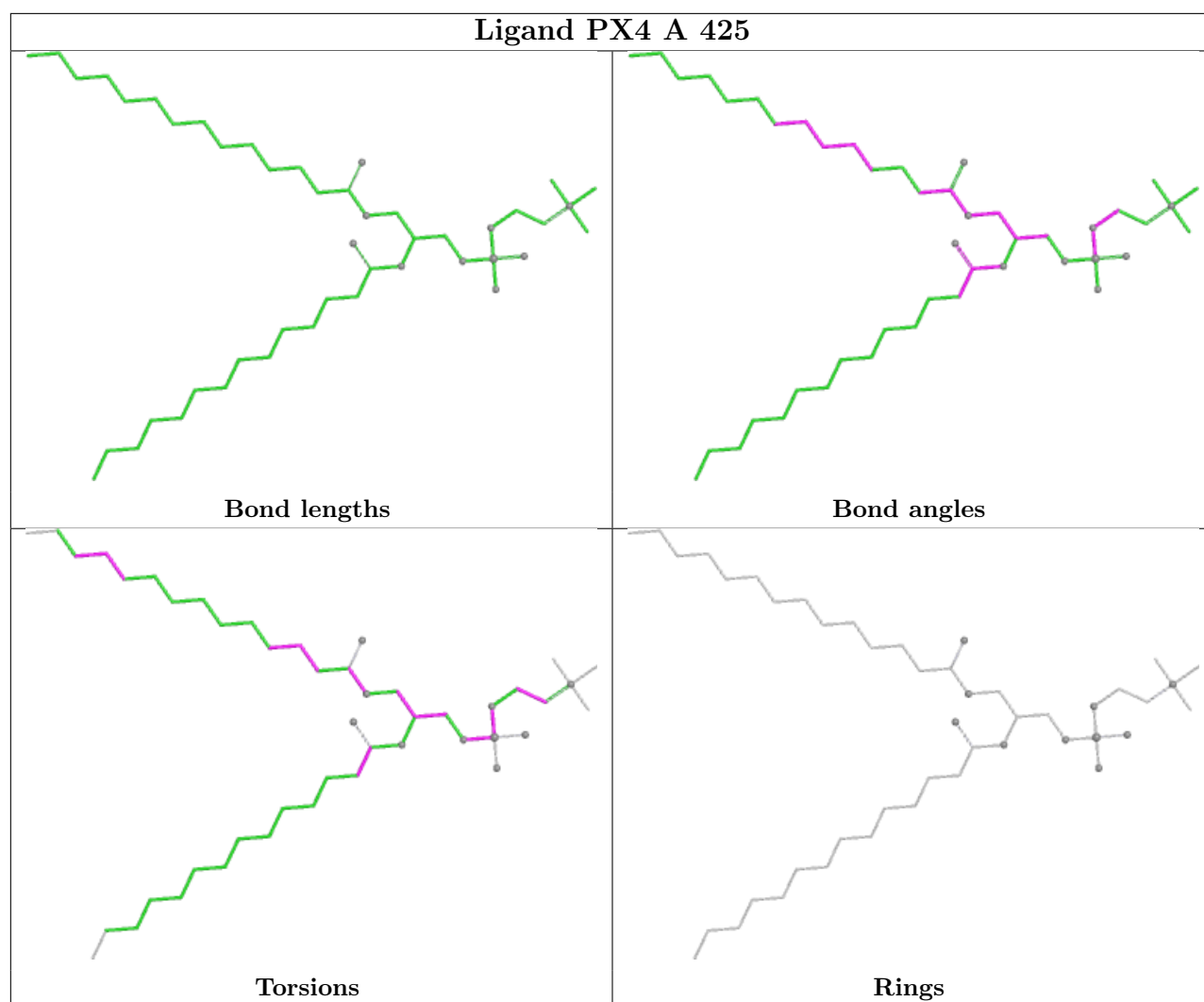


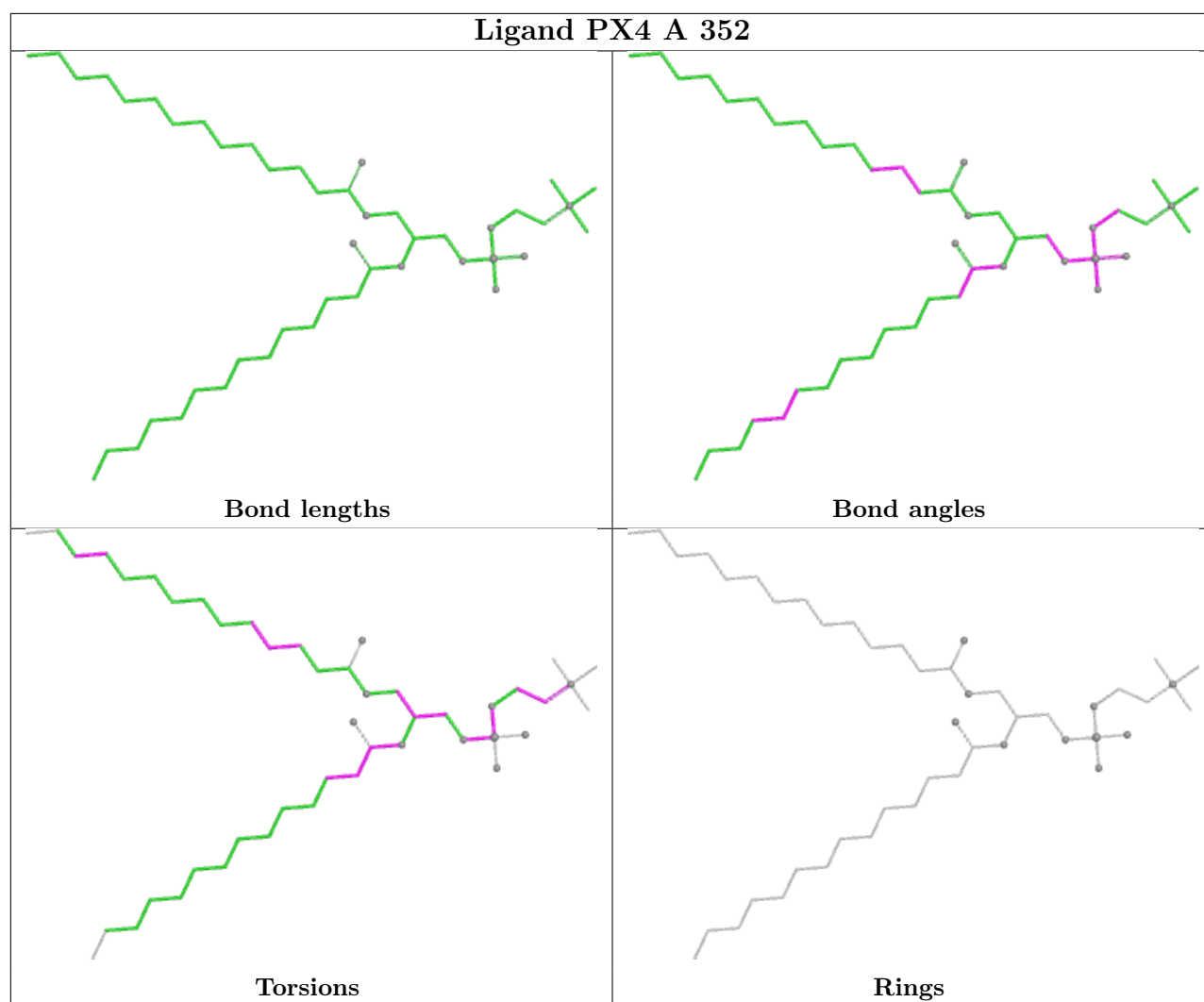


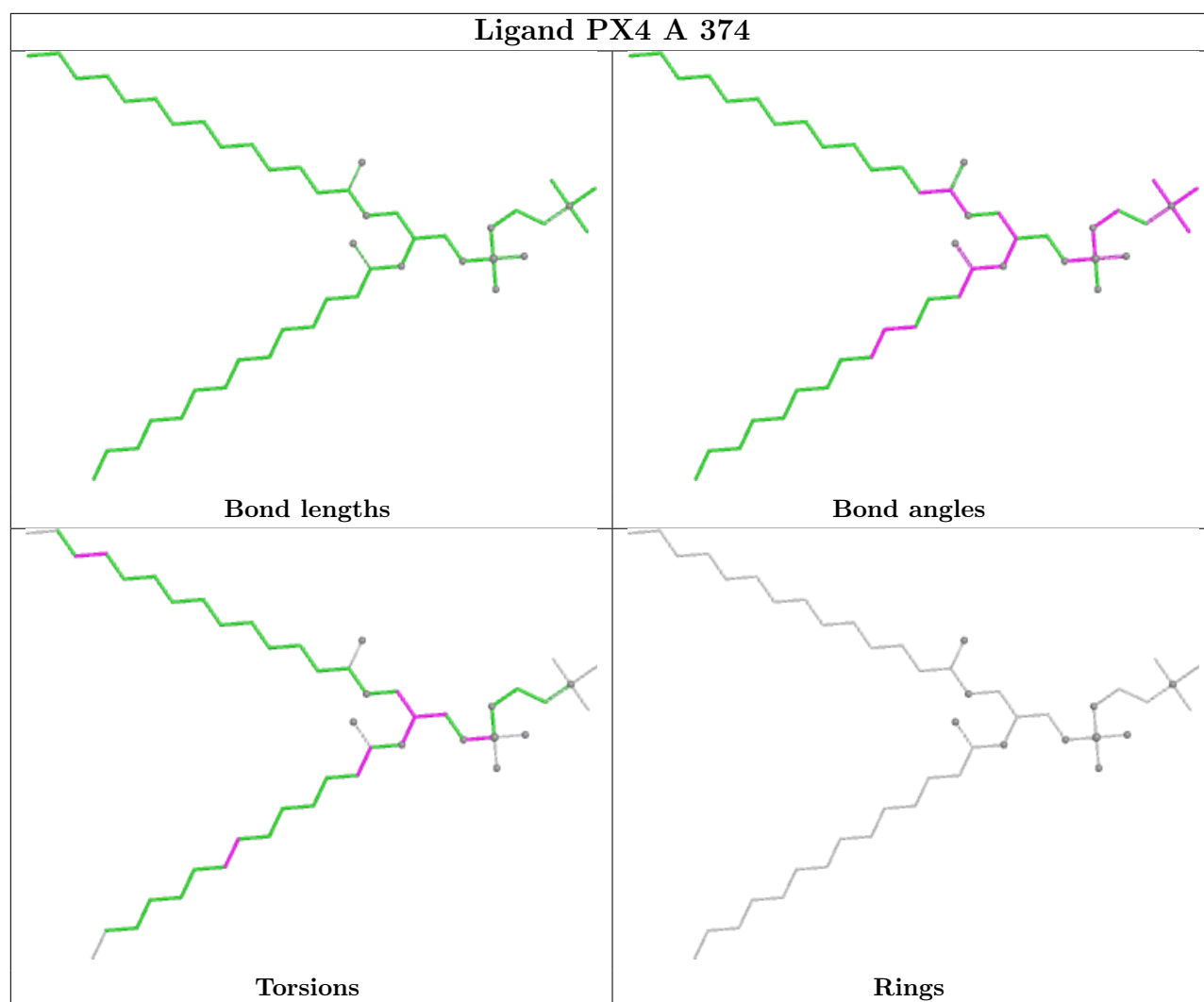


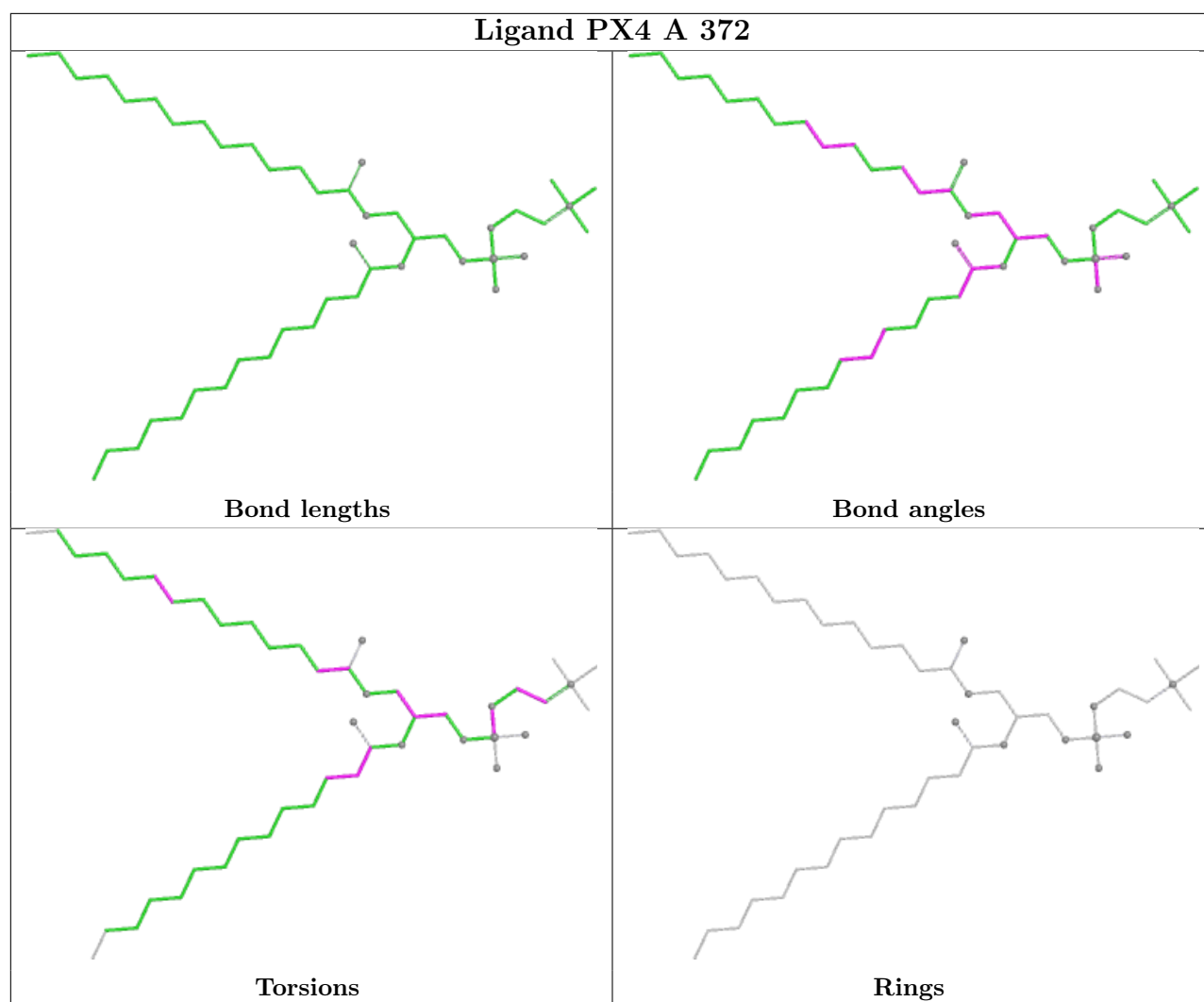


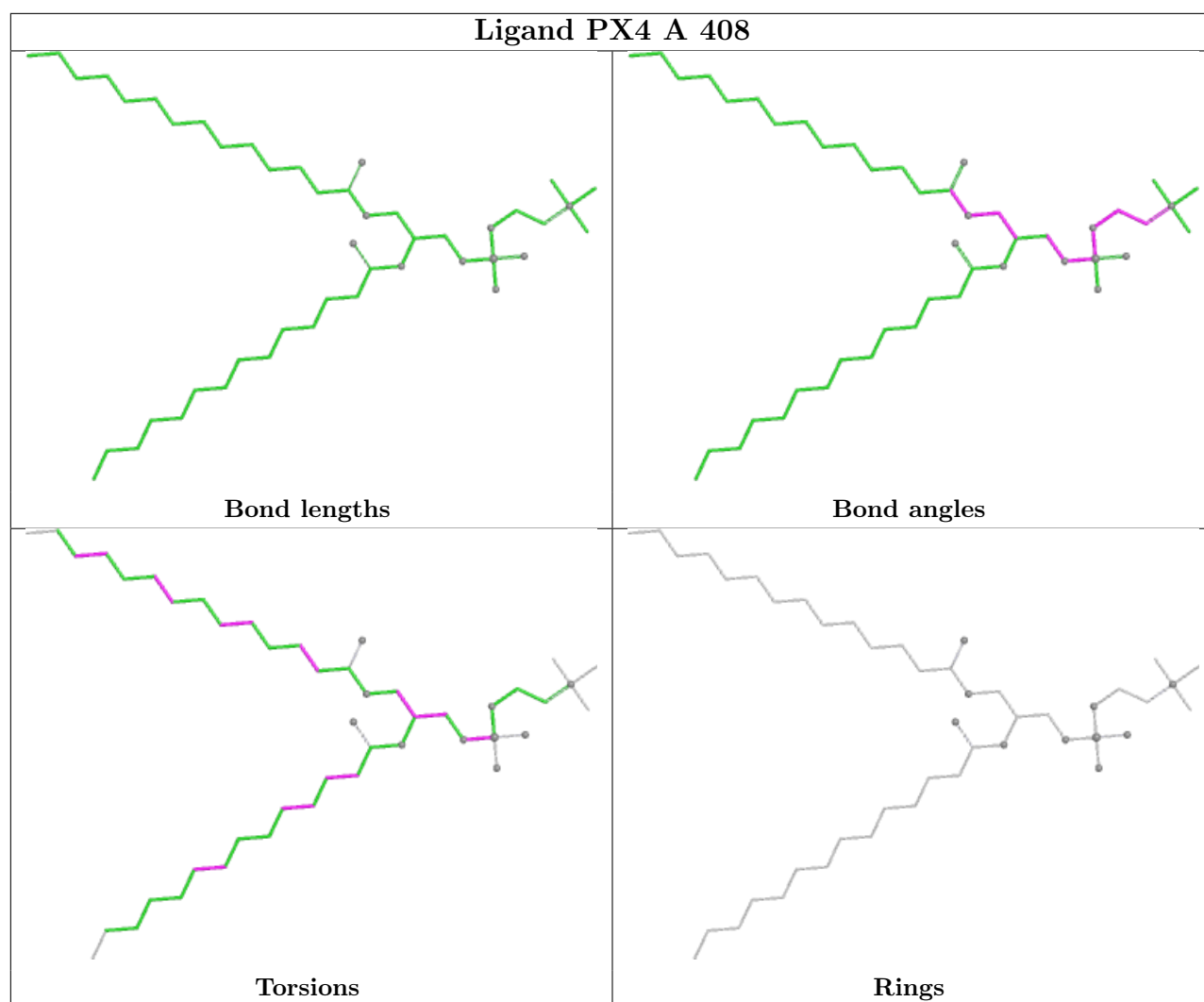


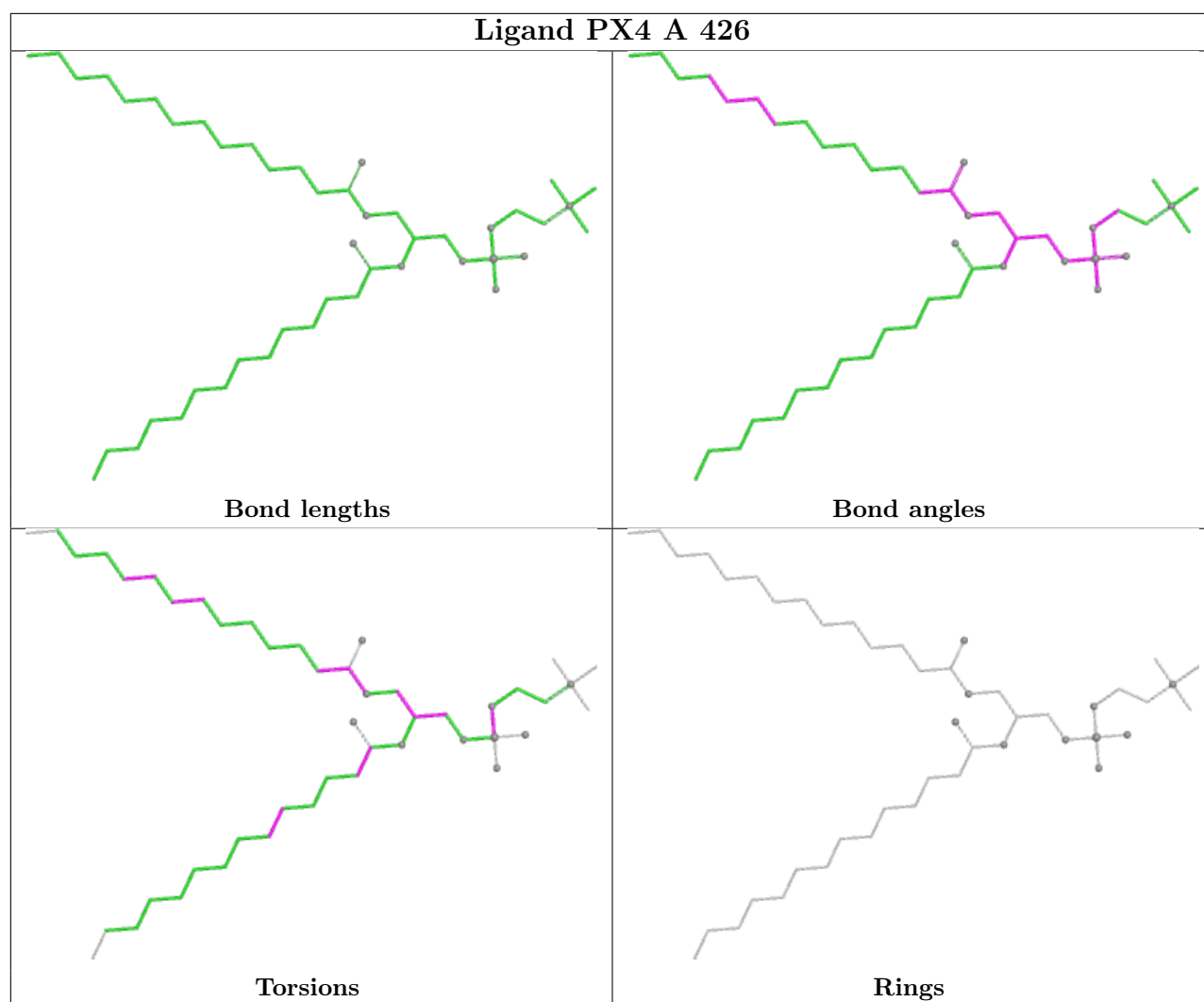


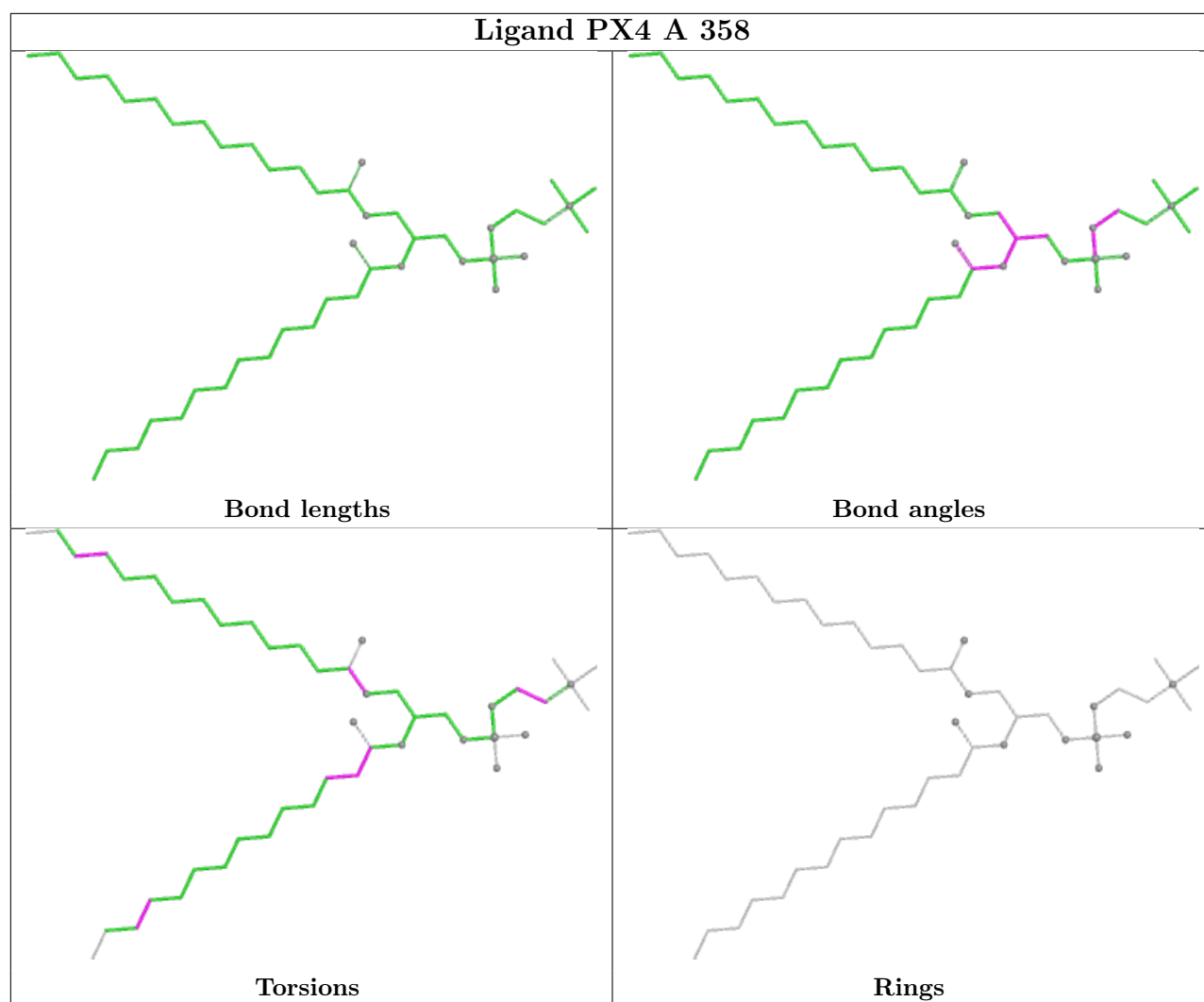




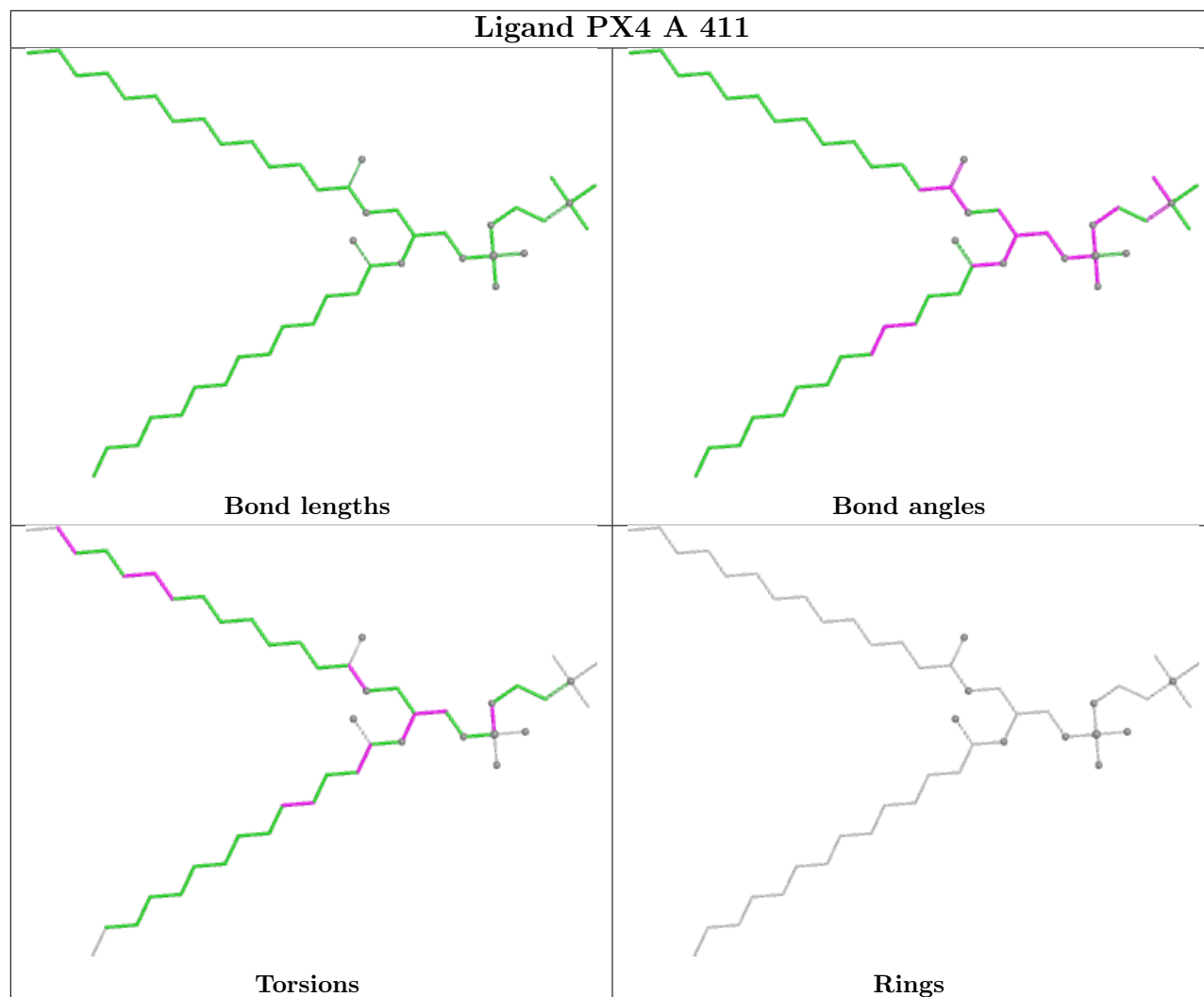




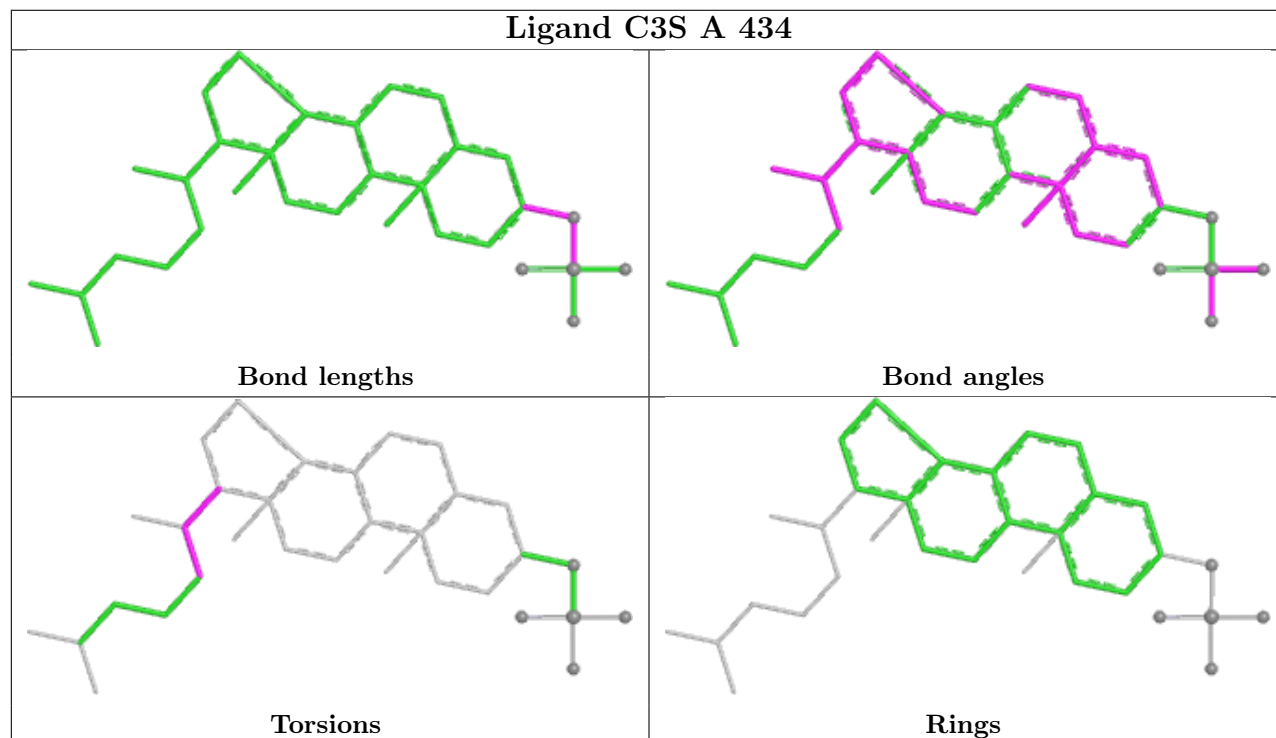


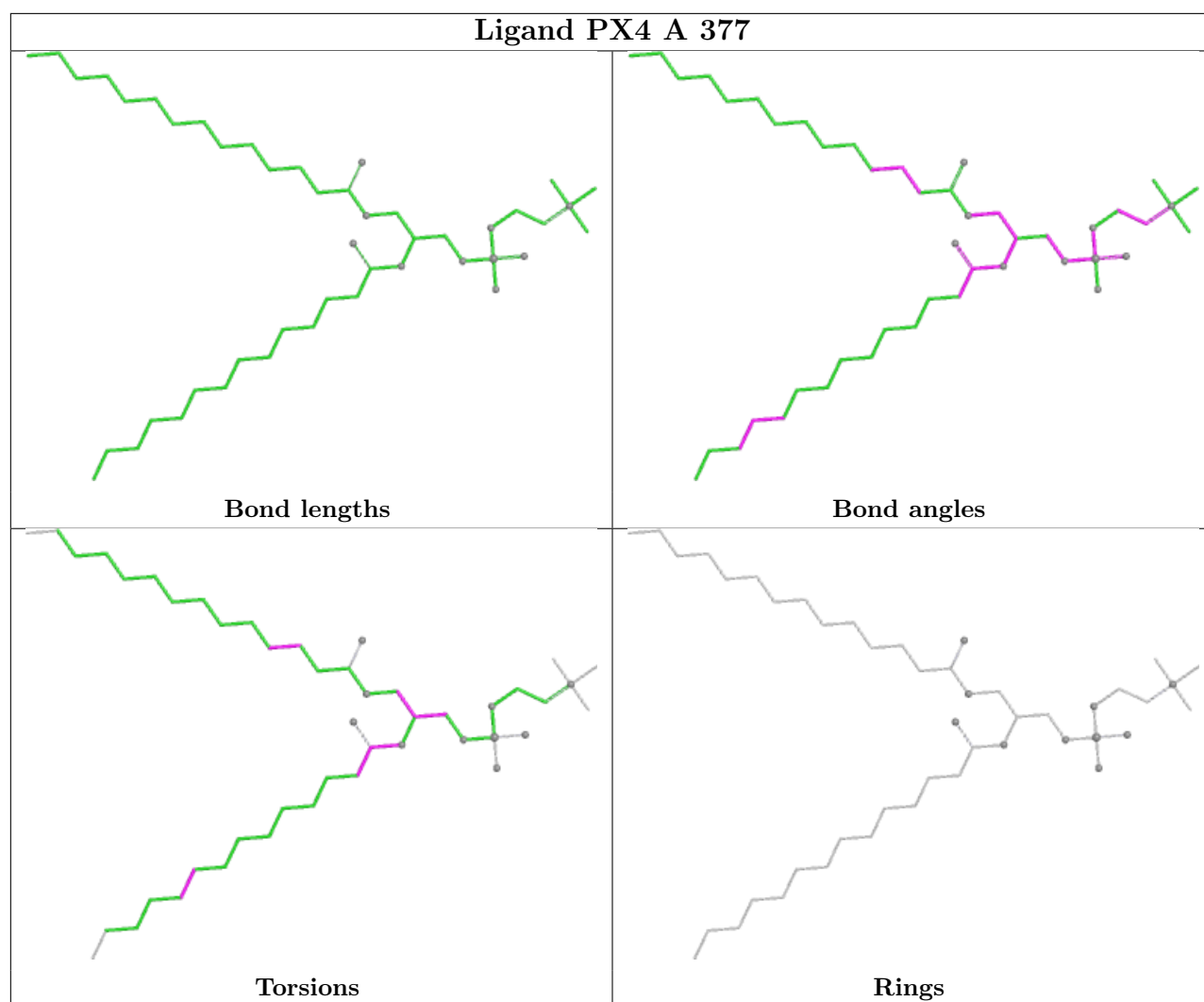


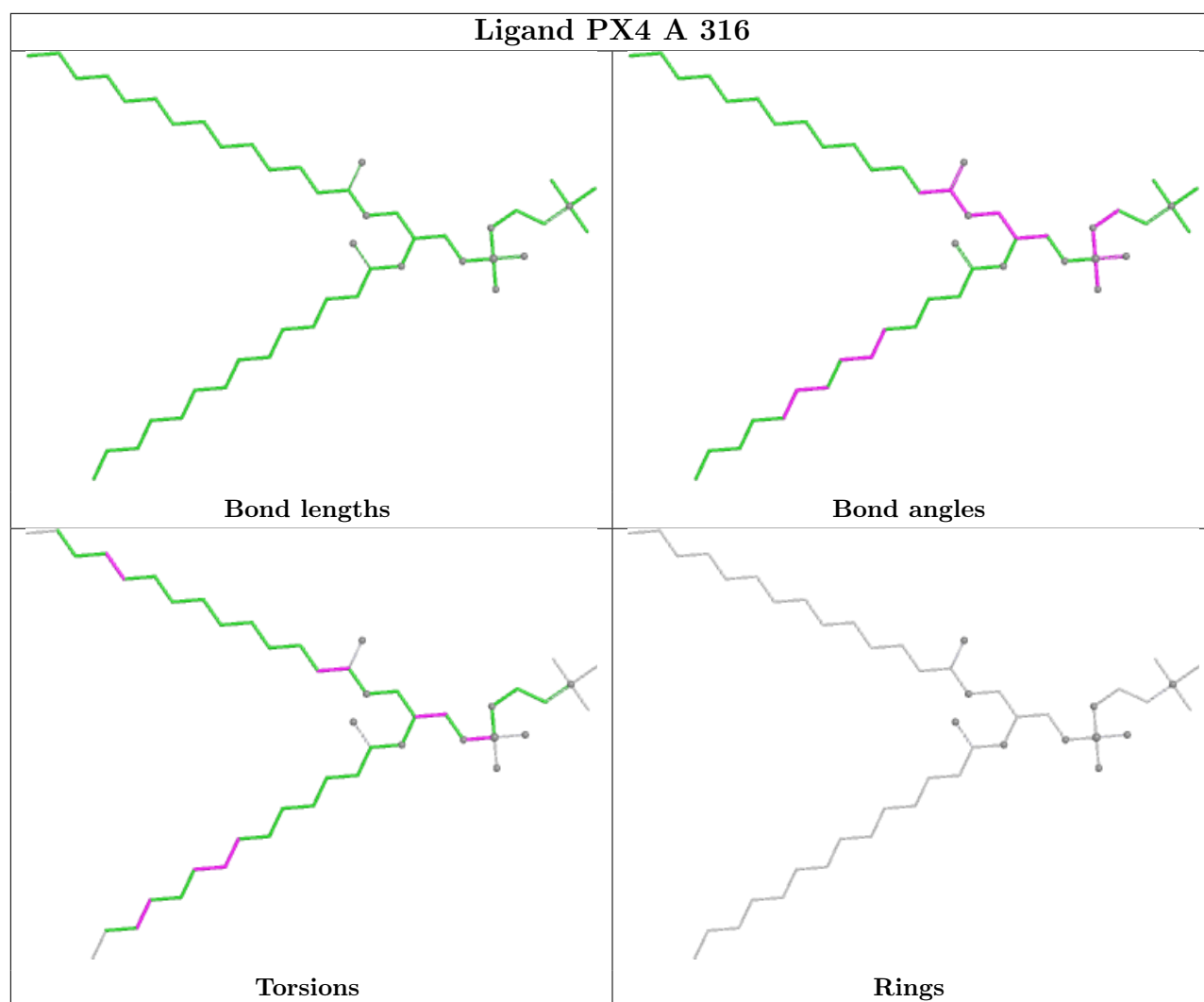
Ligand PX4 A 411

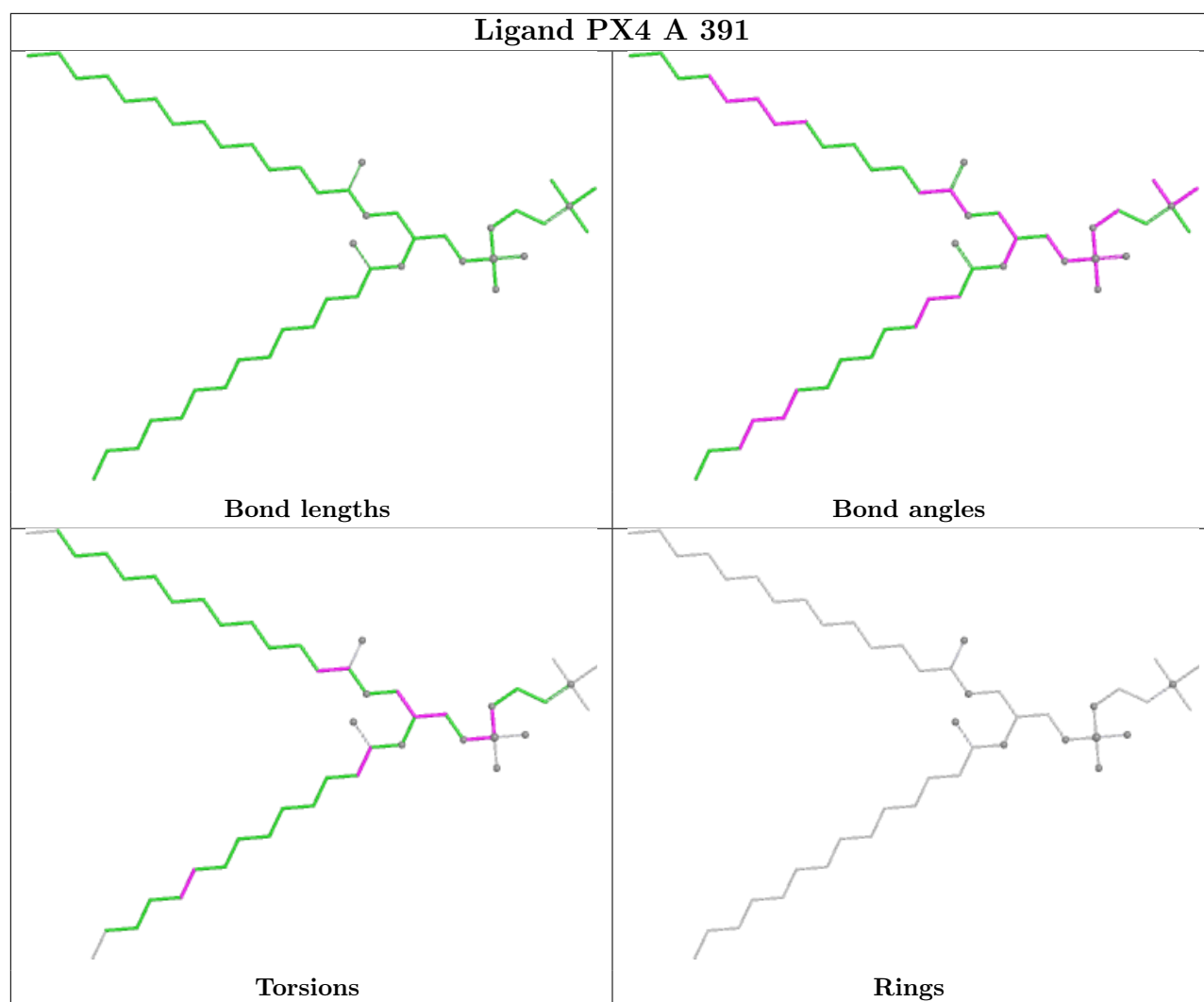


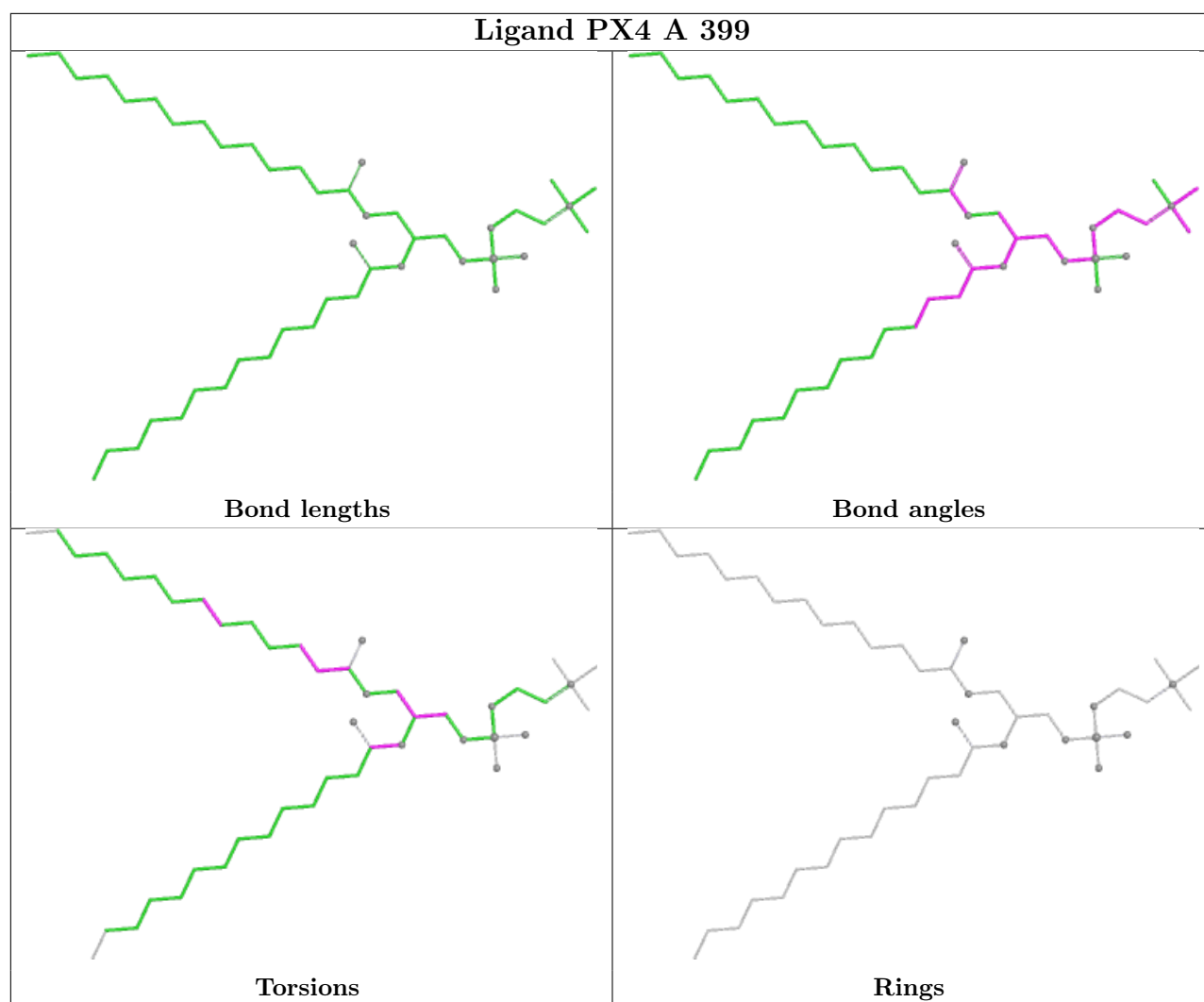
Ligand C3S A 434

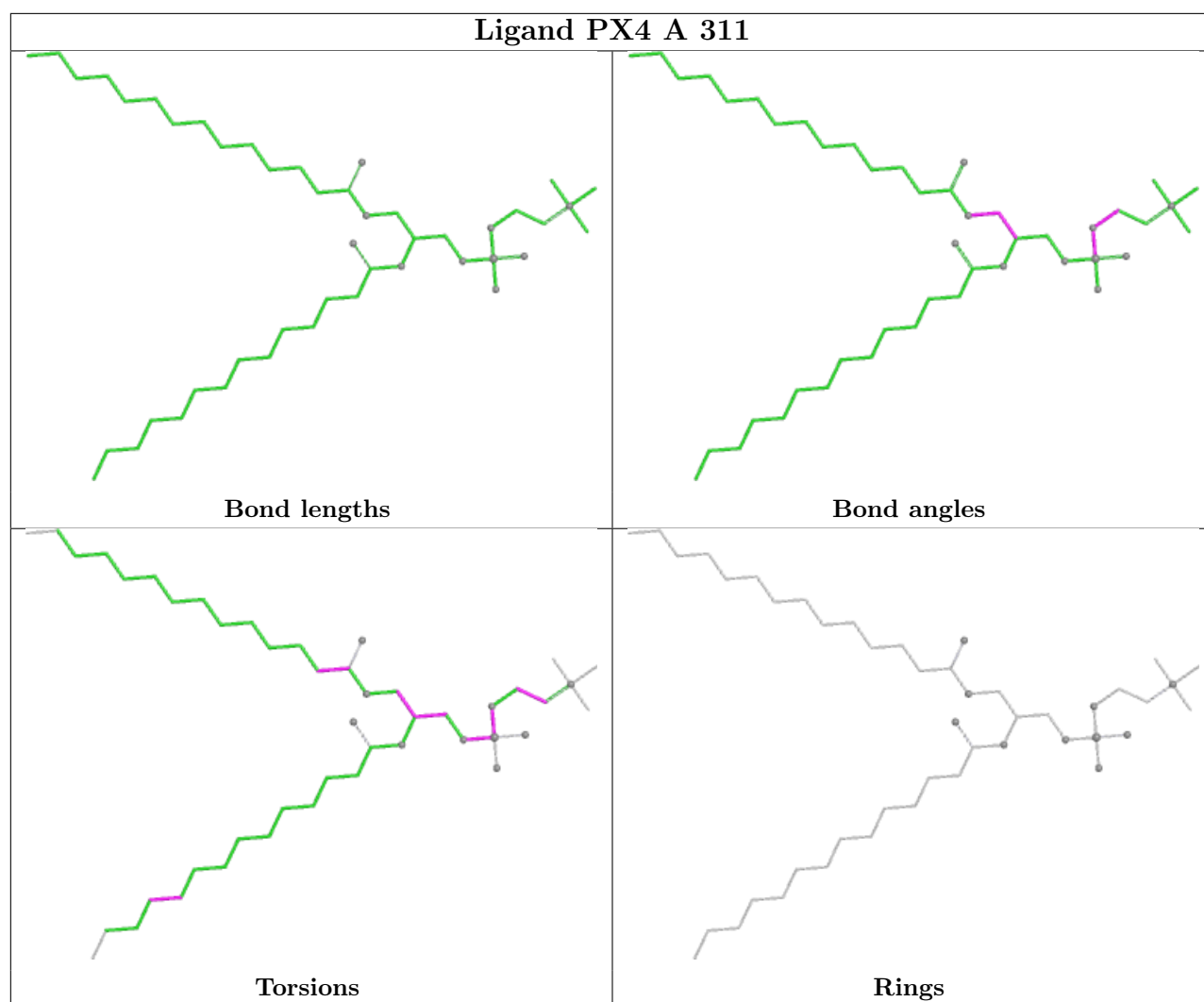


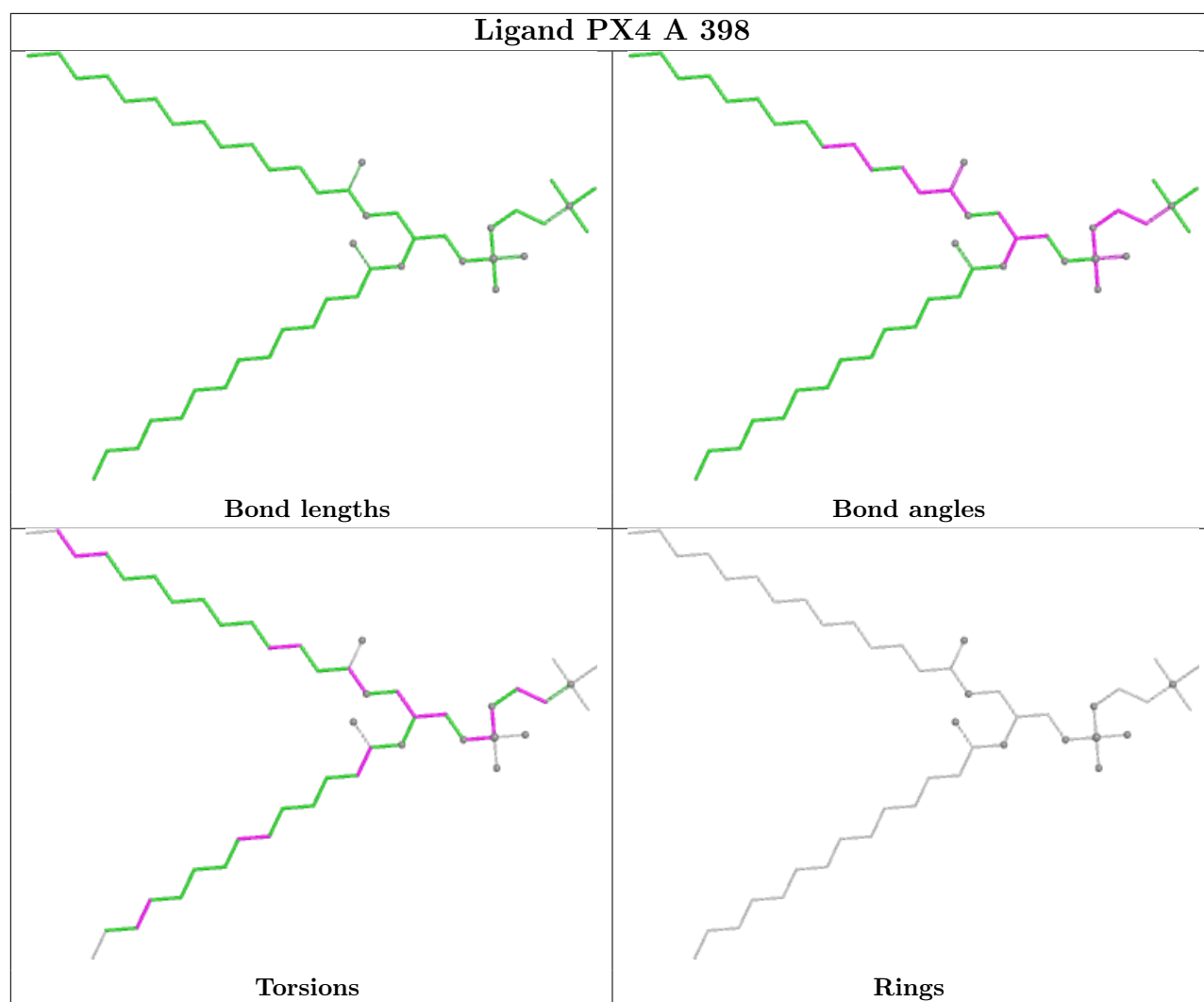


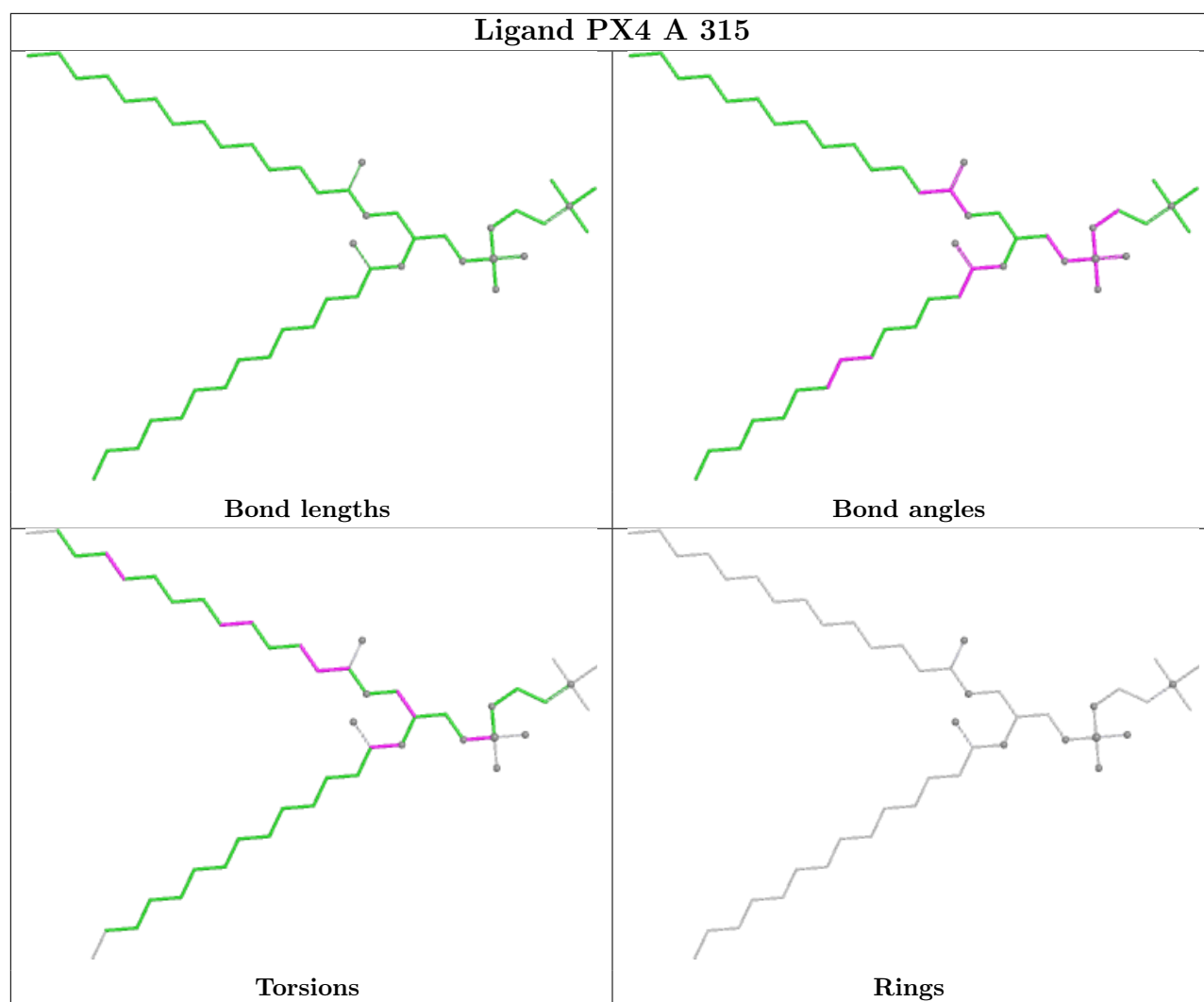


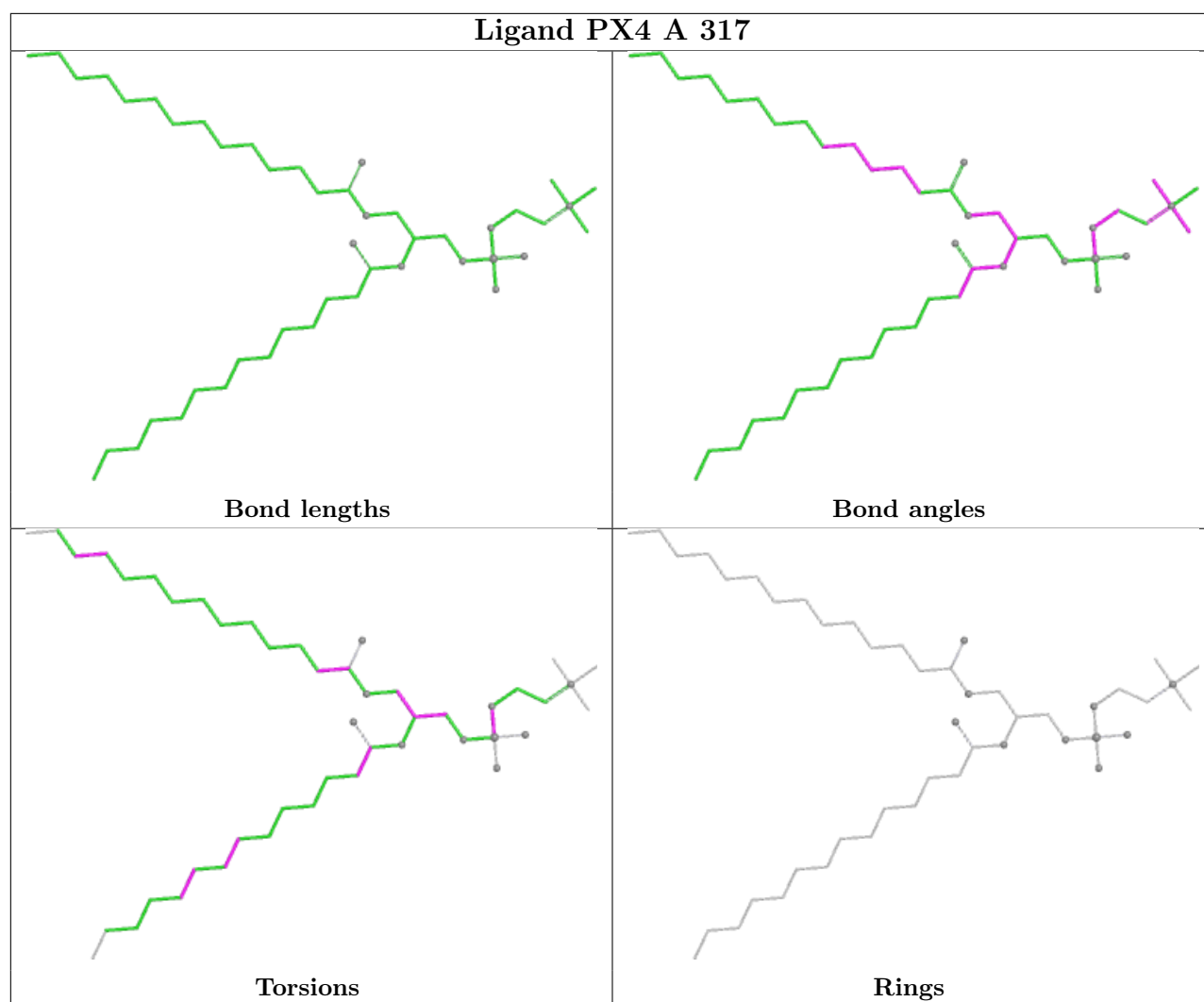


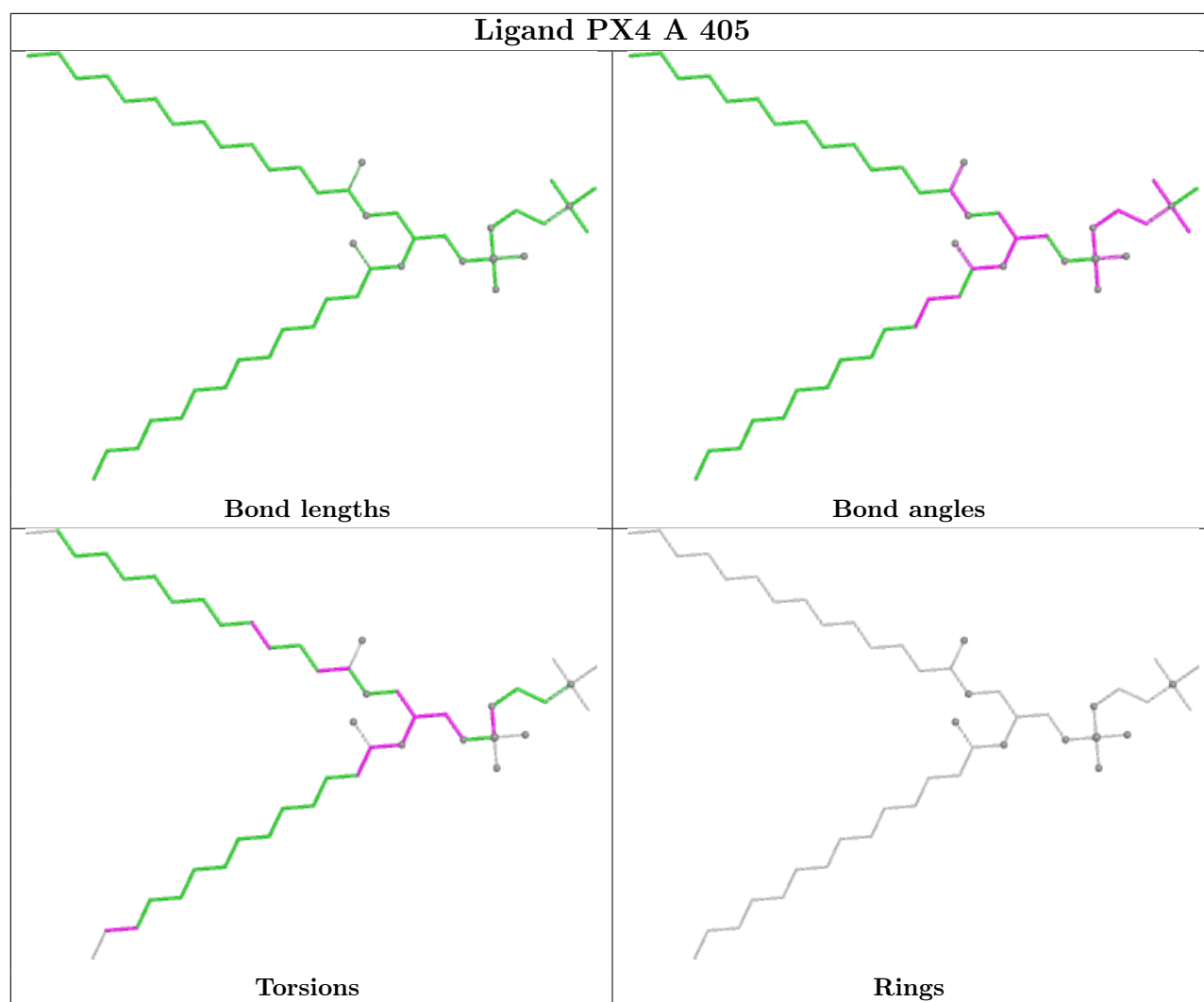


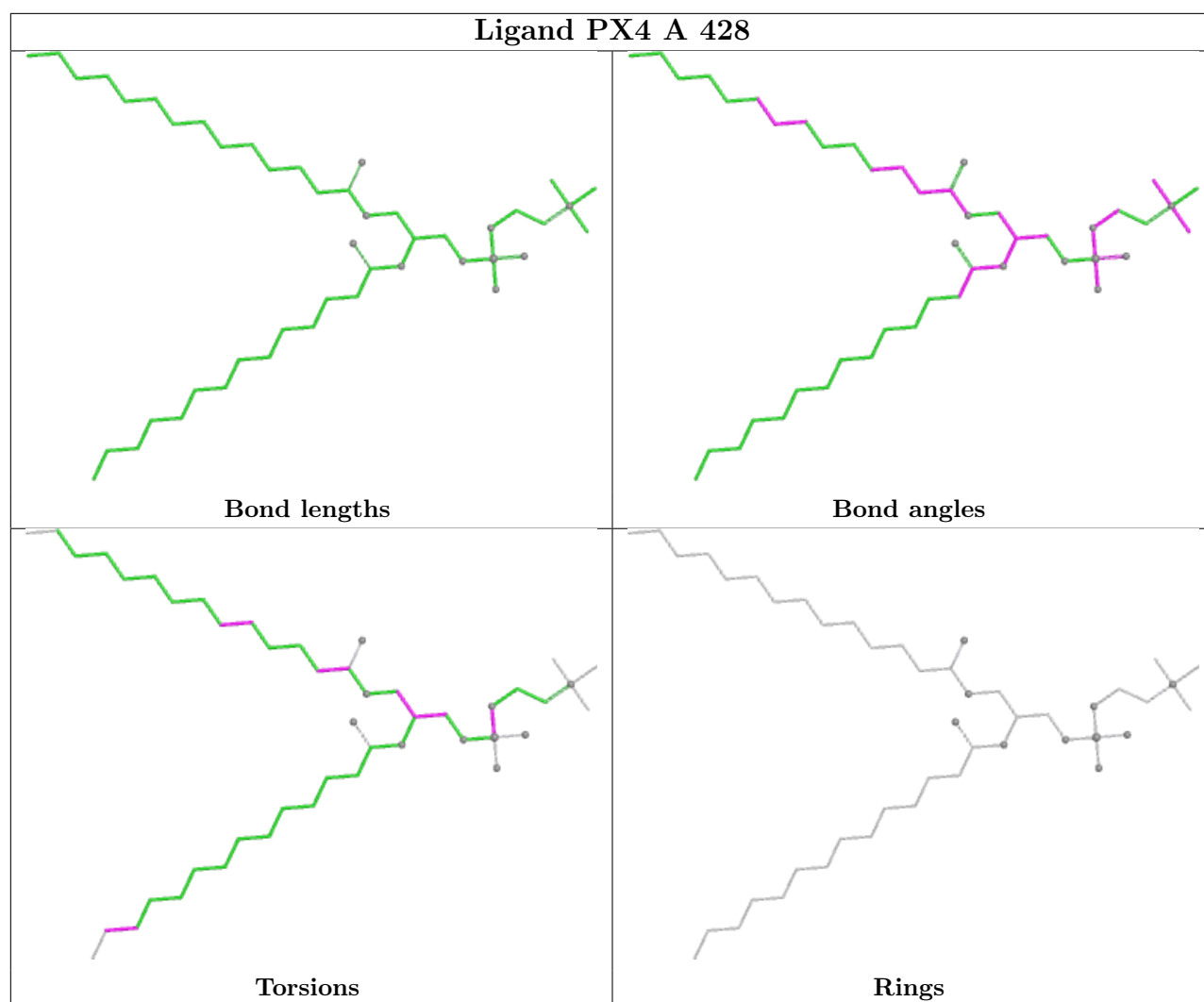


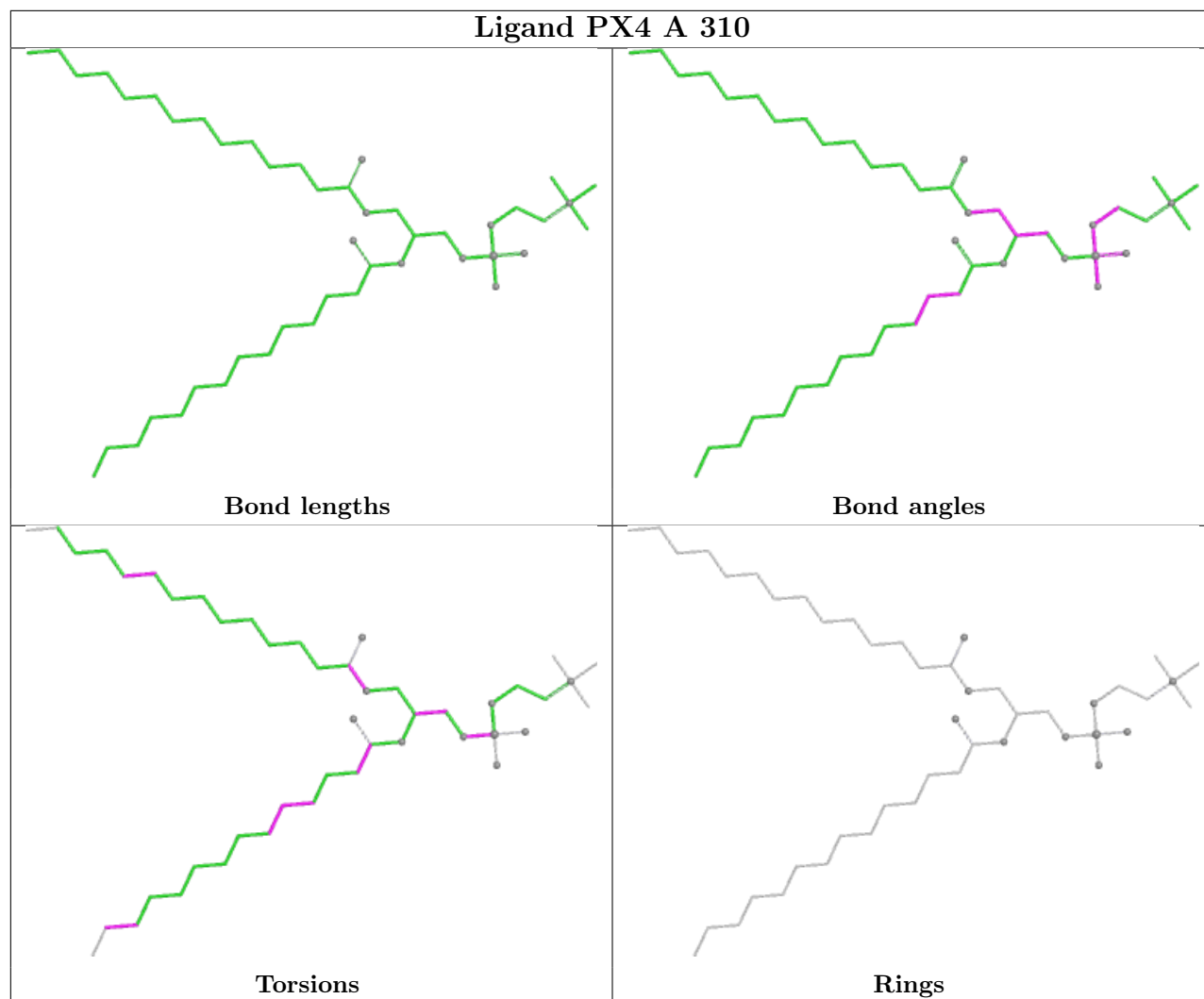




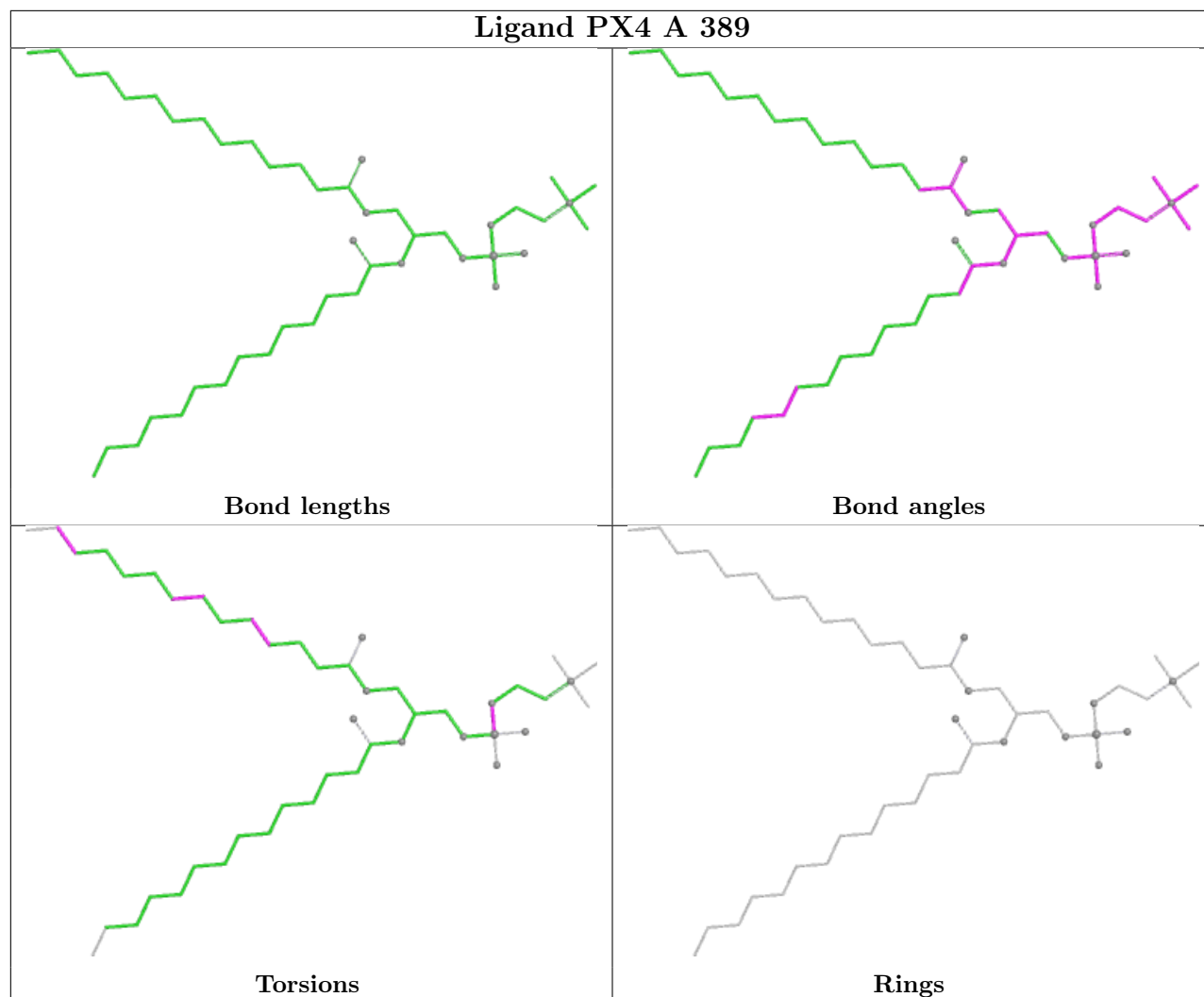




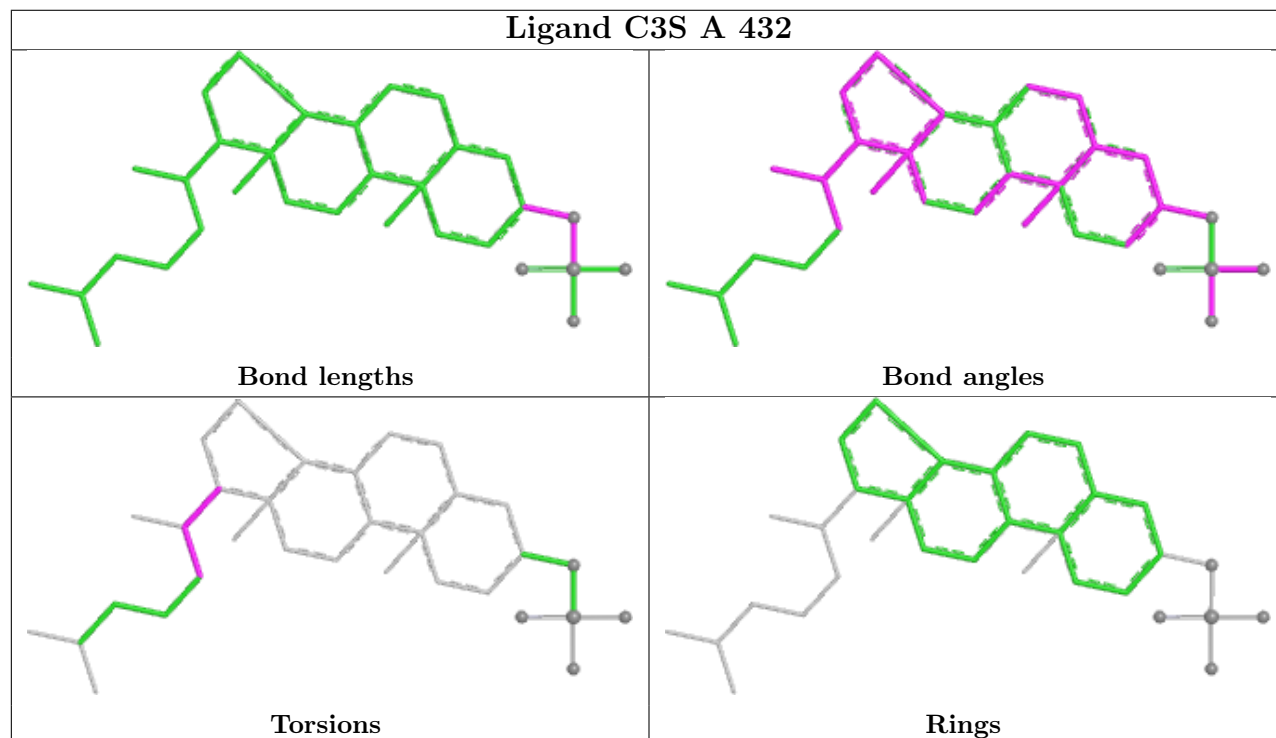


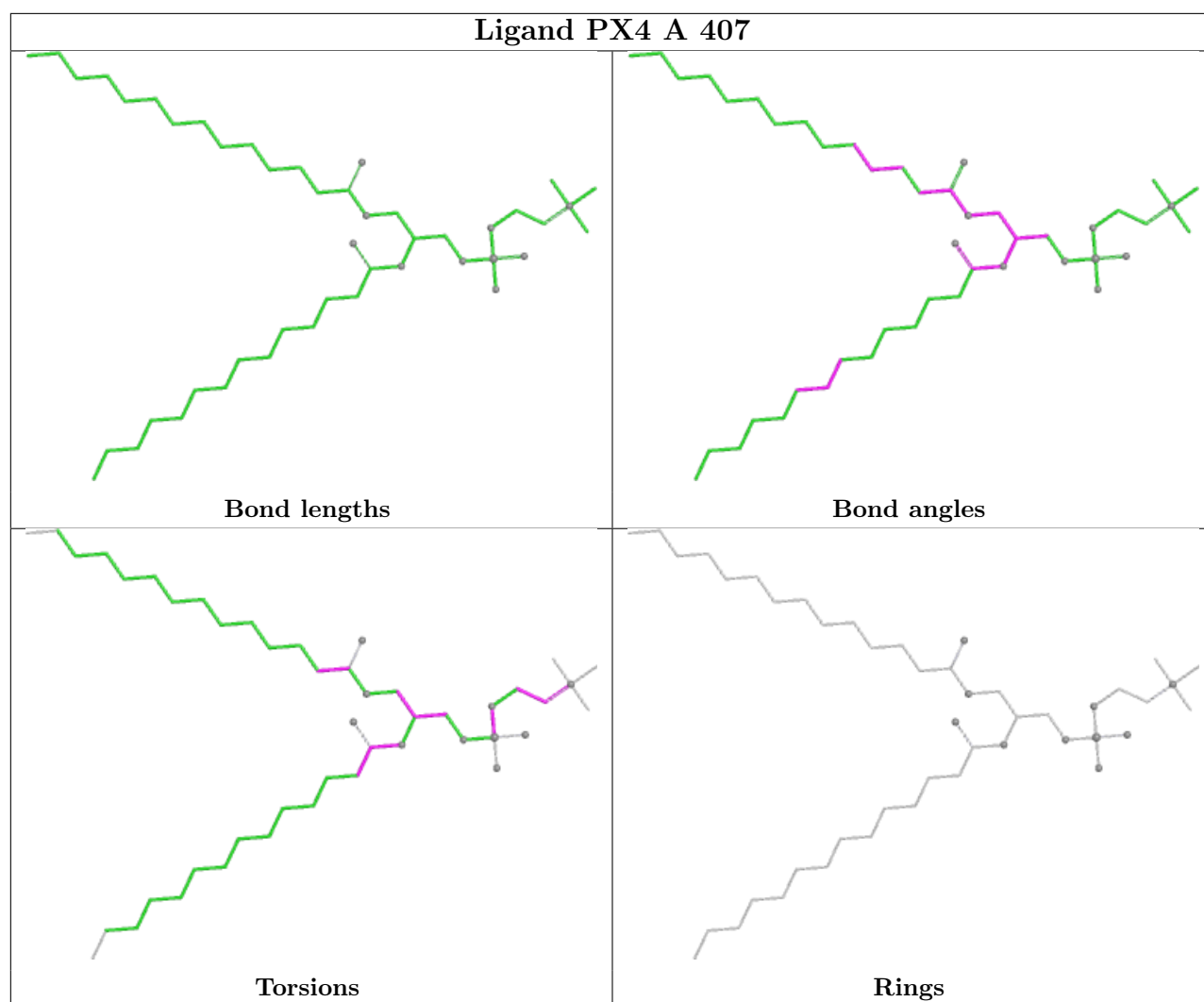


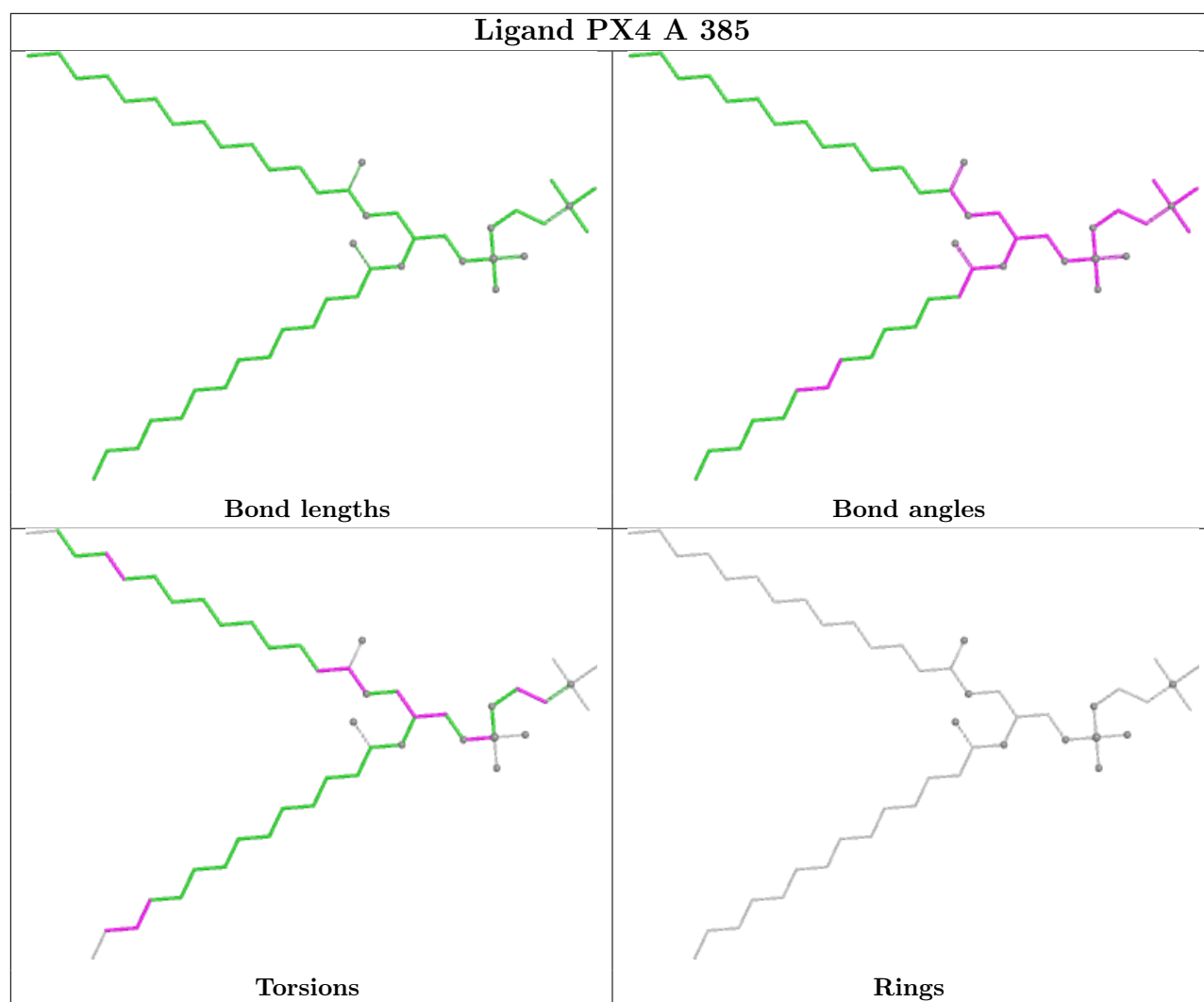
Ligand PX4 A 389

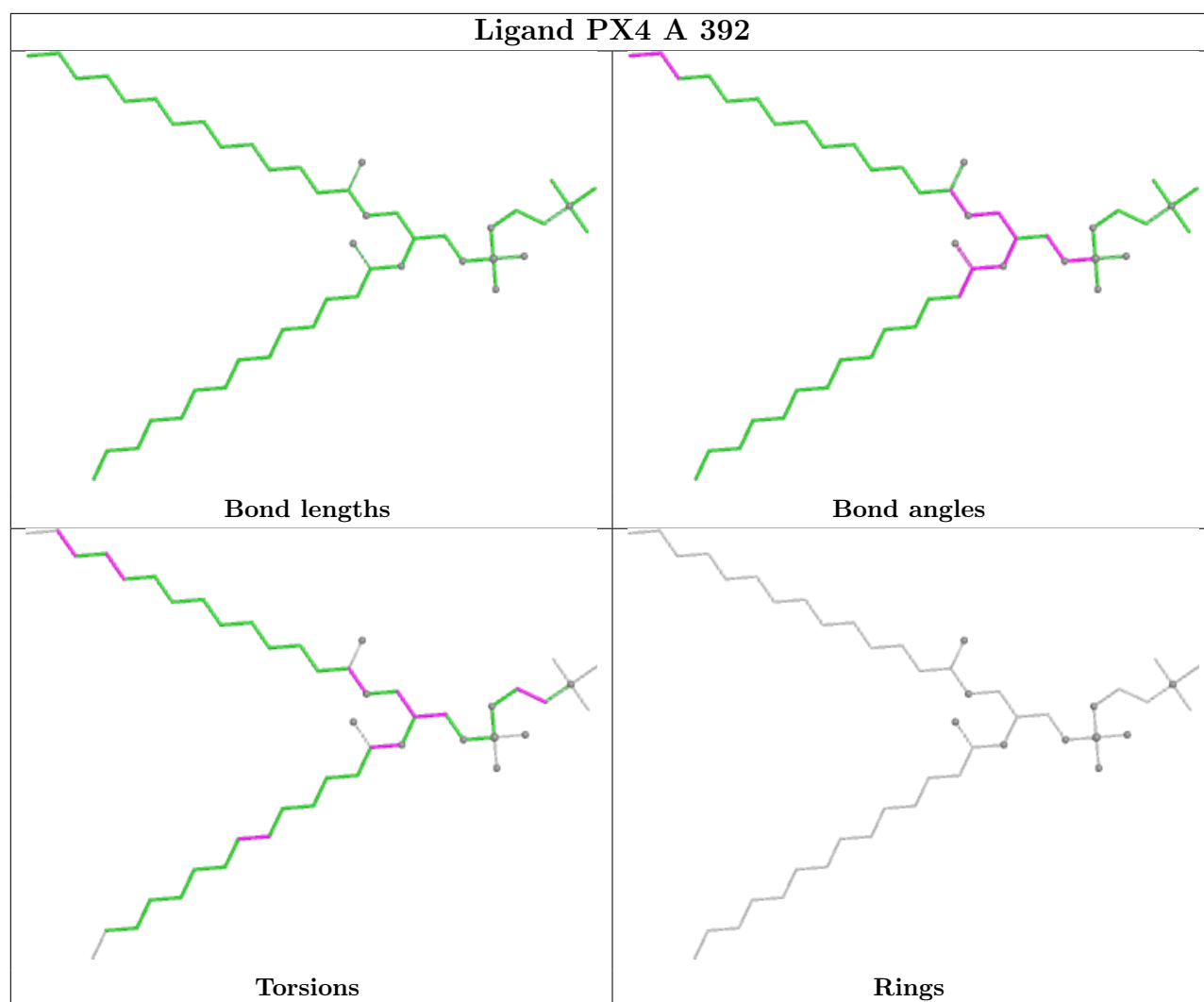


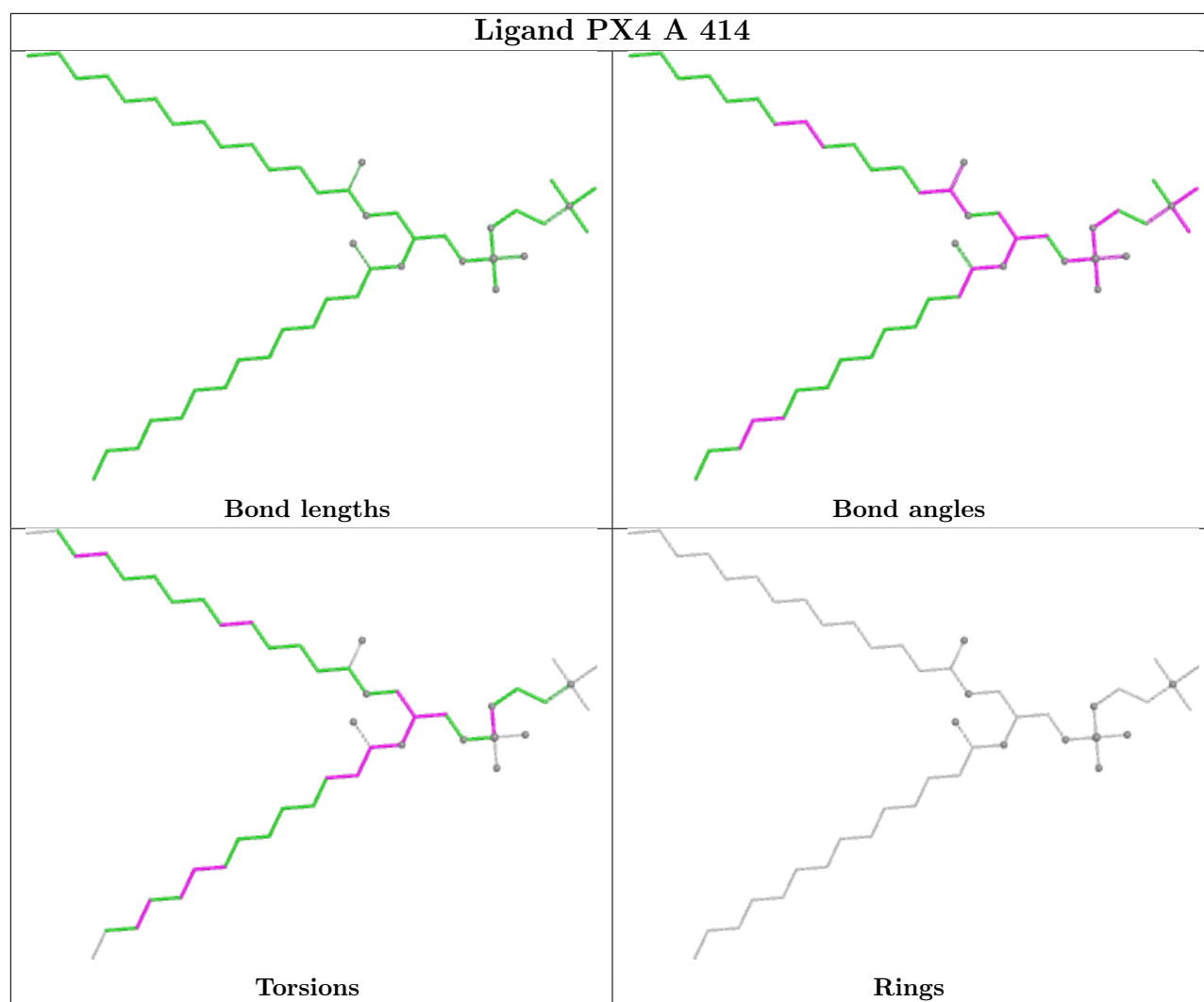
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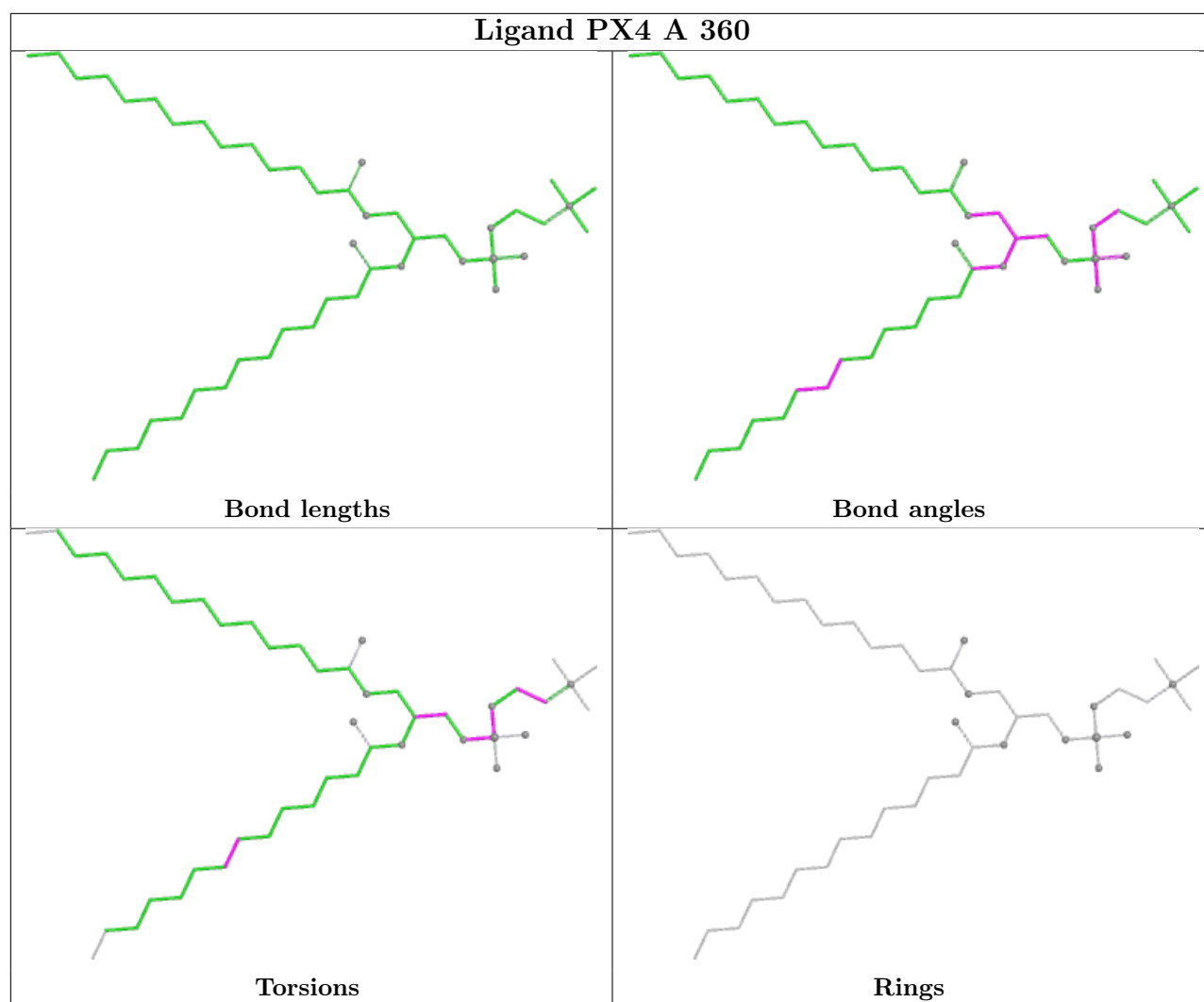


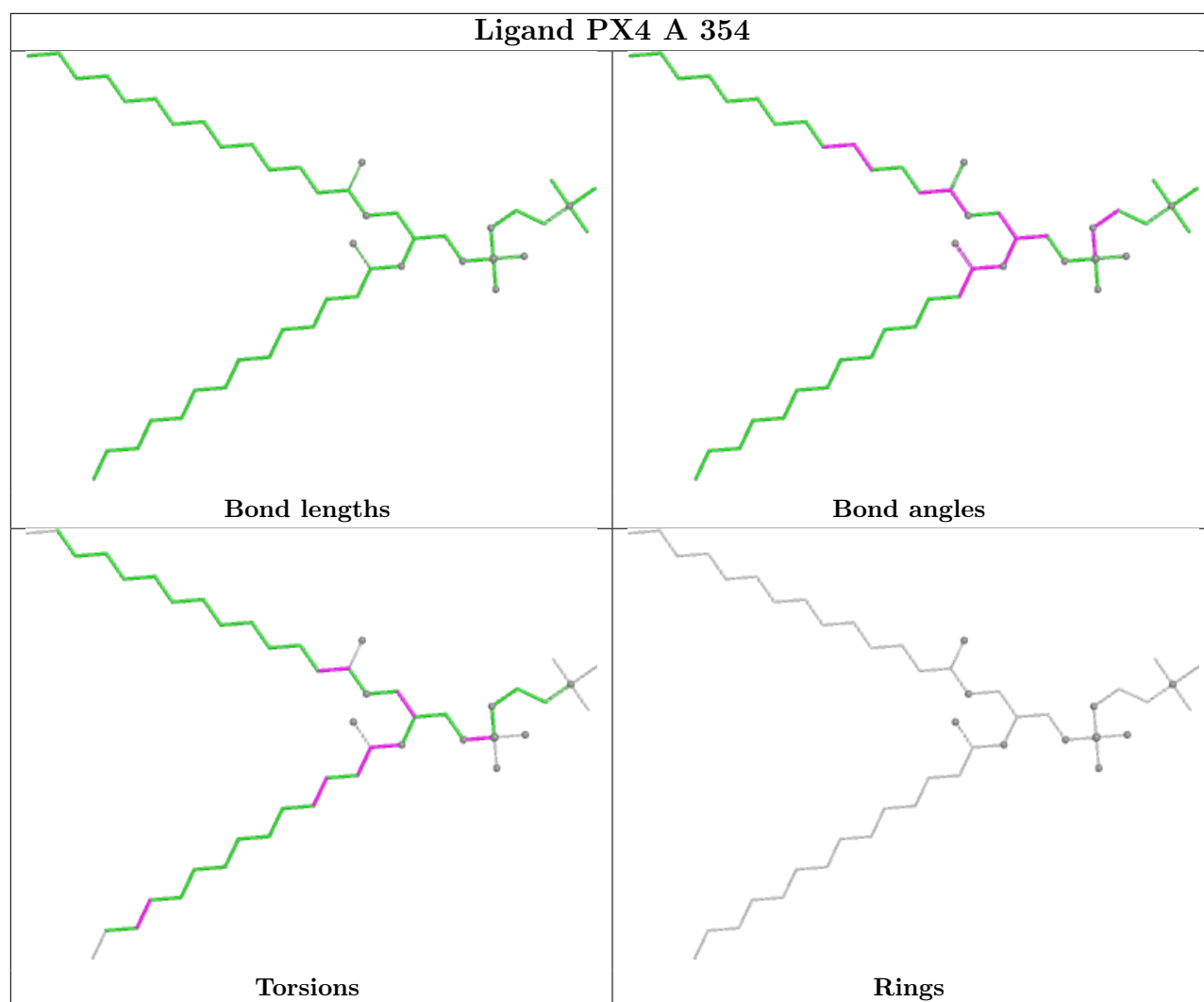


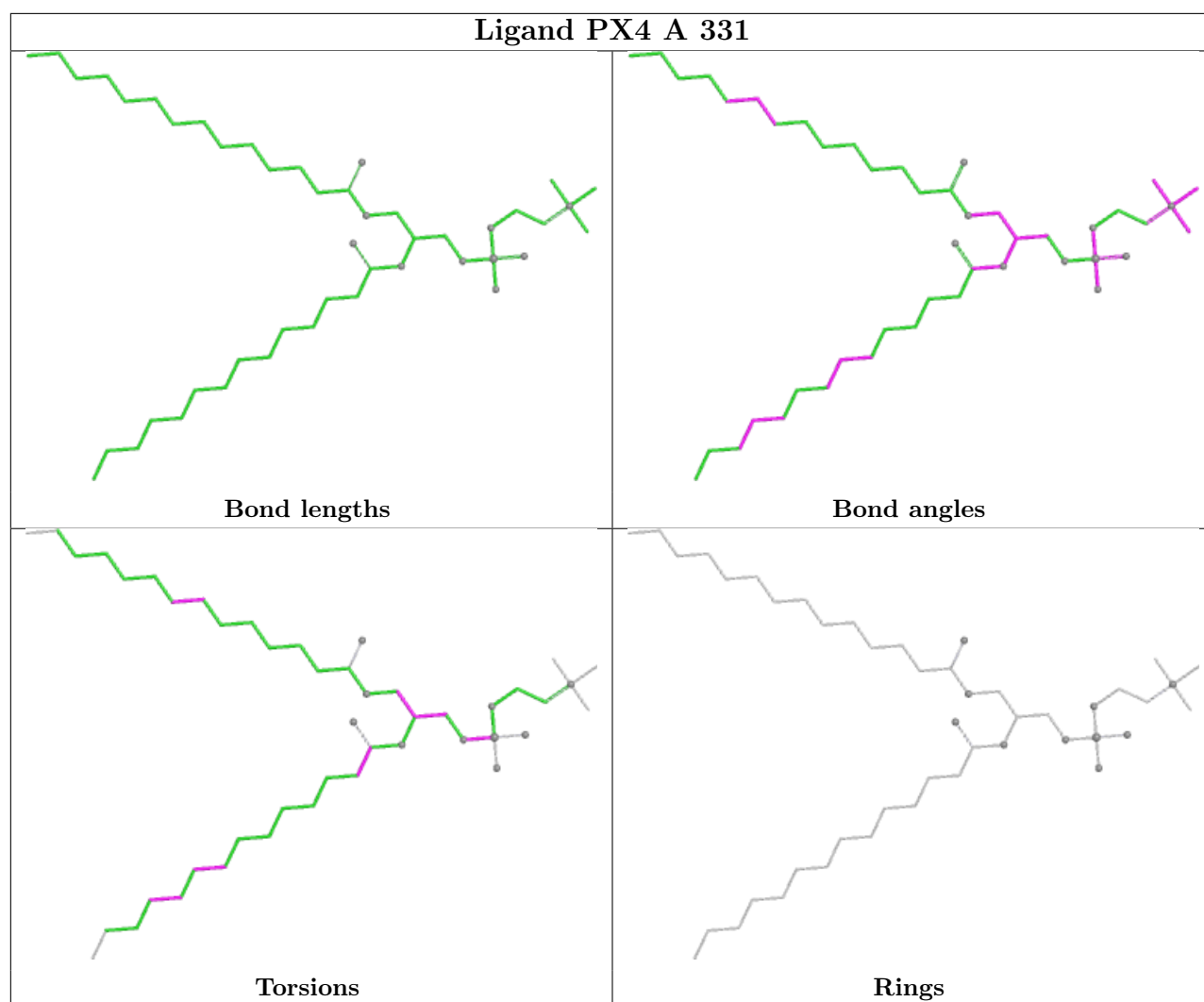


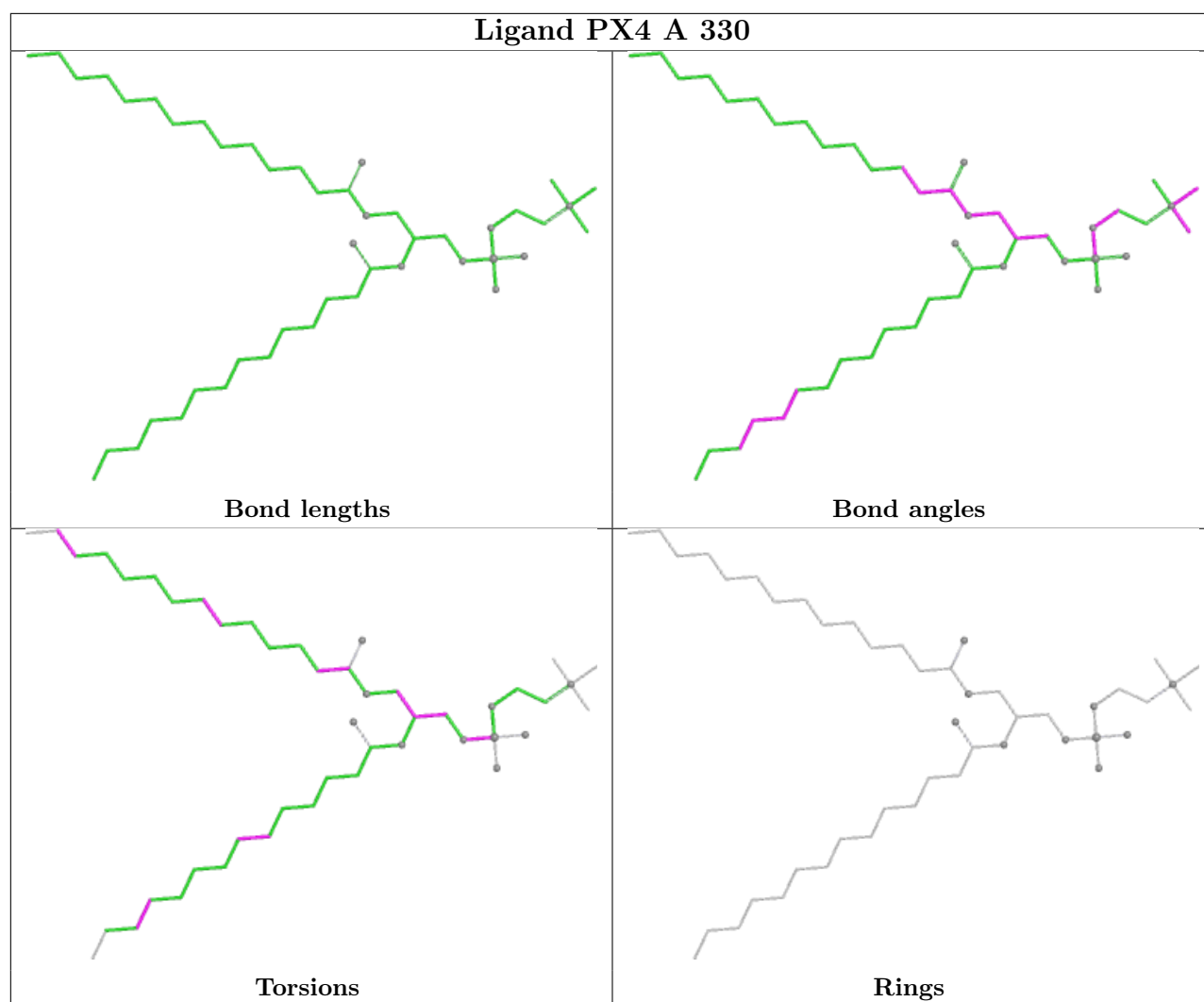


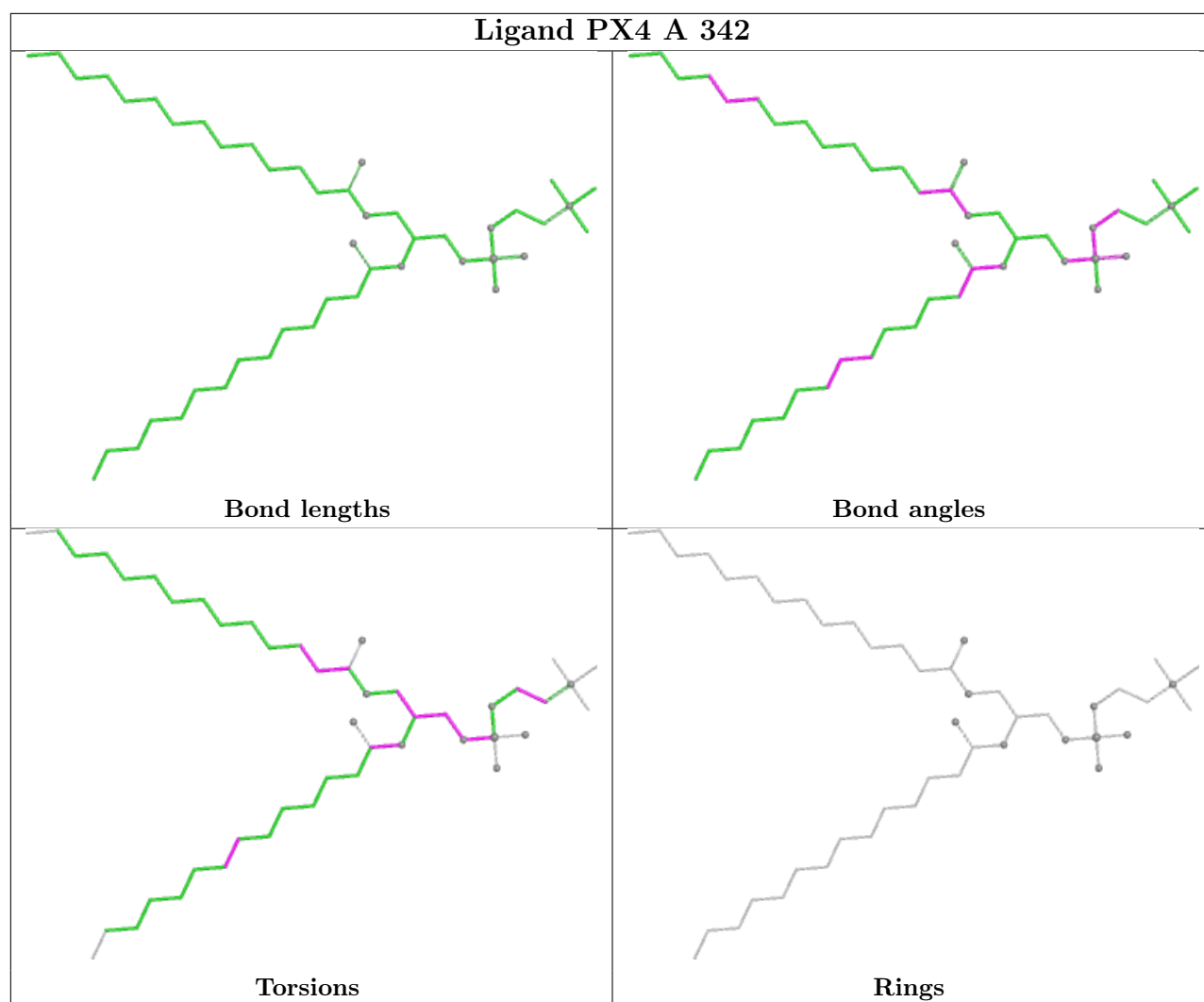


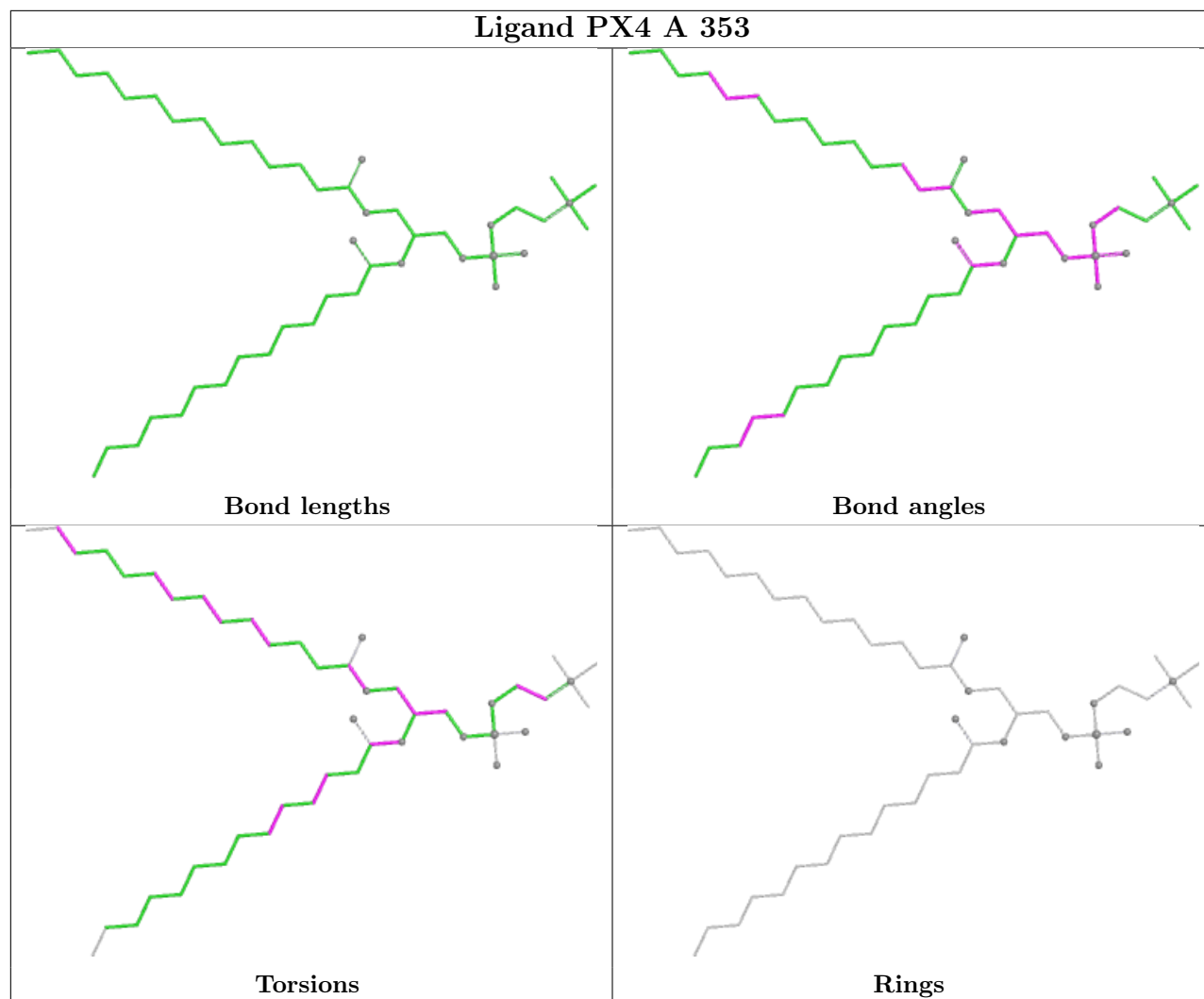


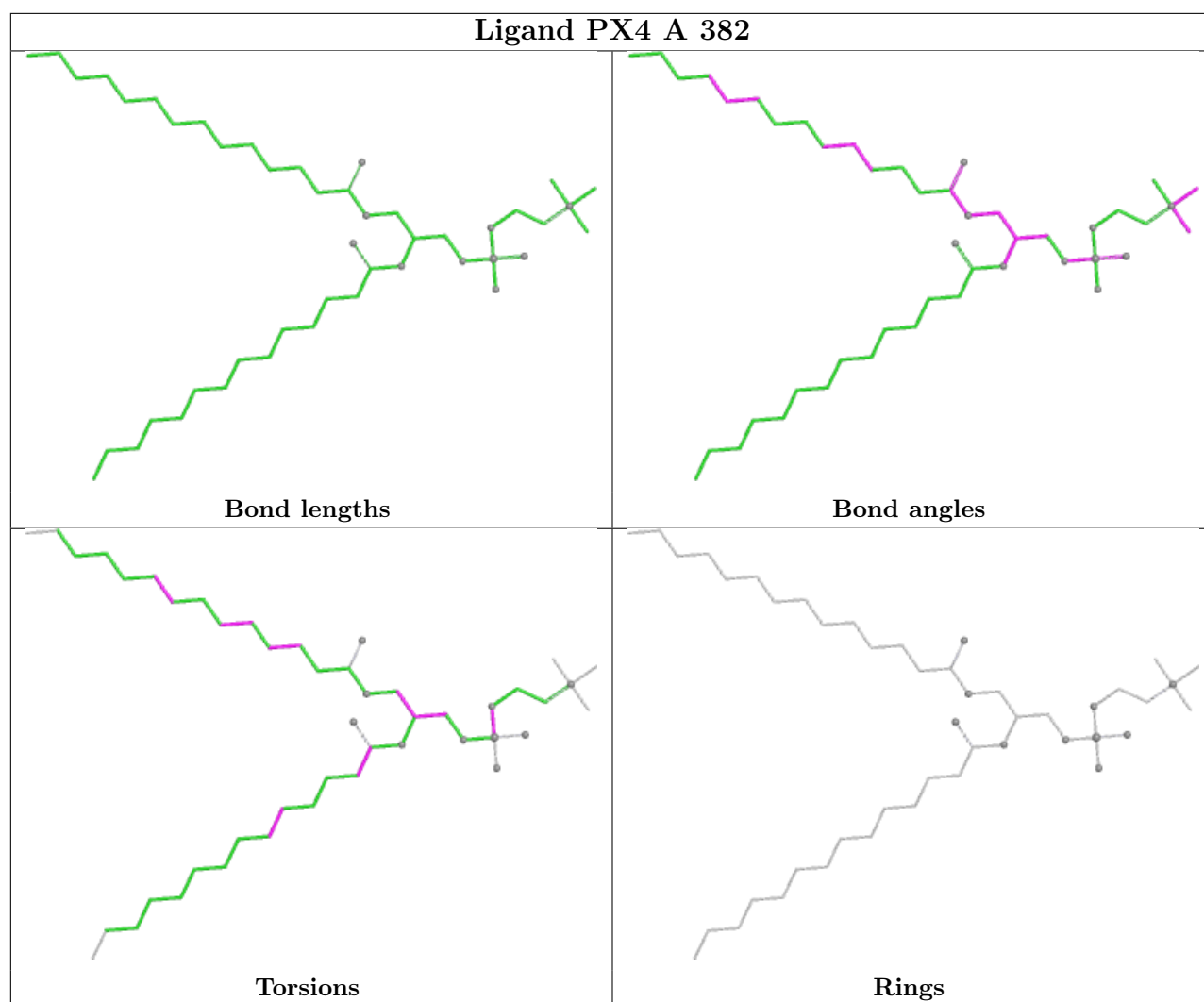




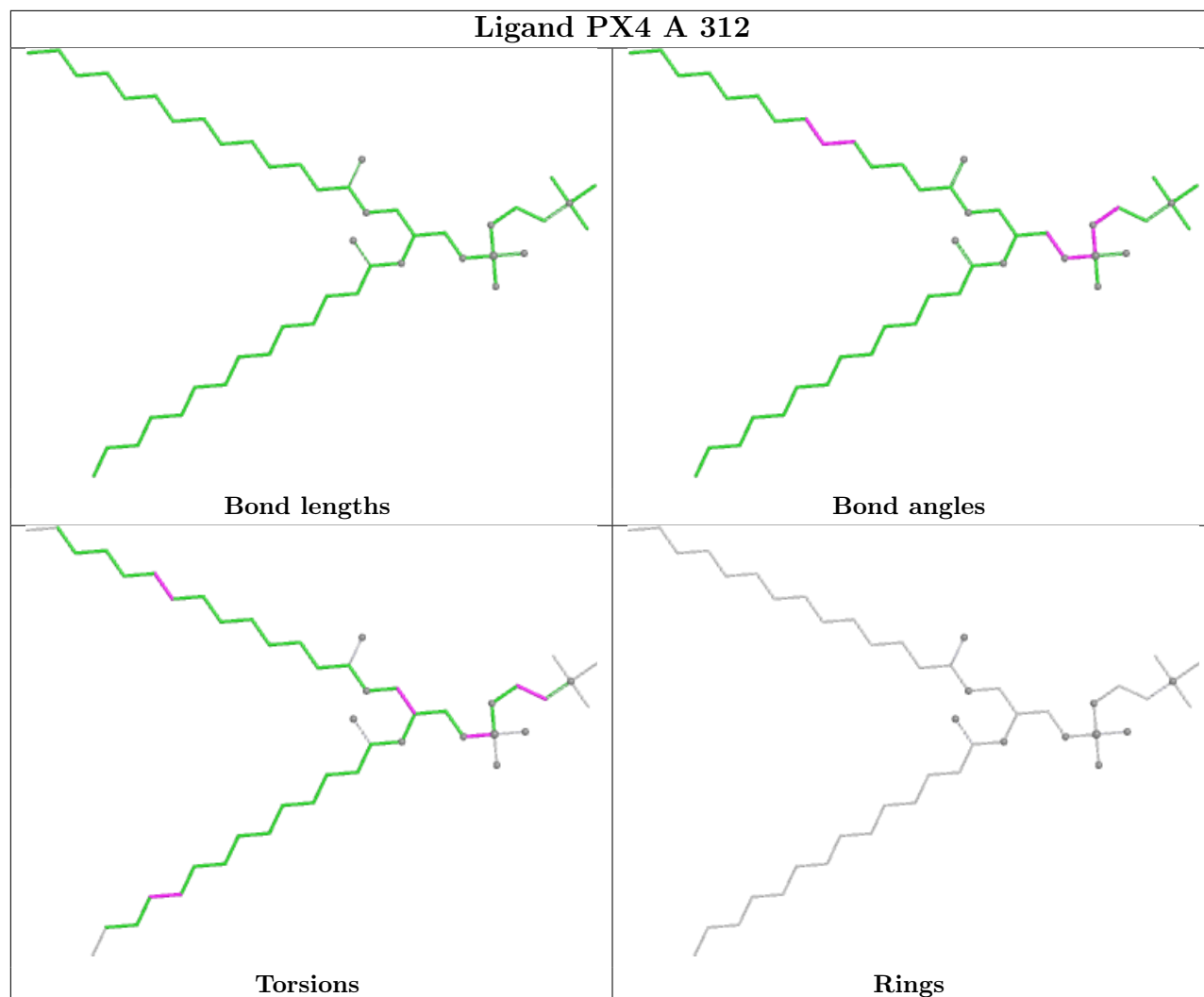




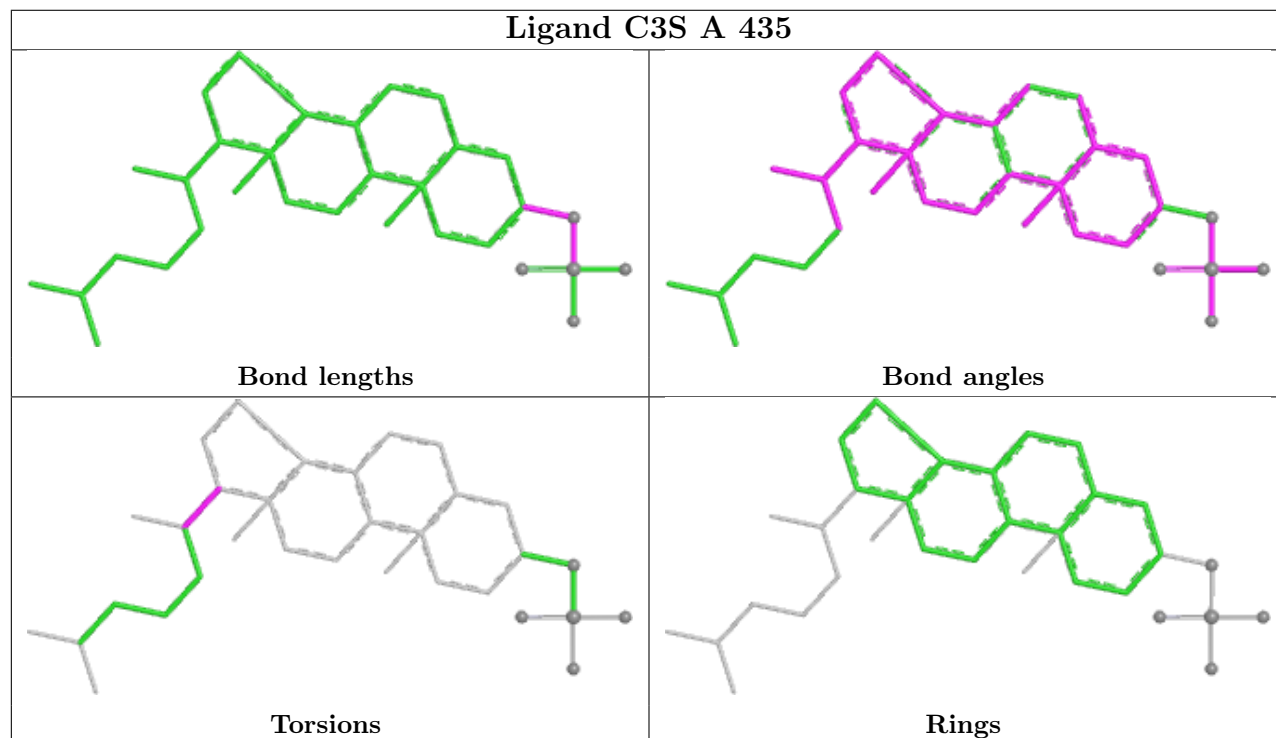


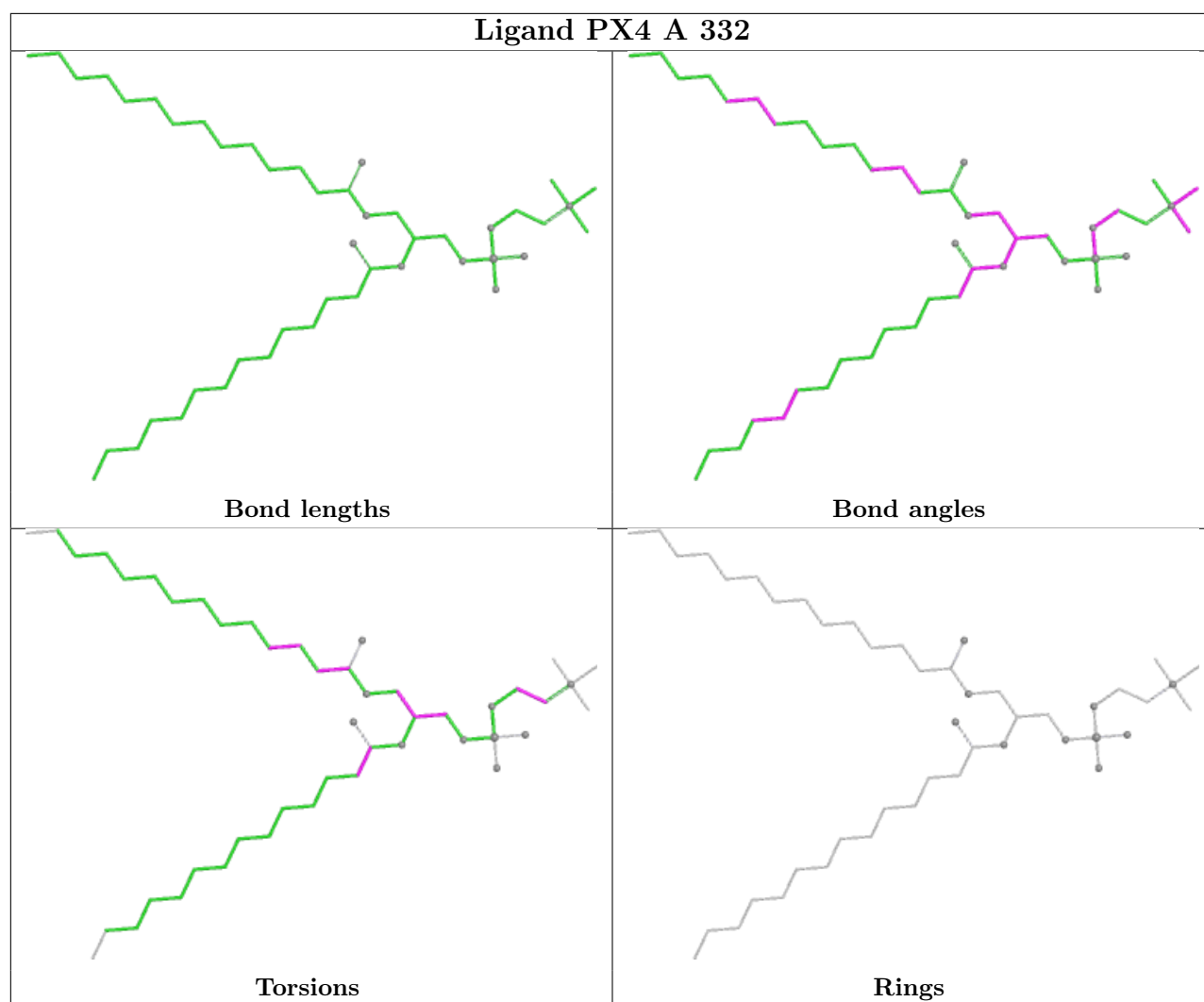


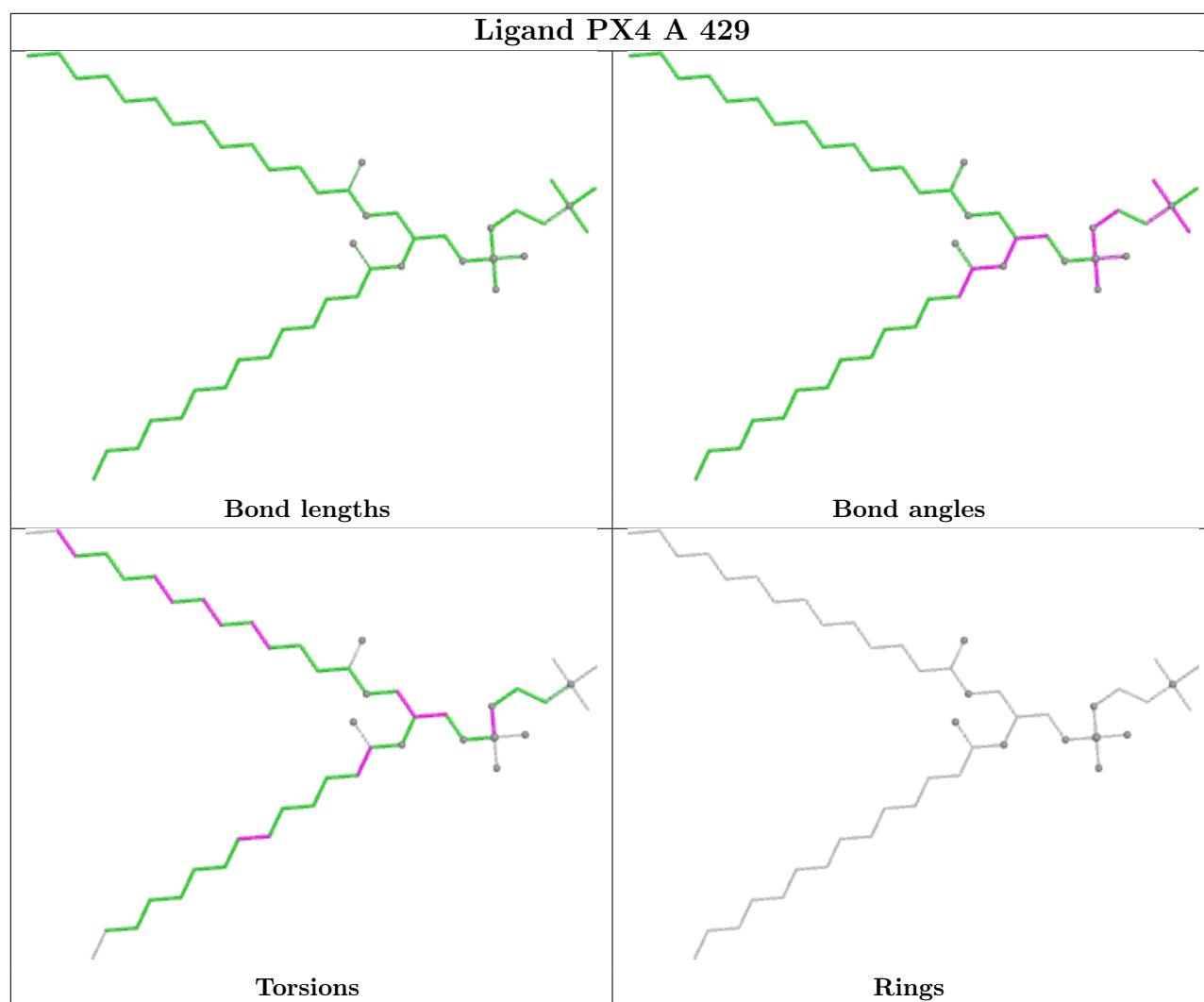
Ligand PX4 A 312

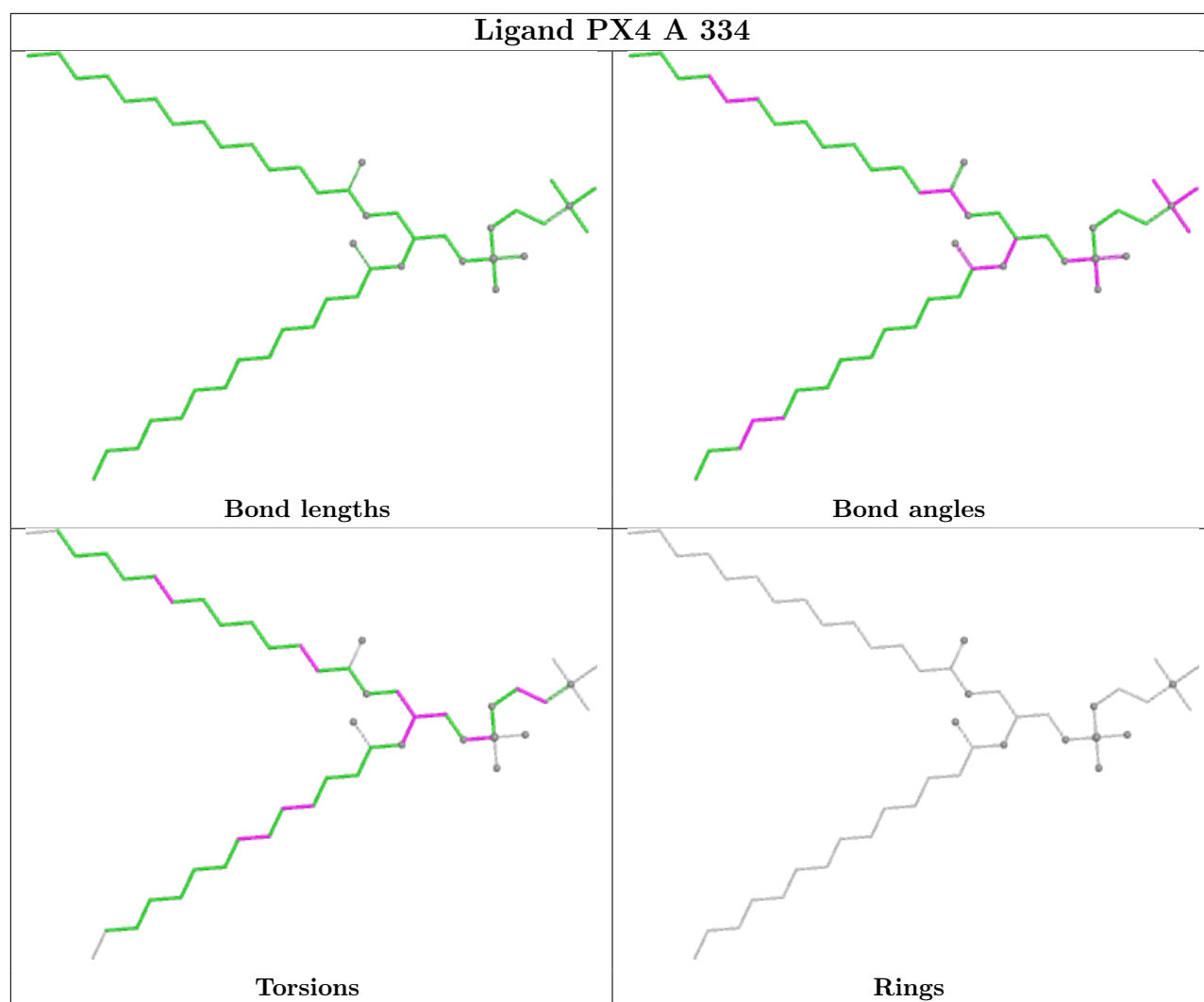


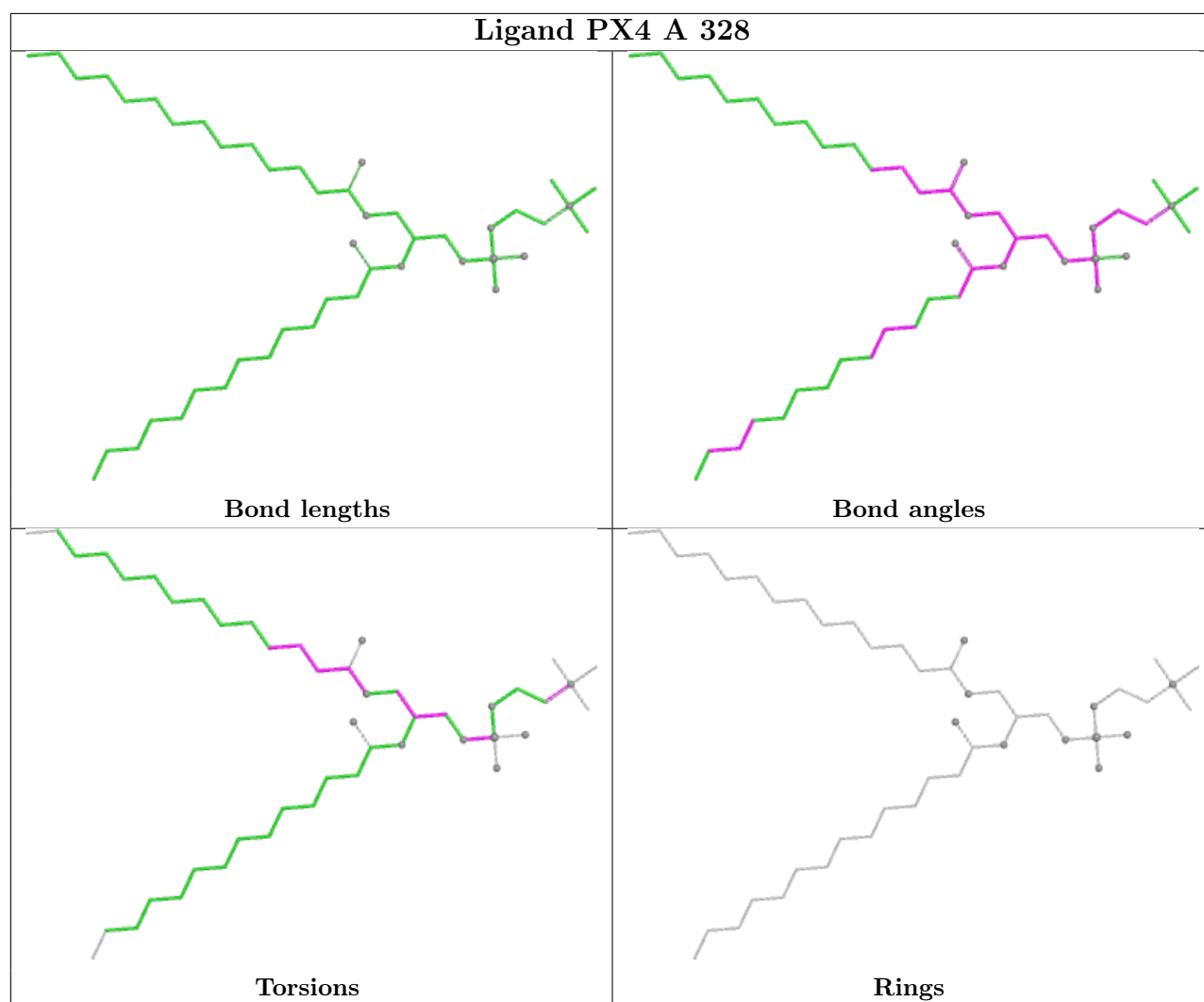
Ligand C3S A 435

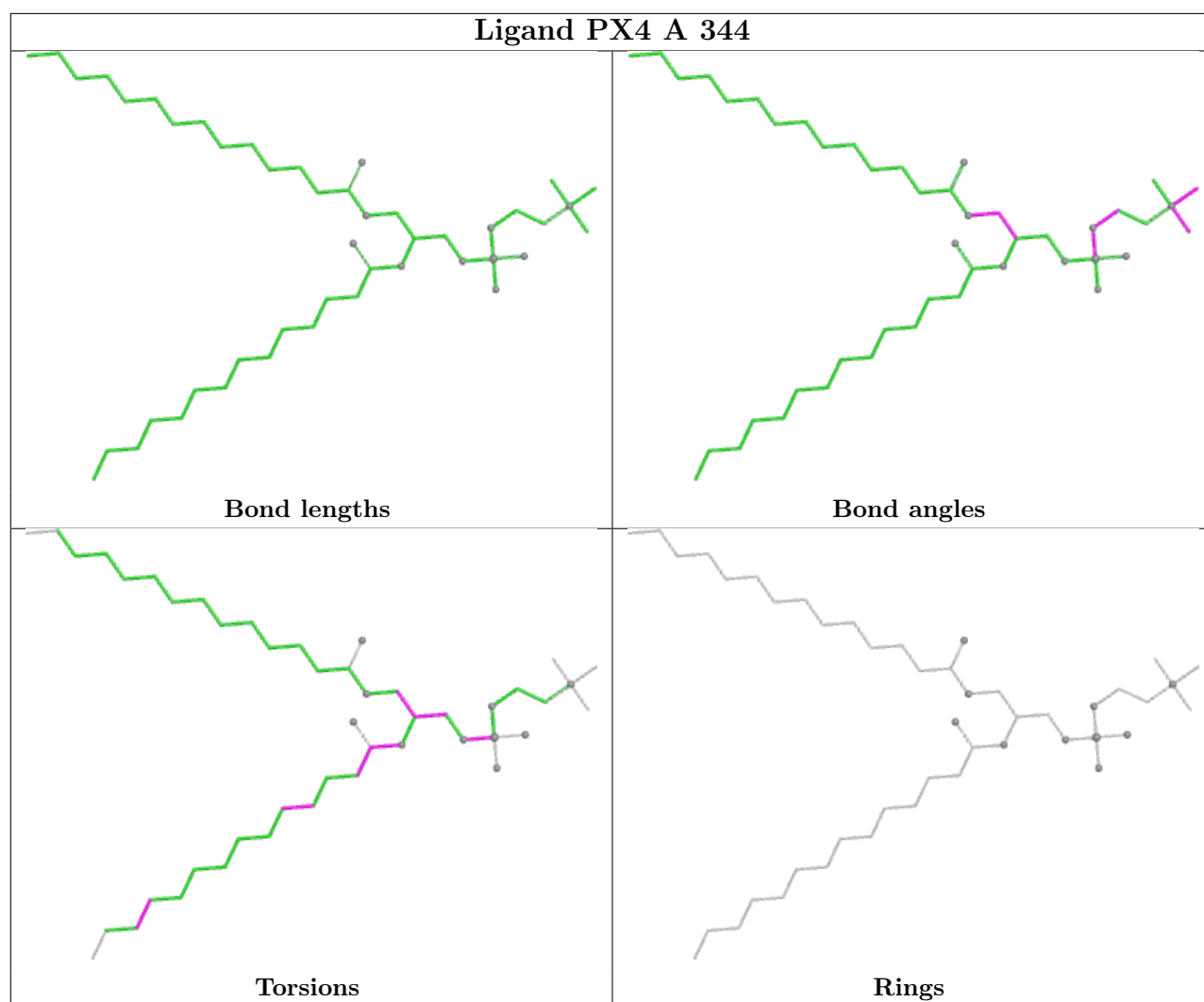


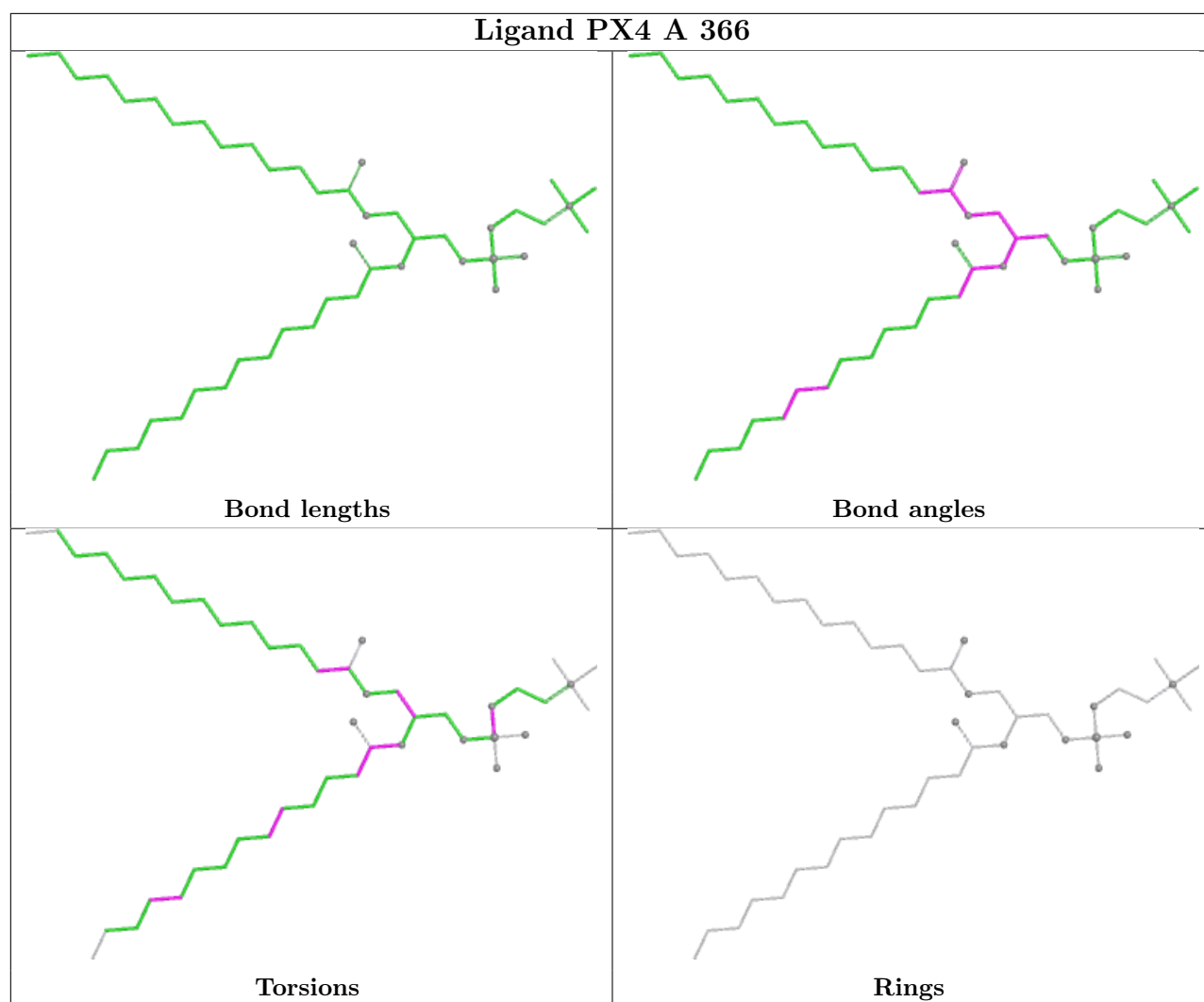


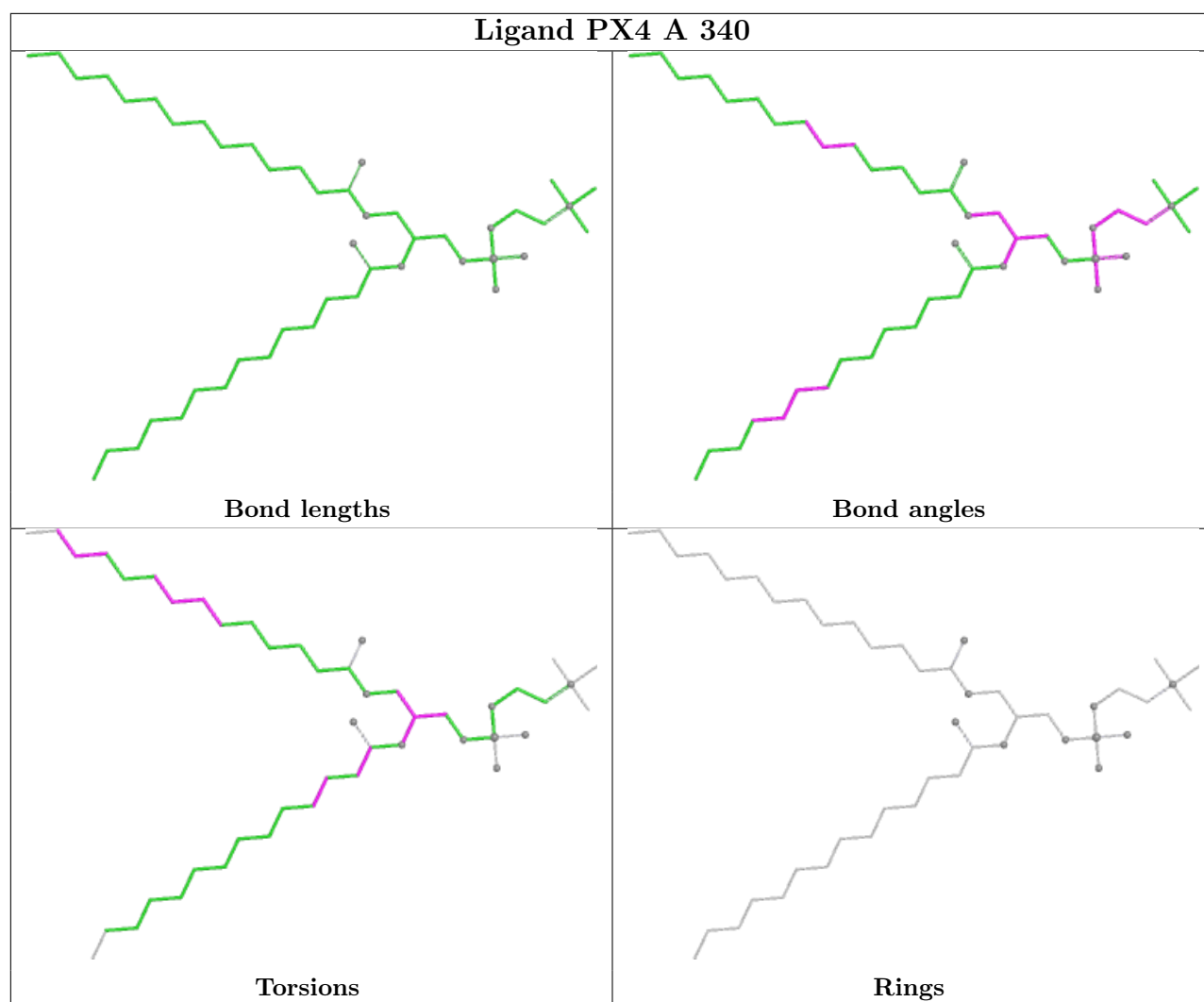


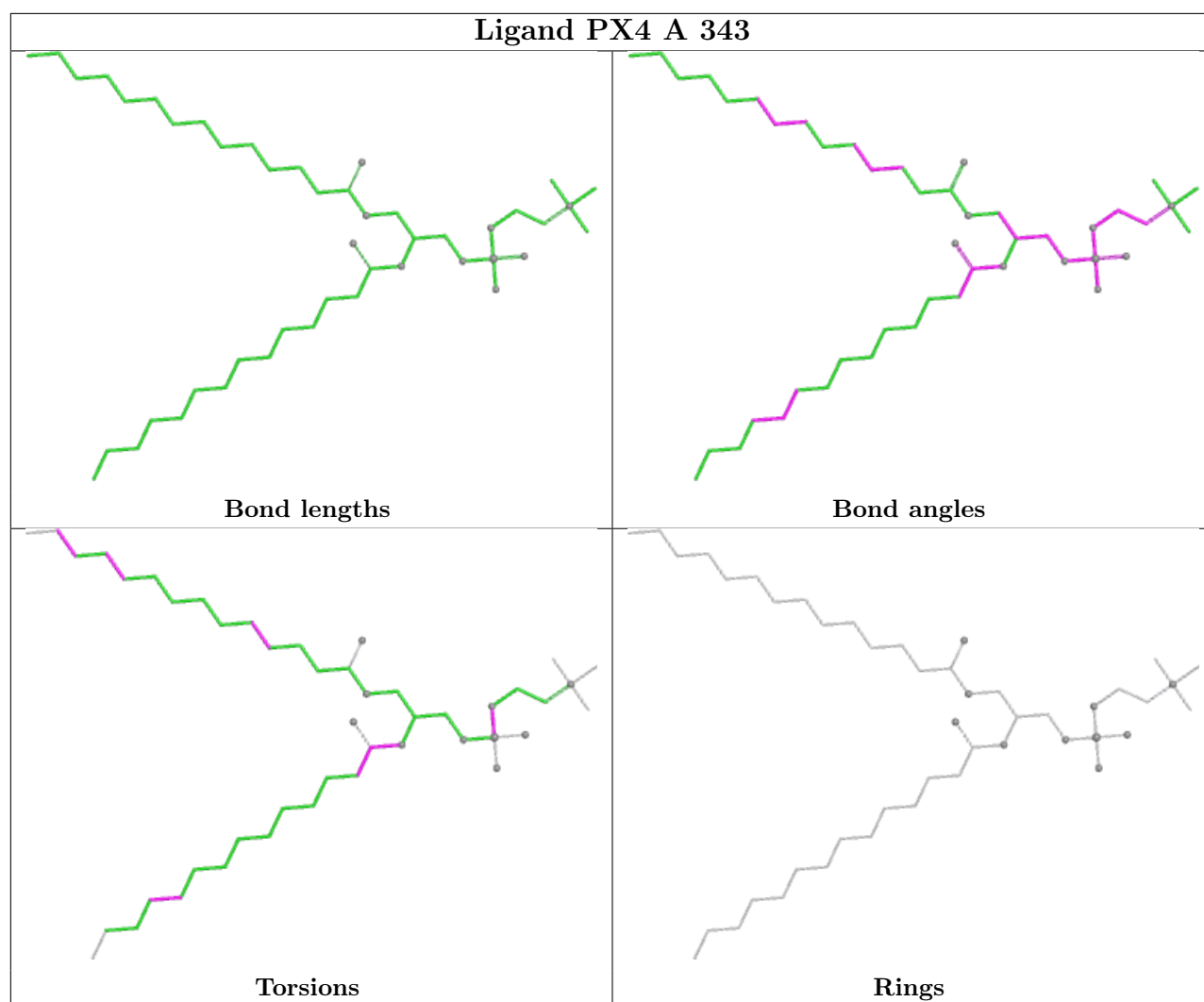


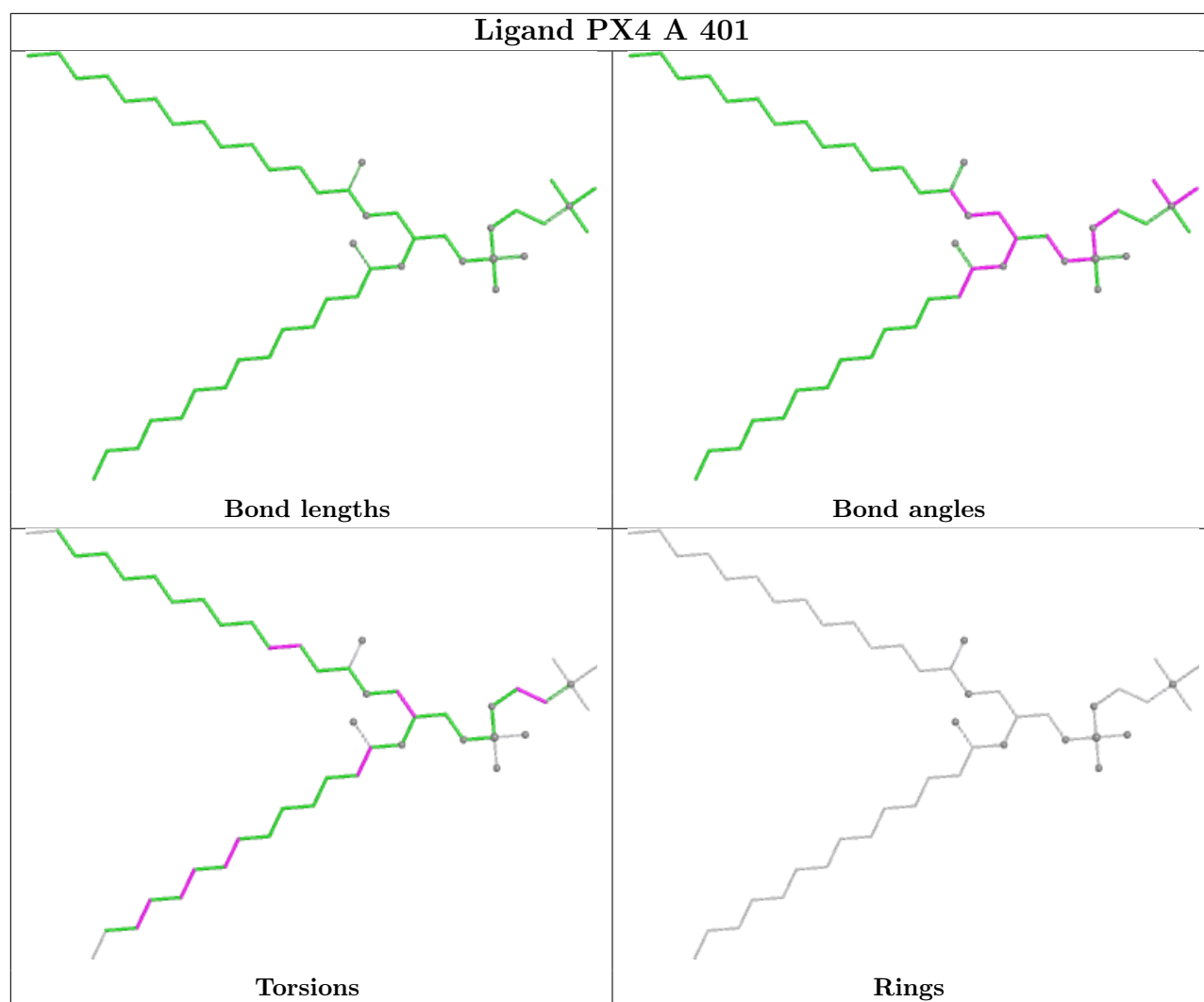


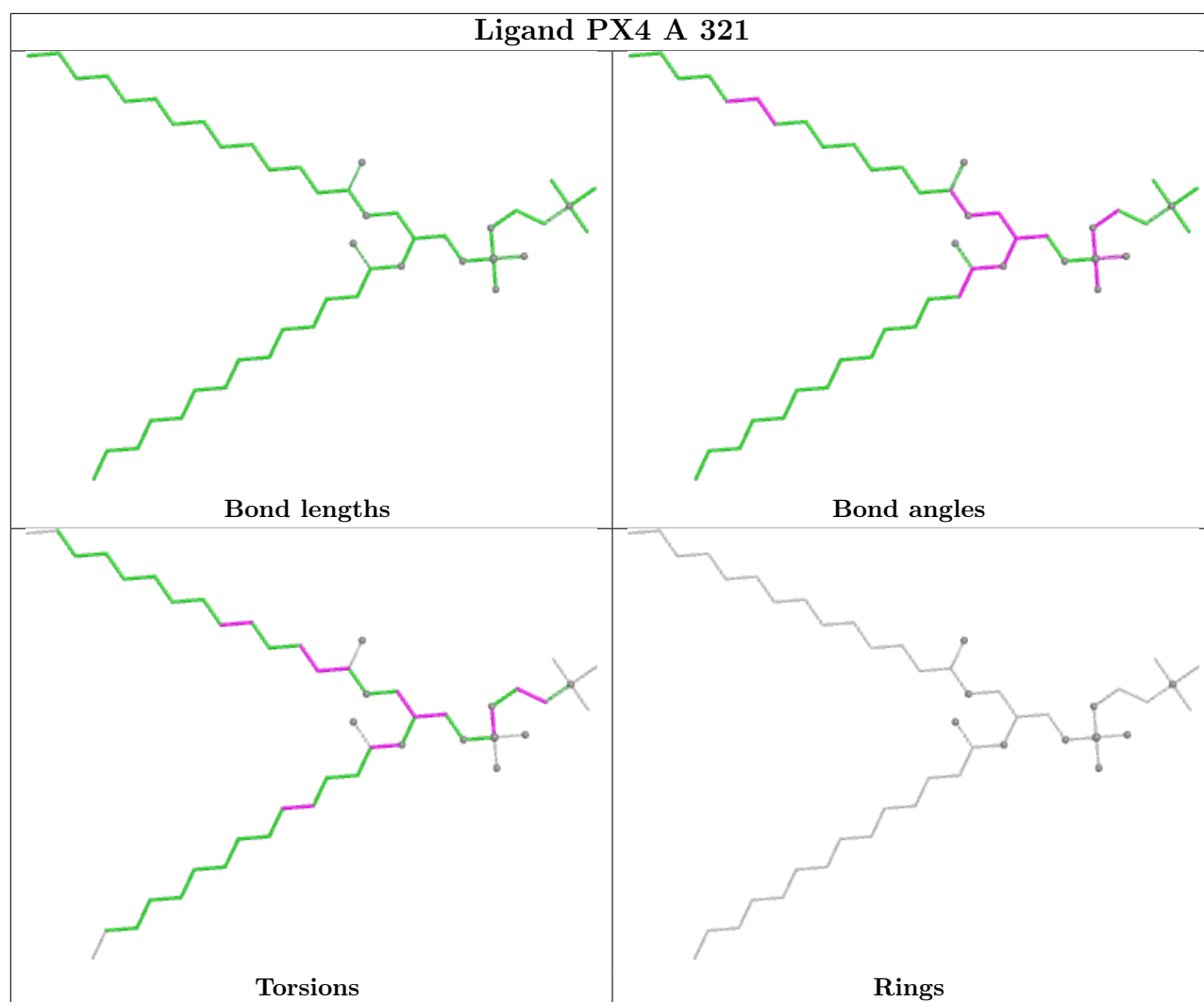


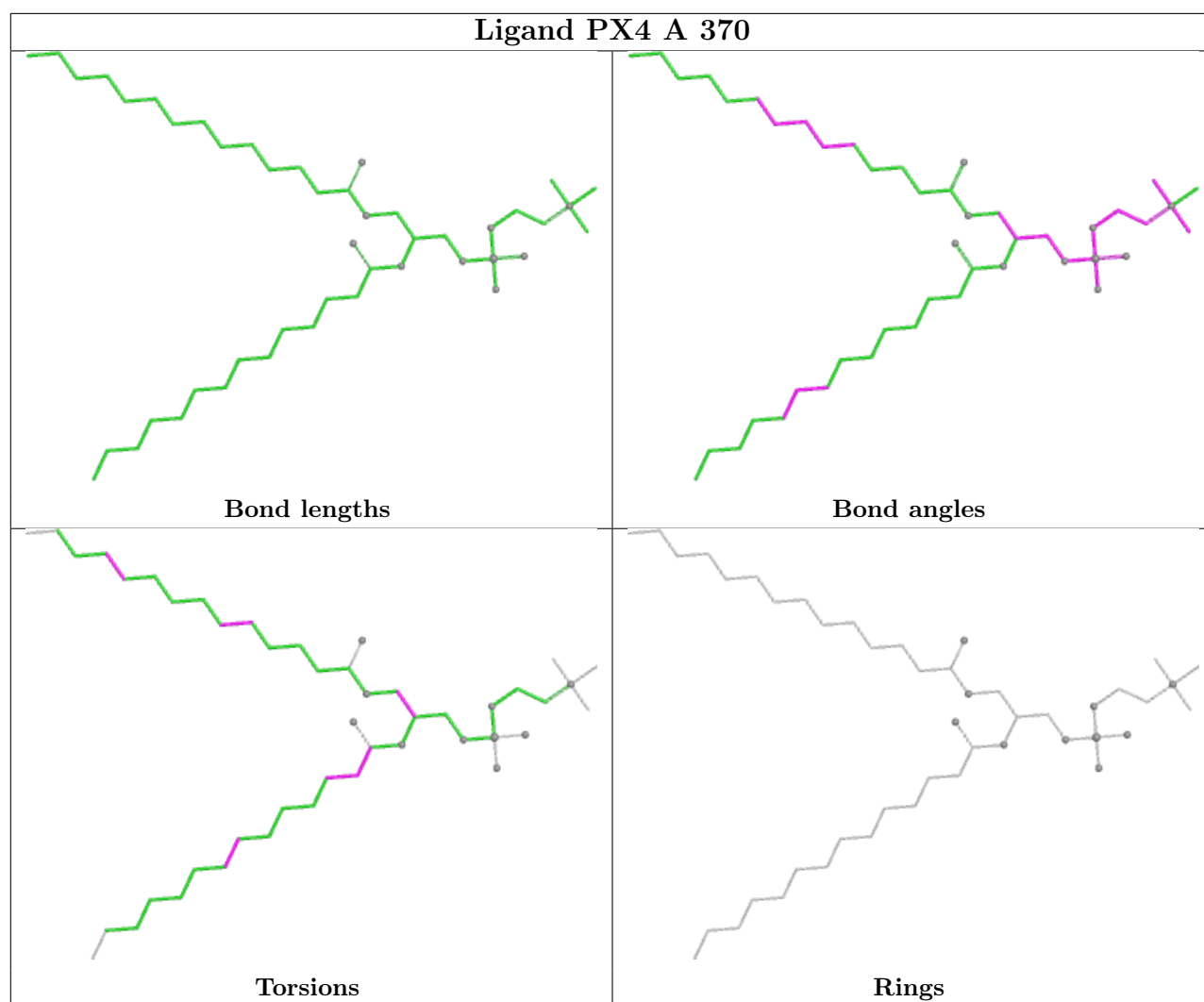


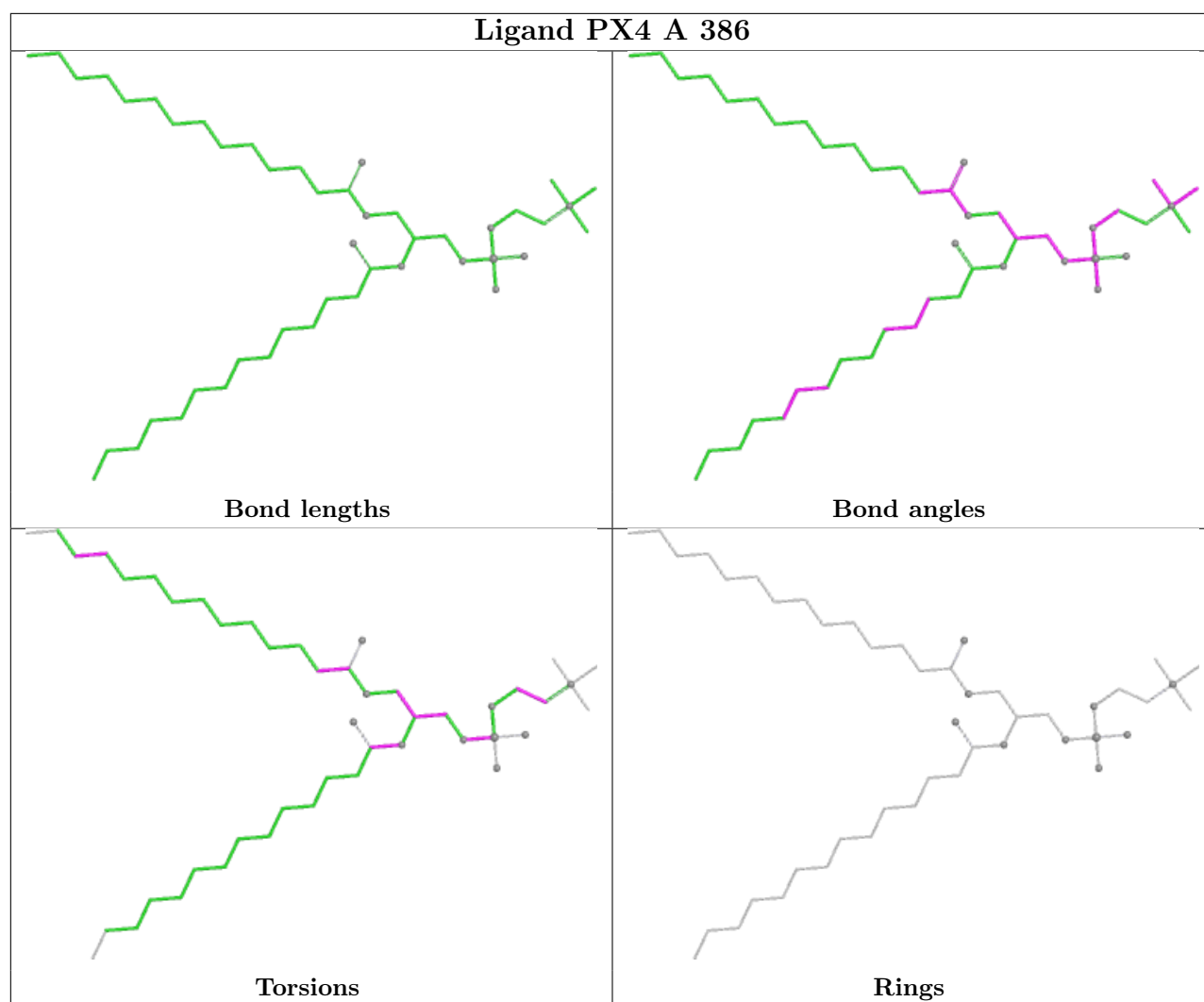


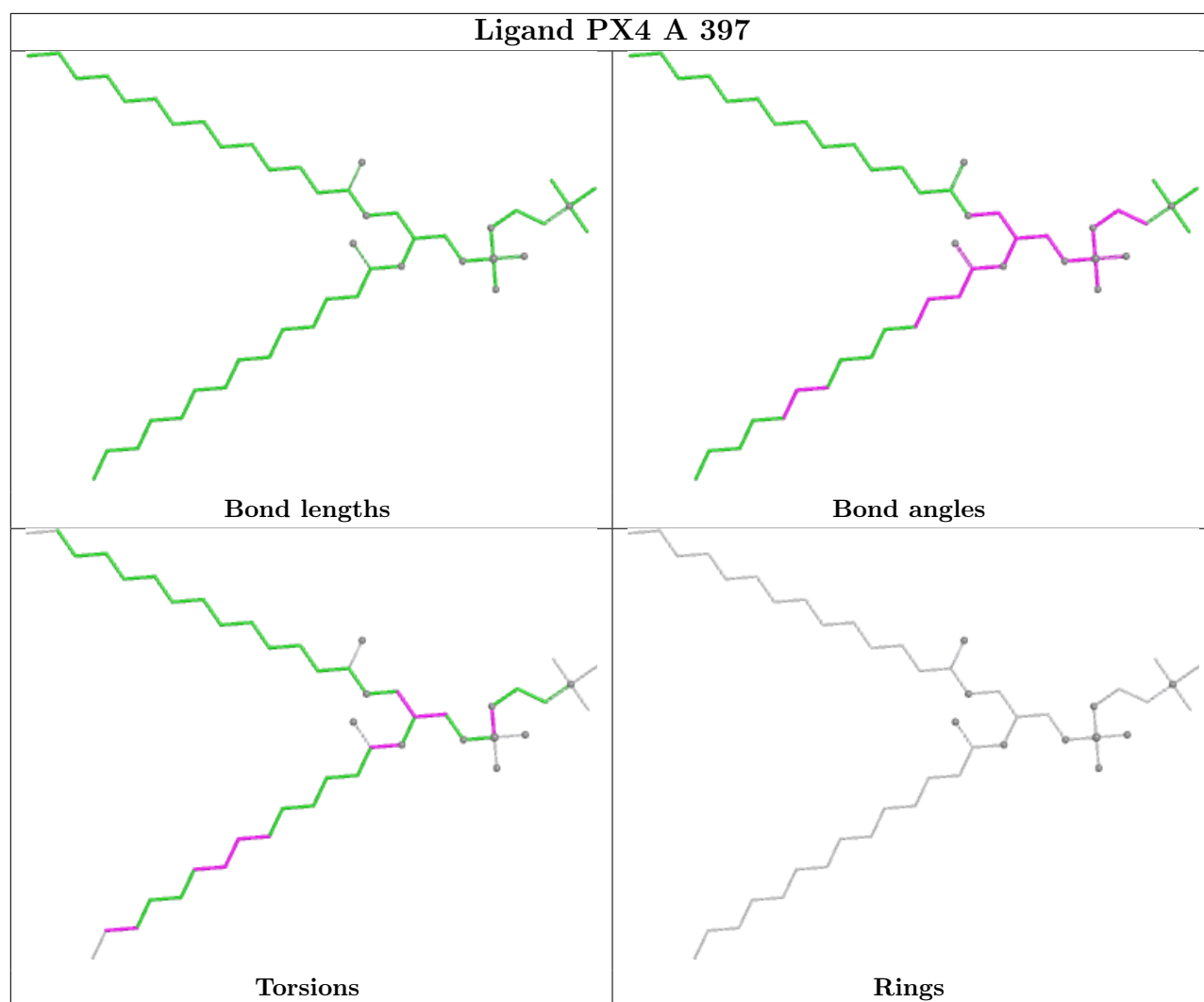


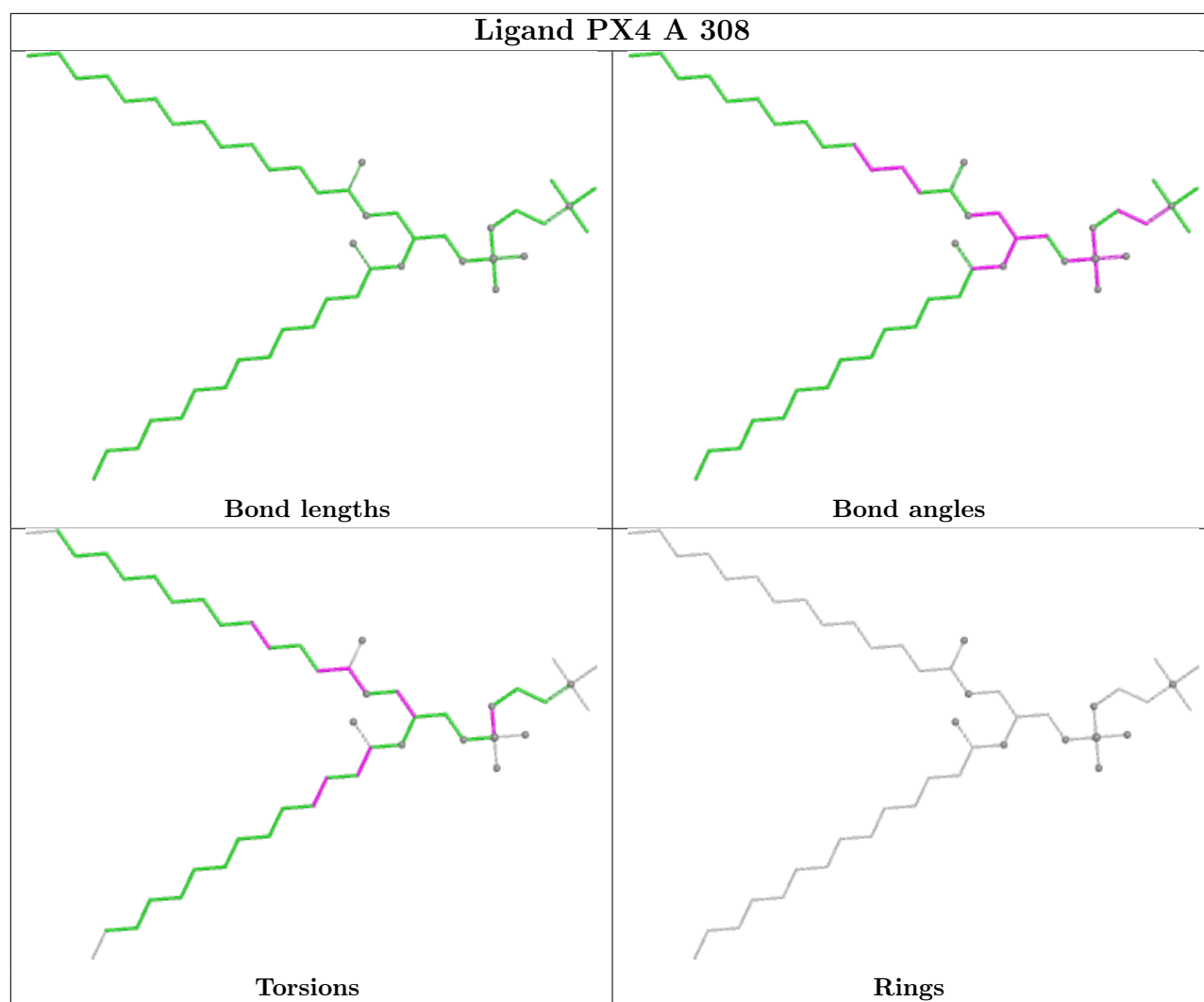


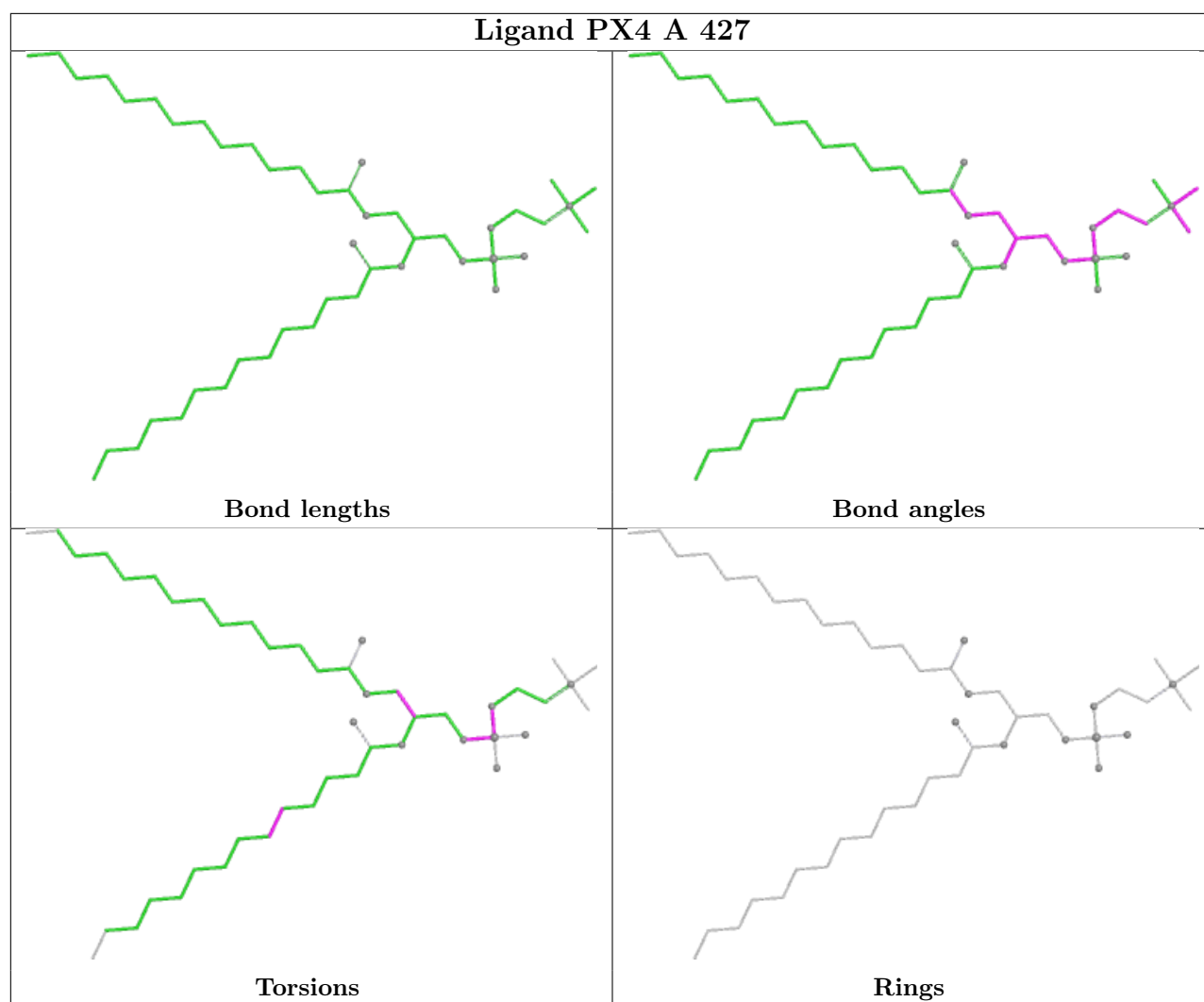


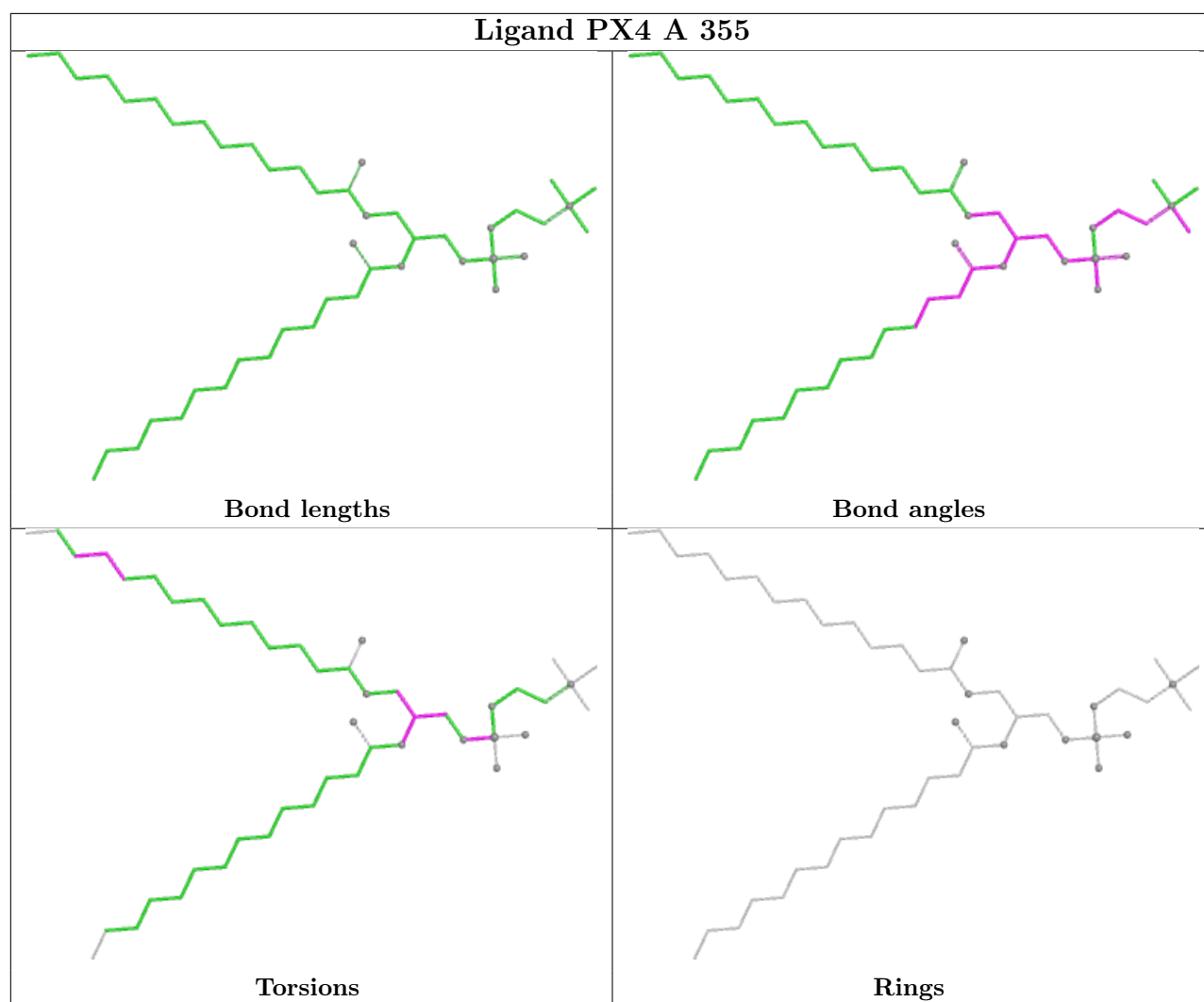


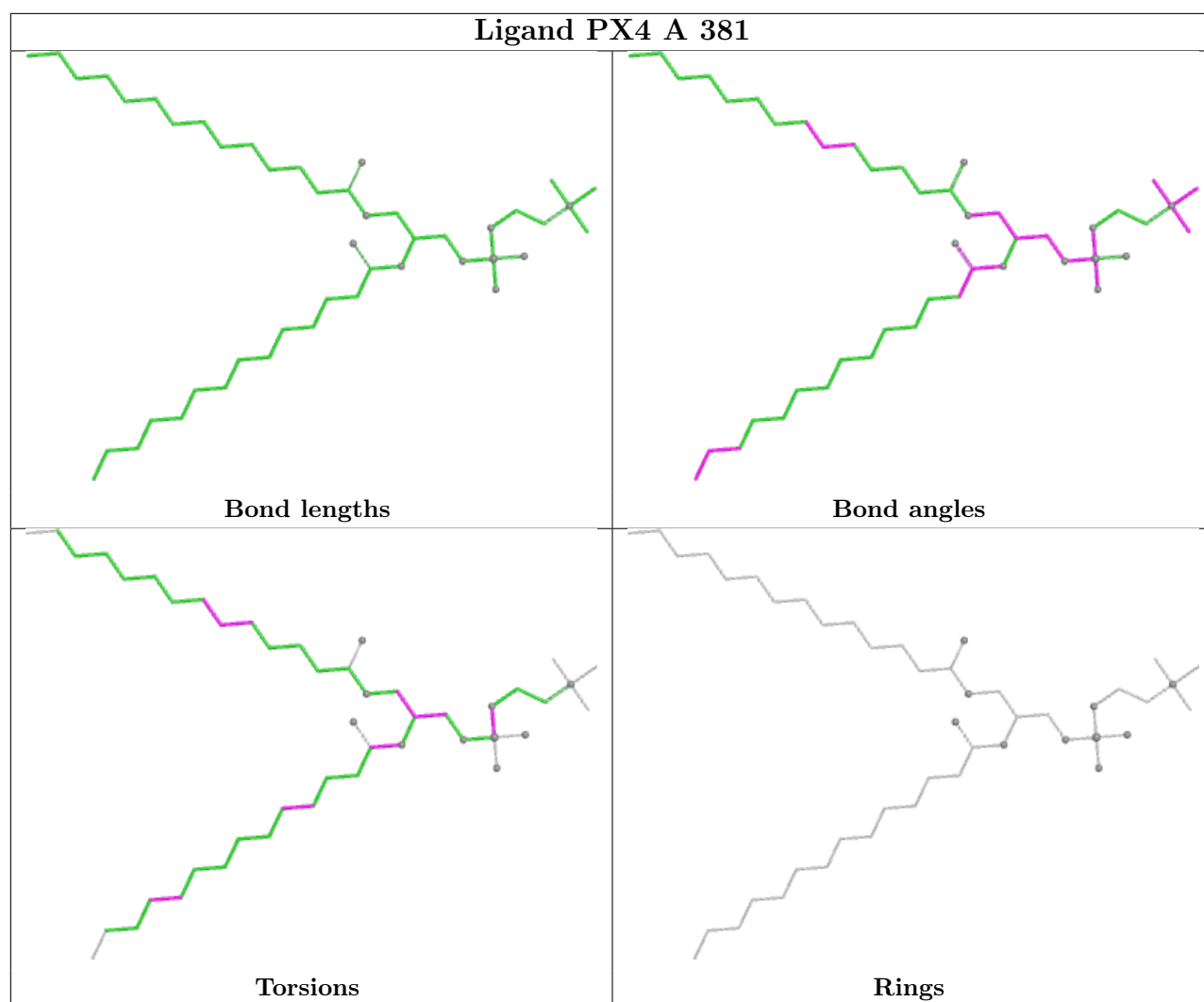


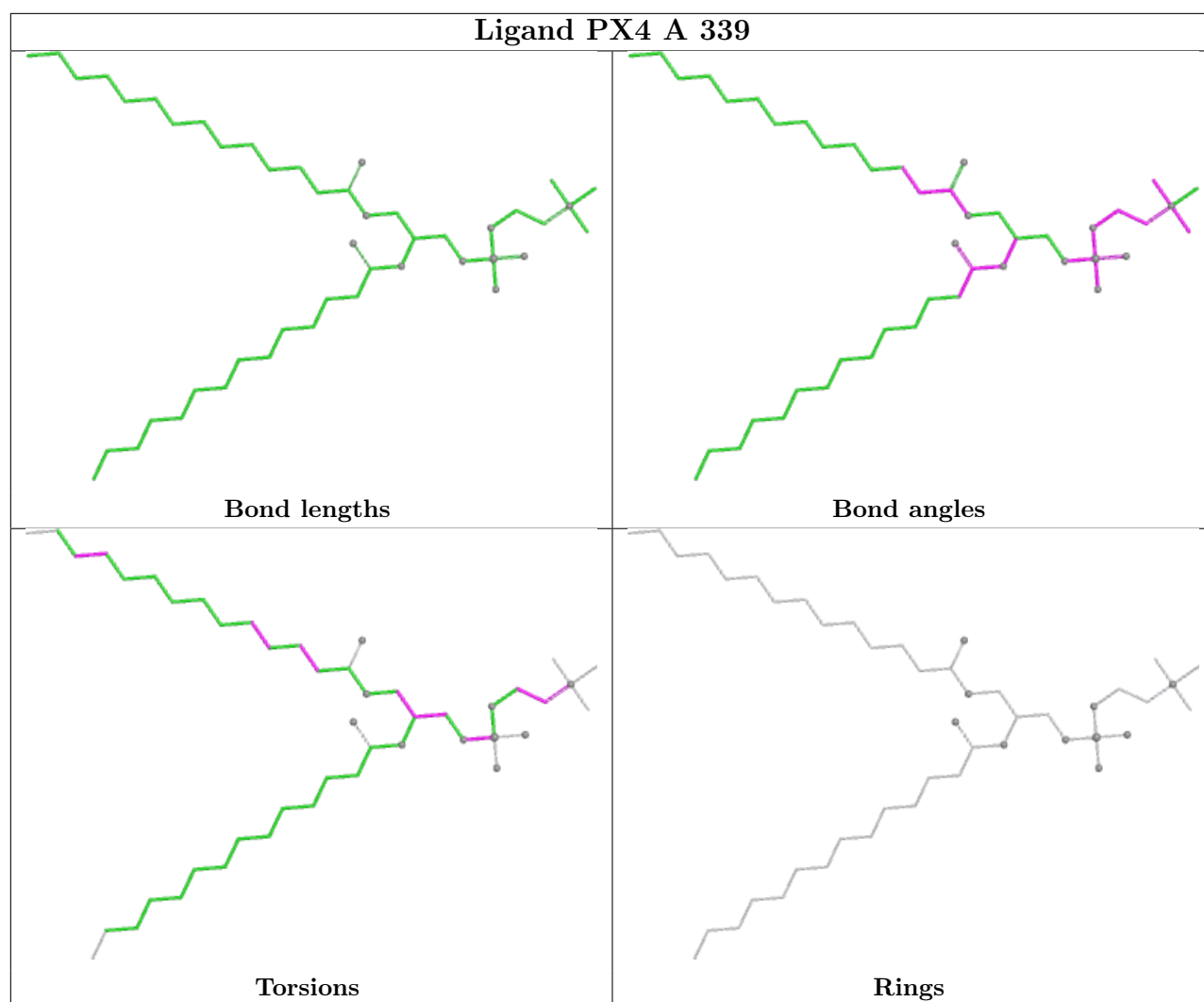


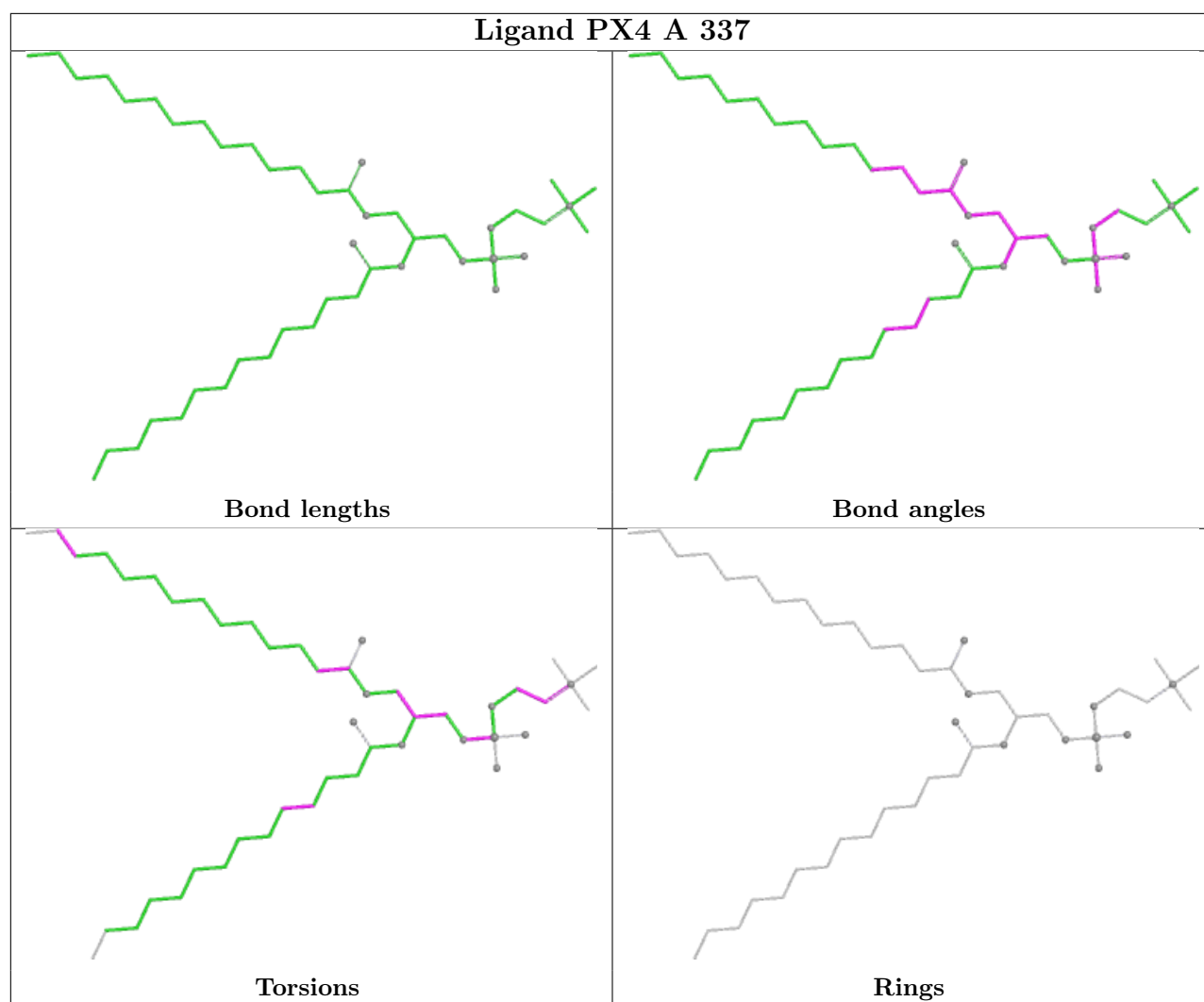


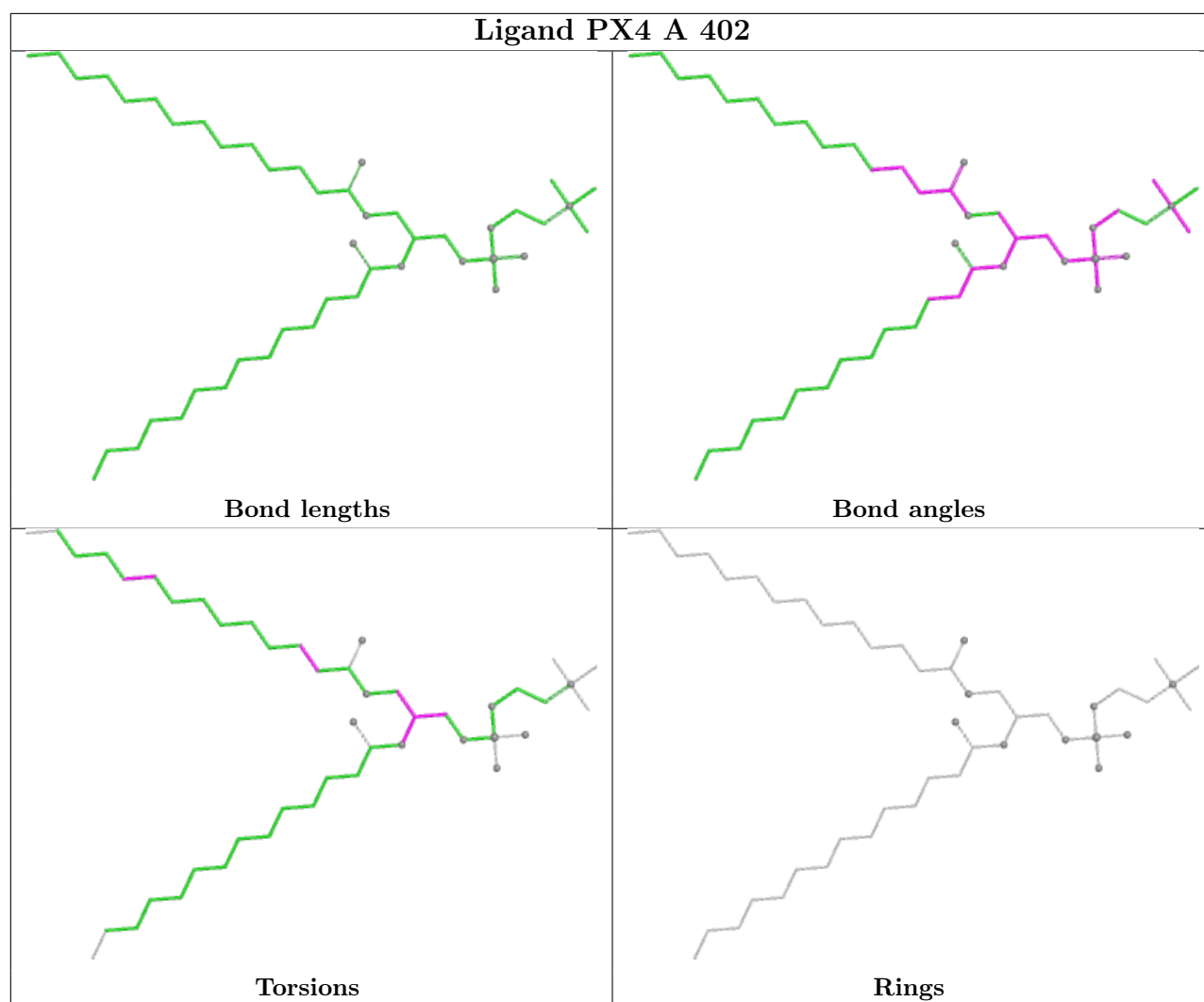


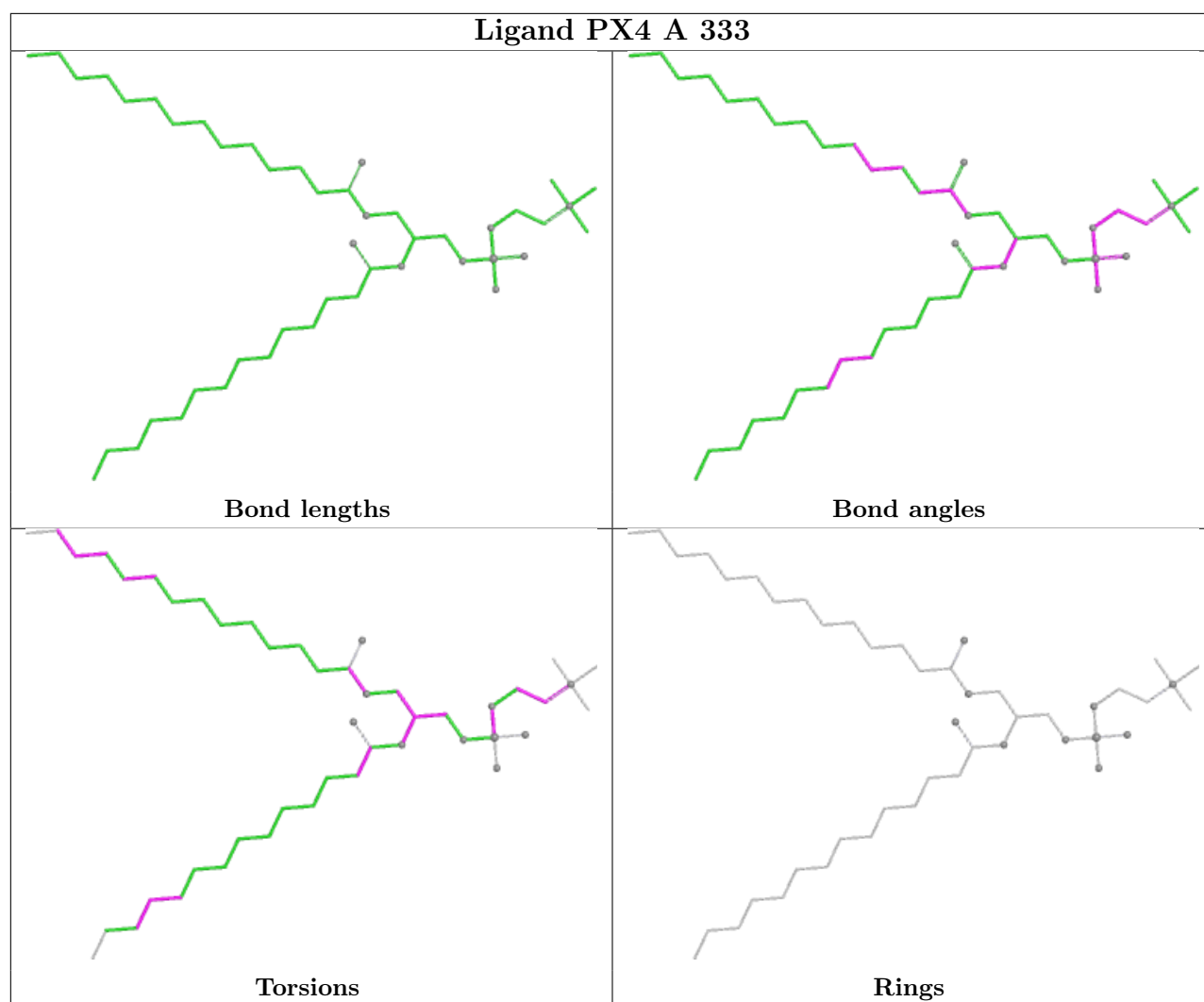


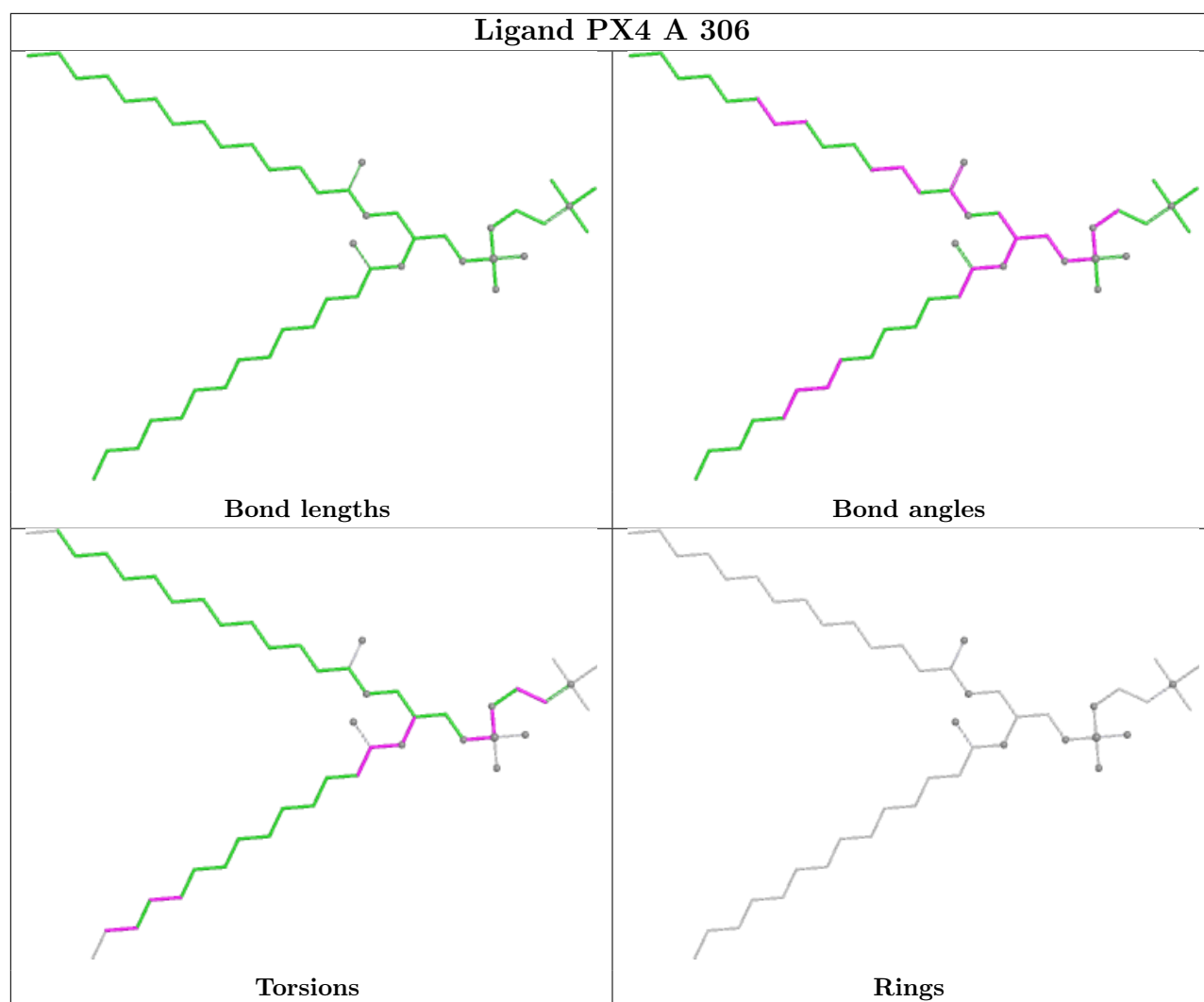


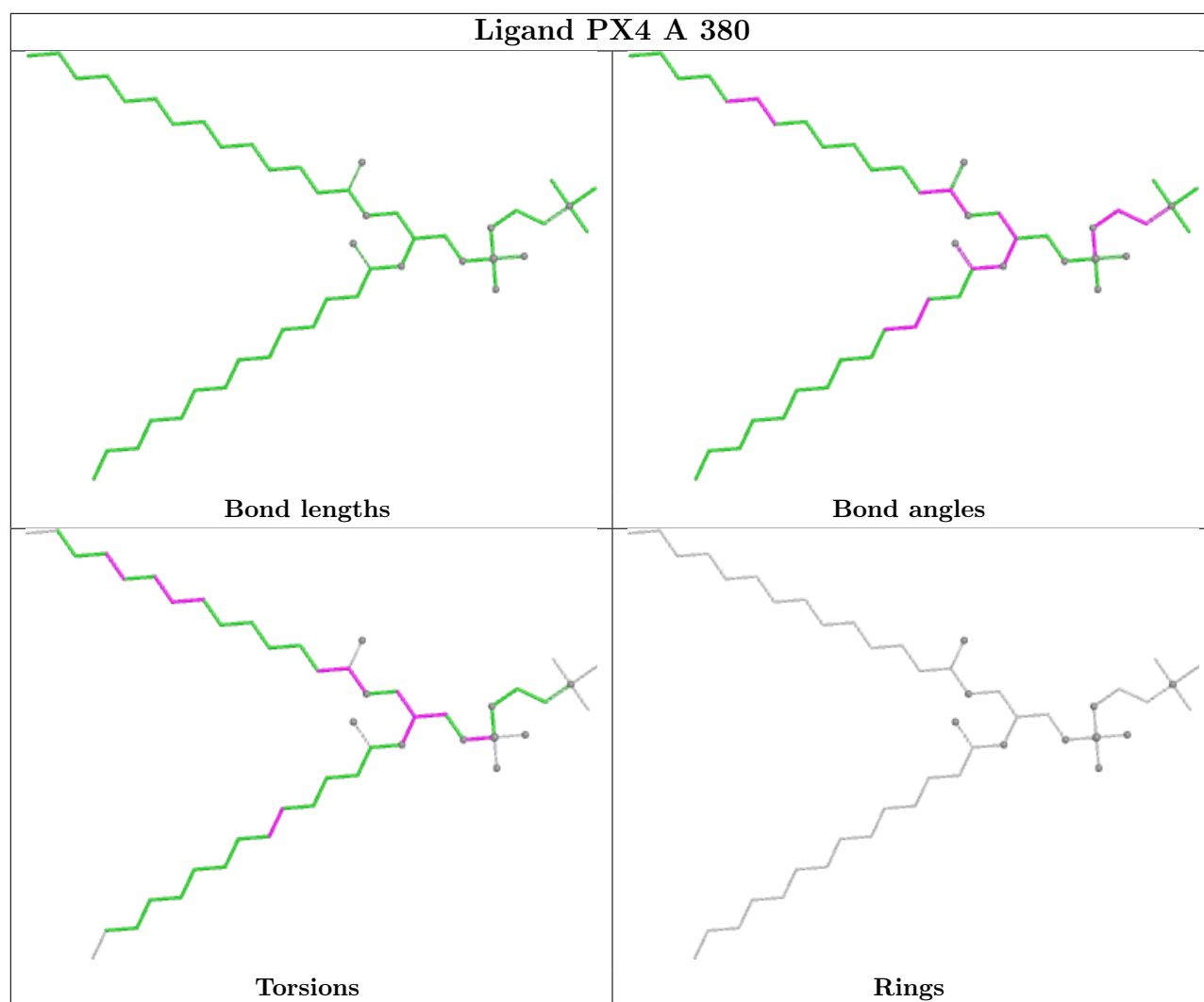


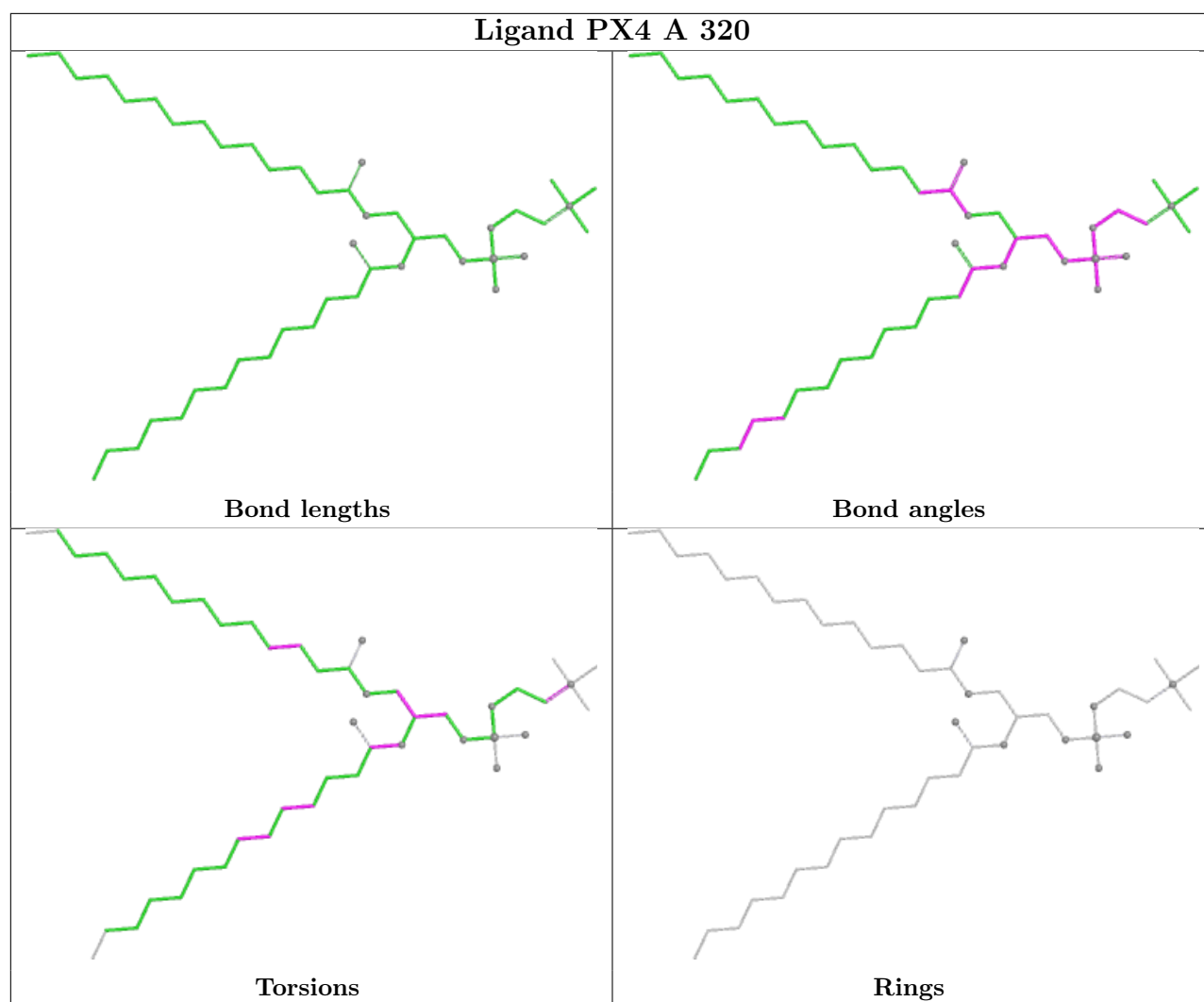


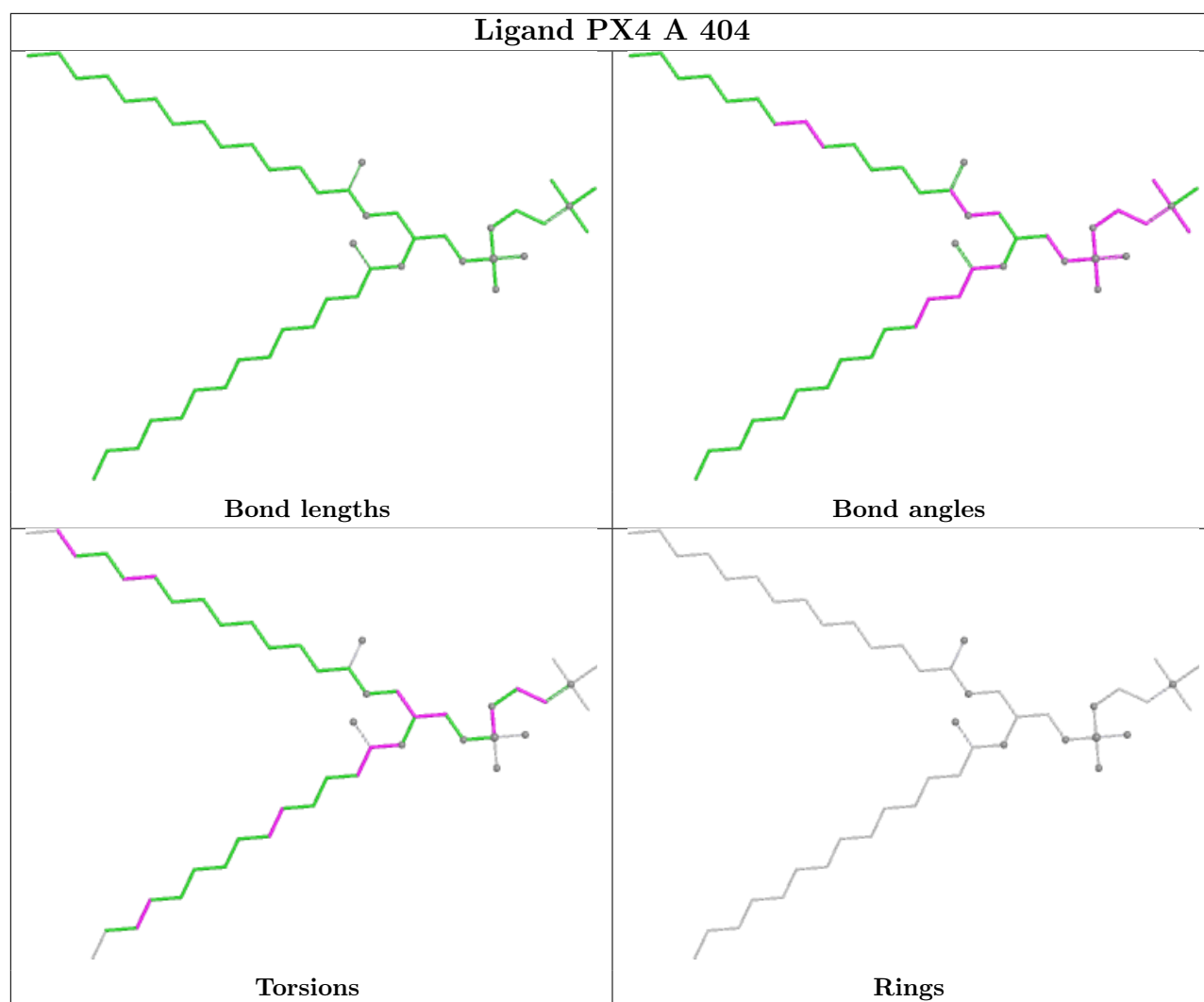


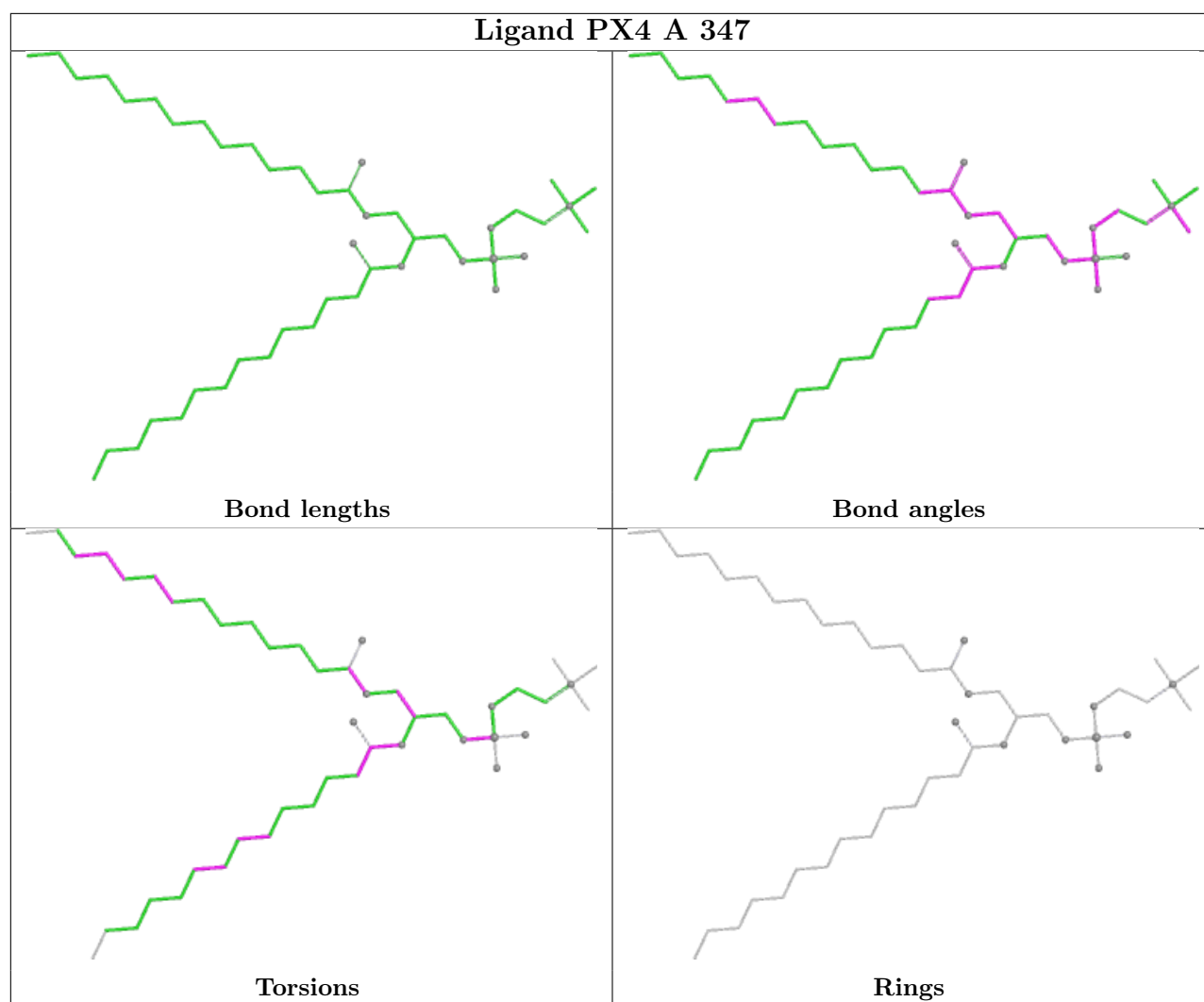


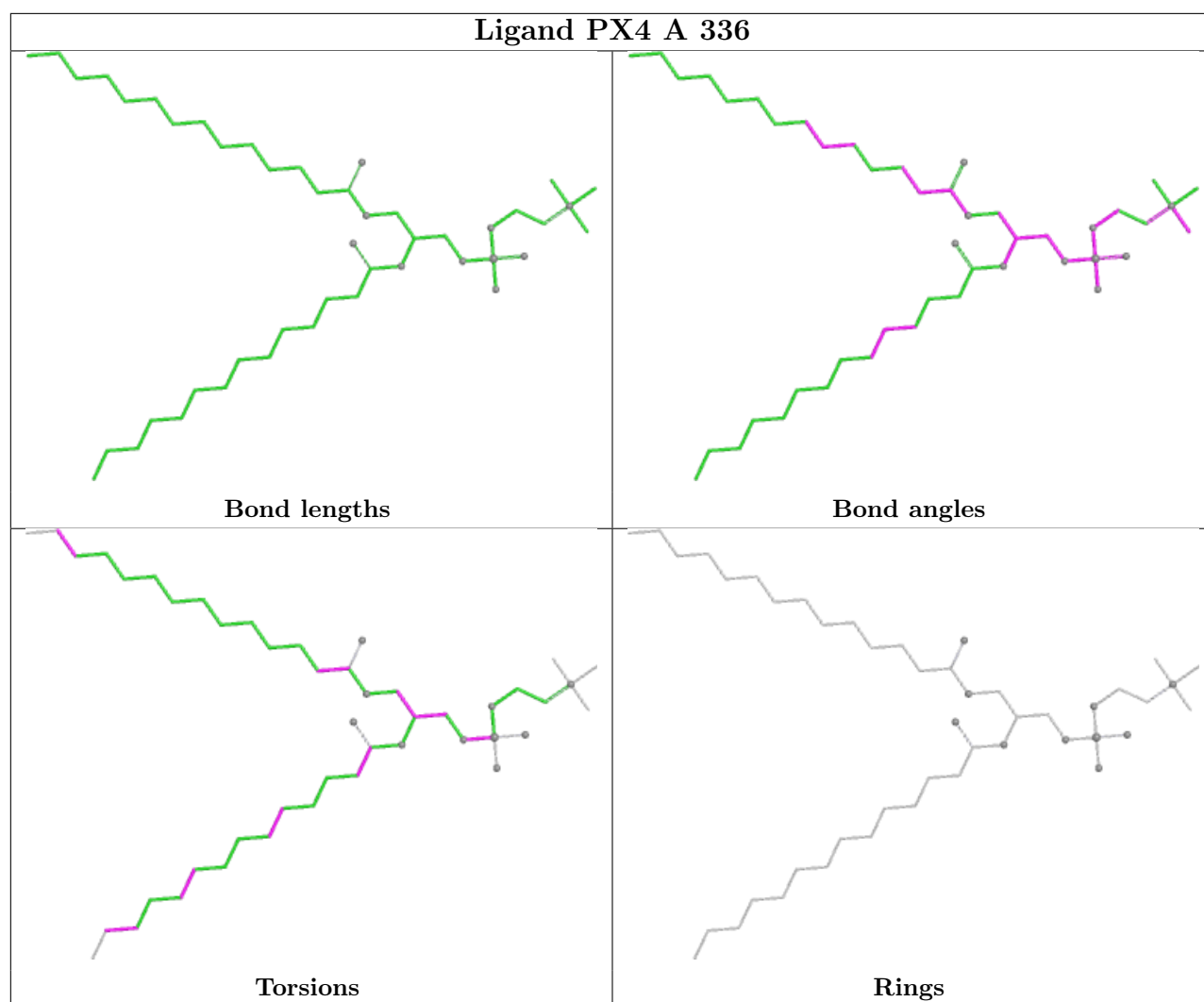


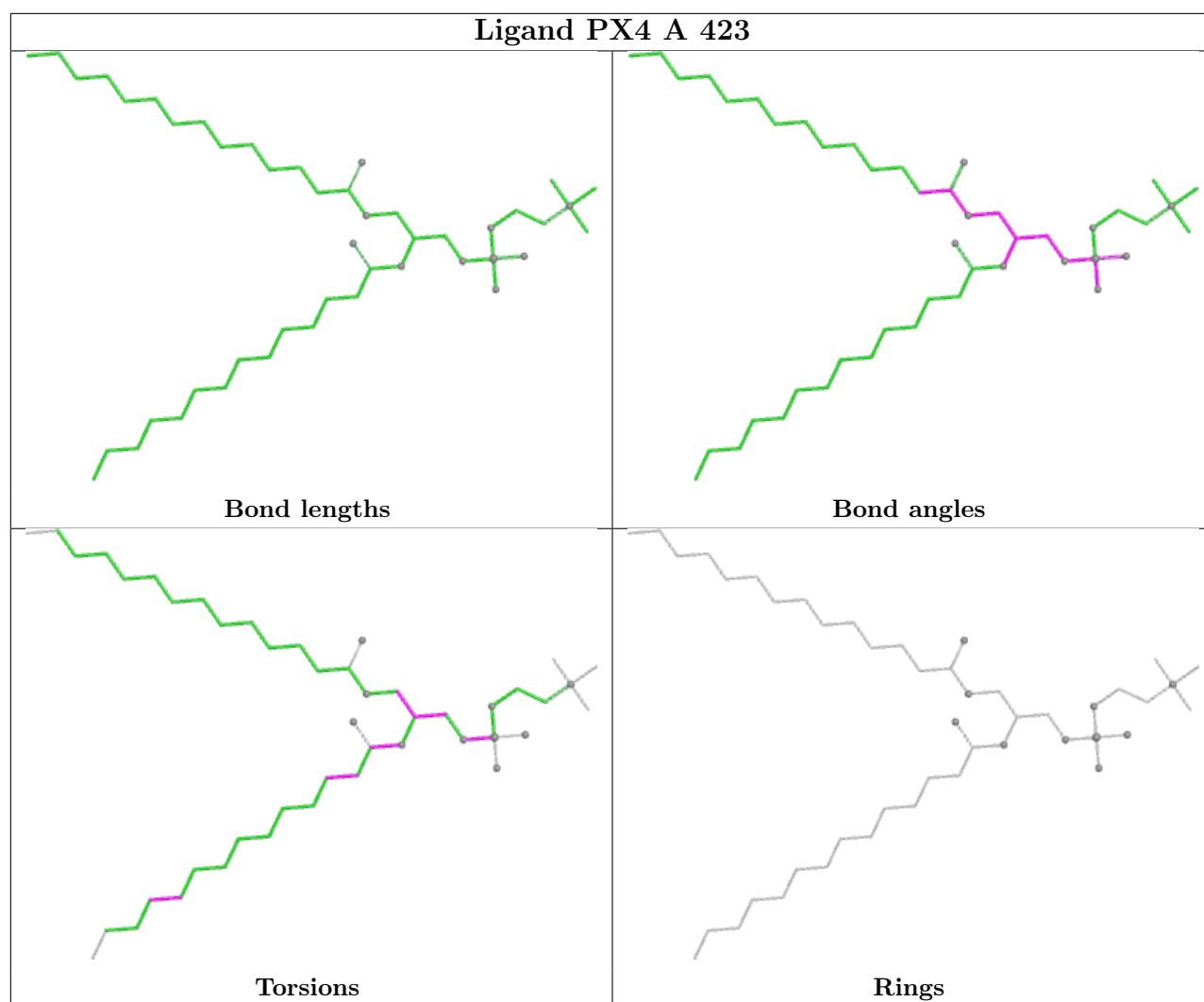


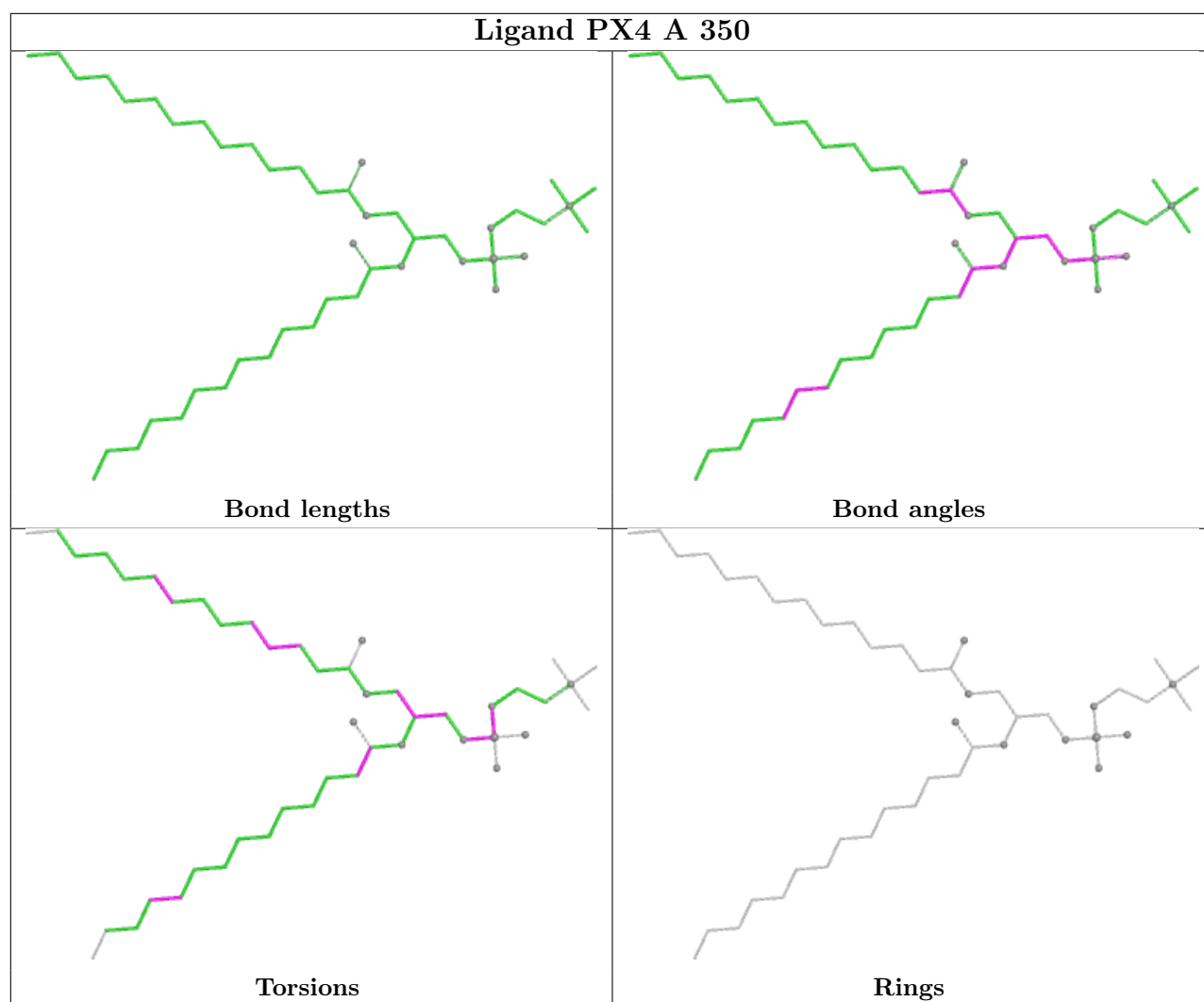


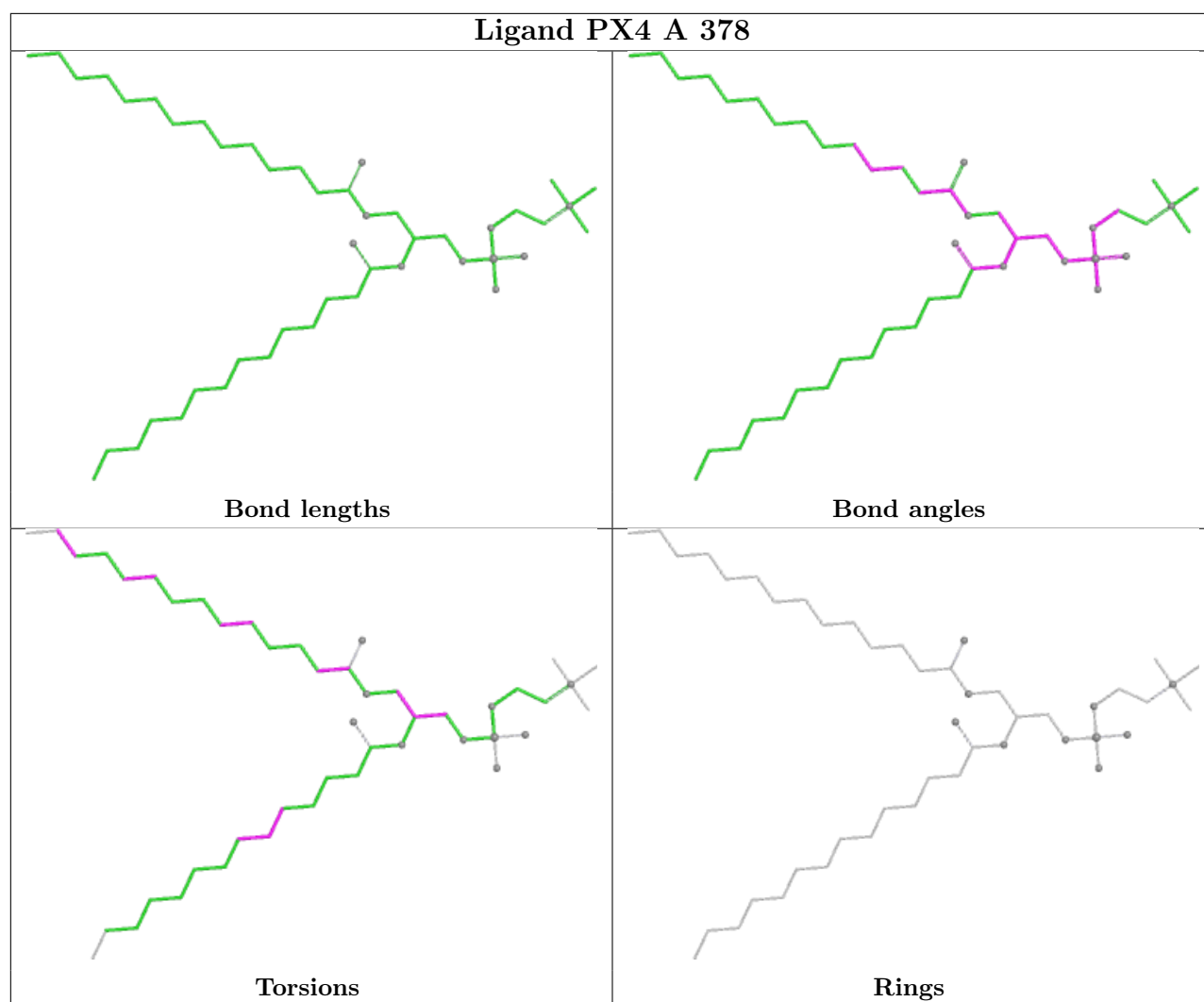


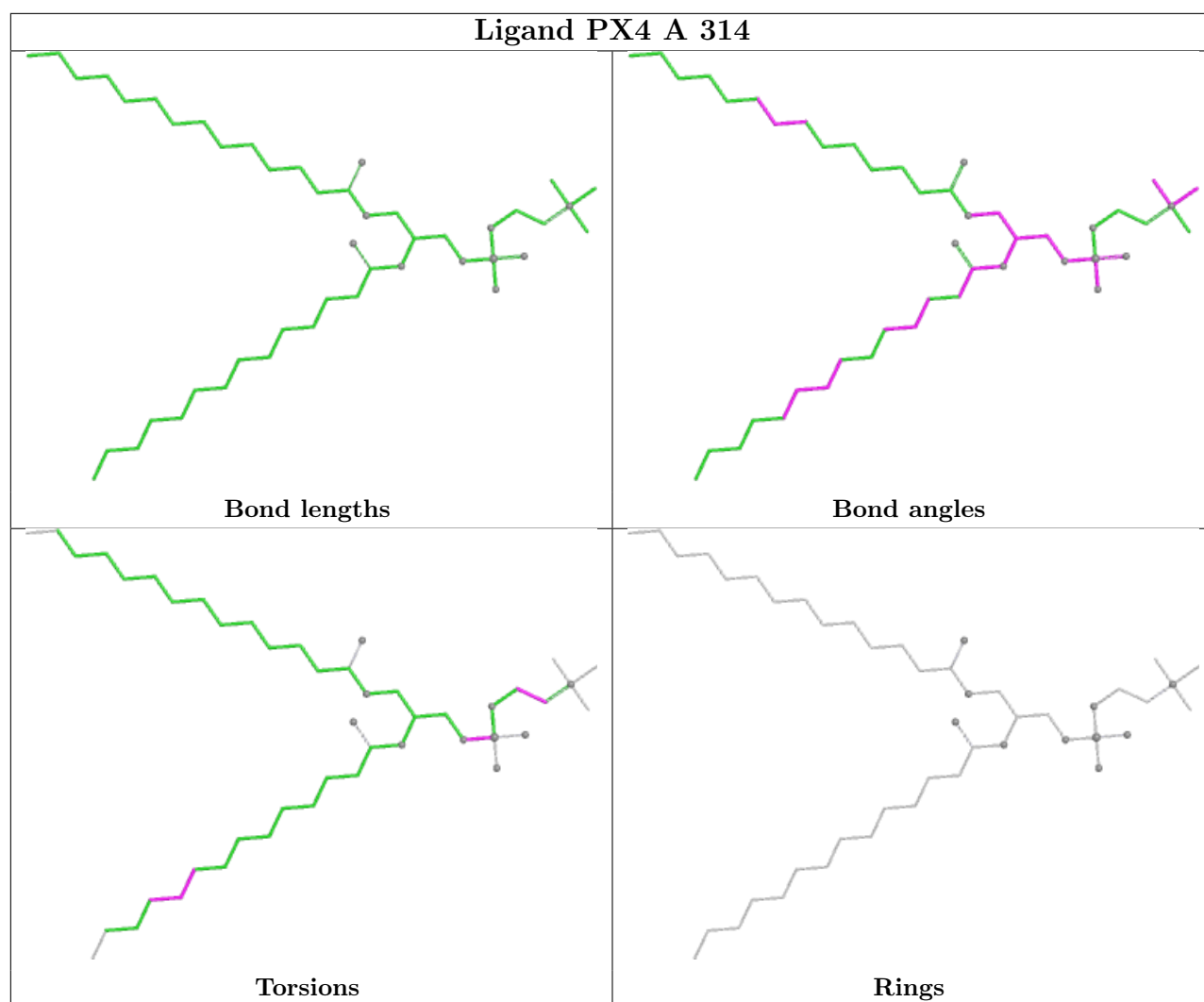


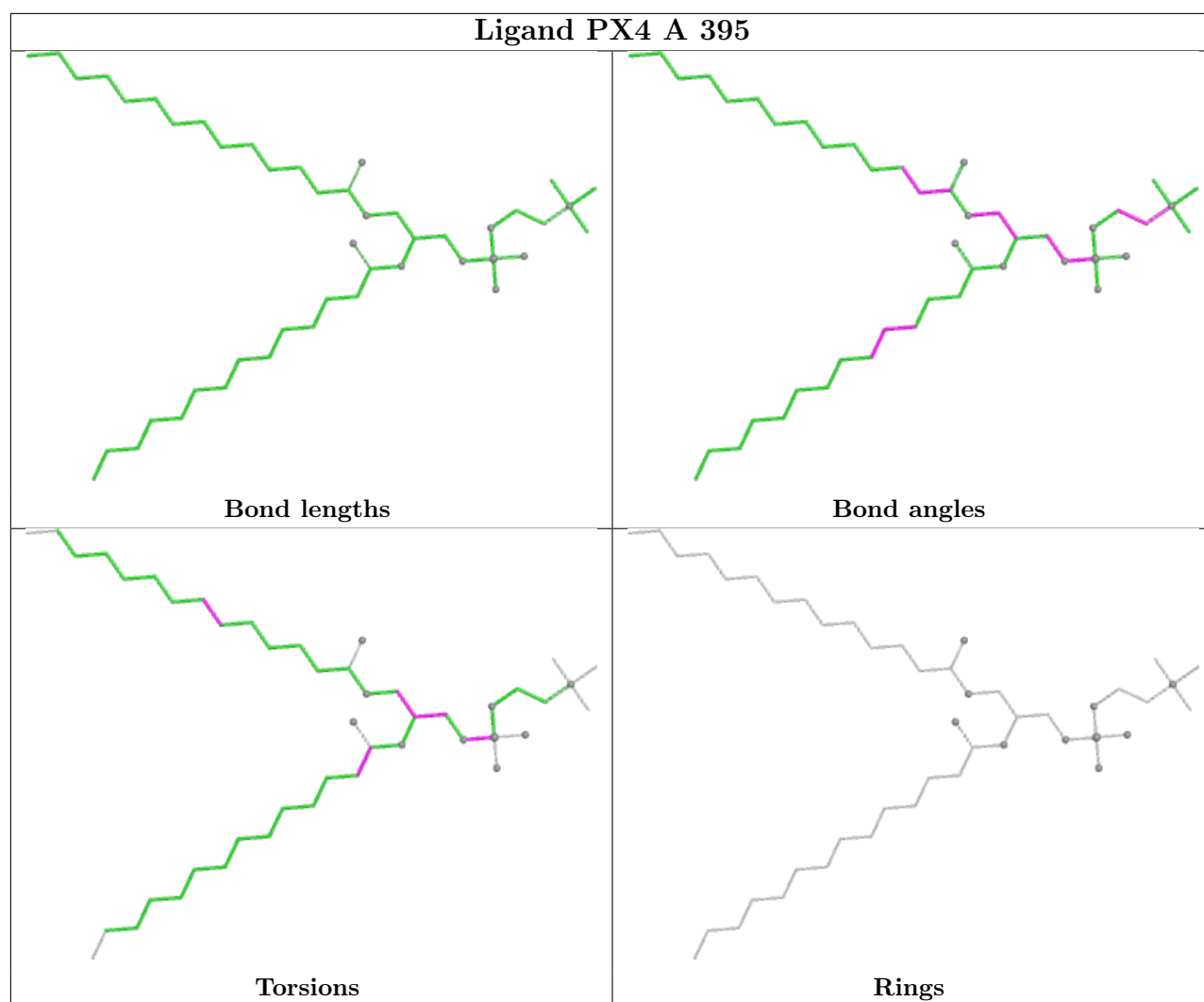


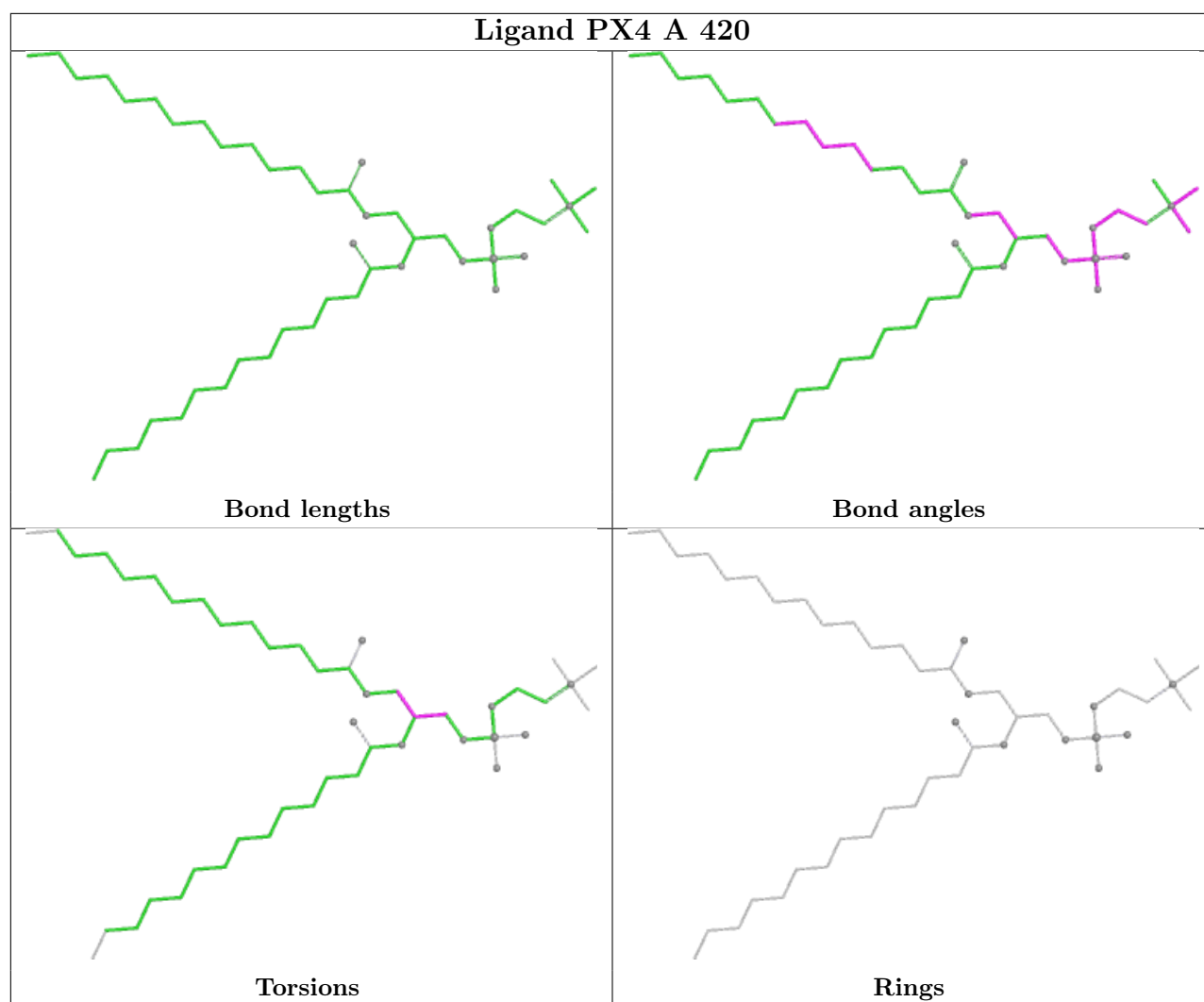


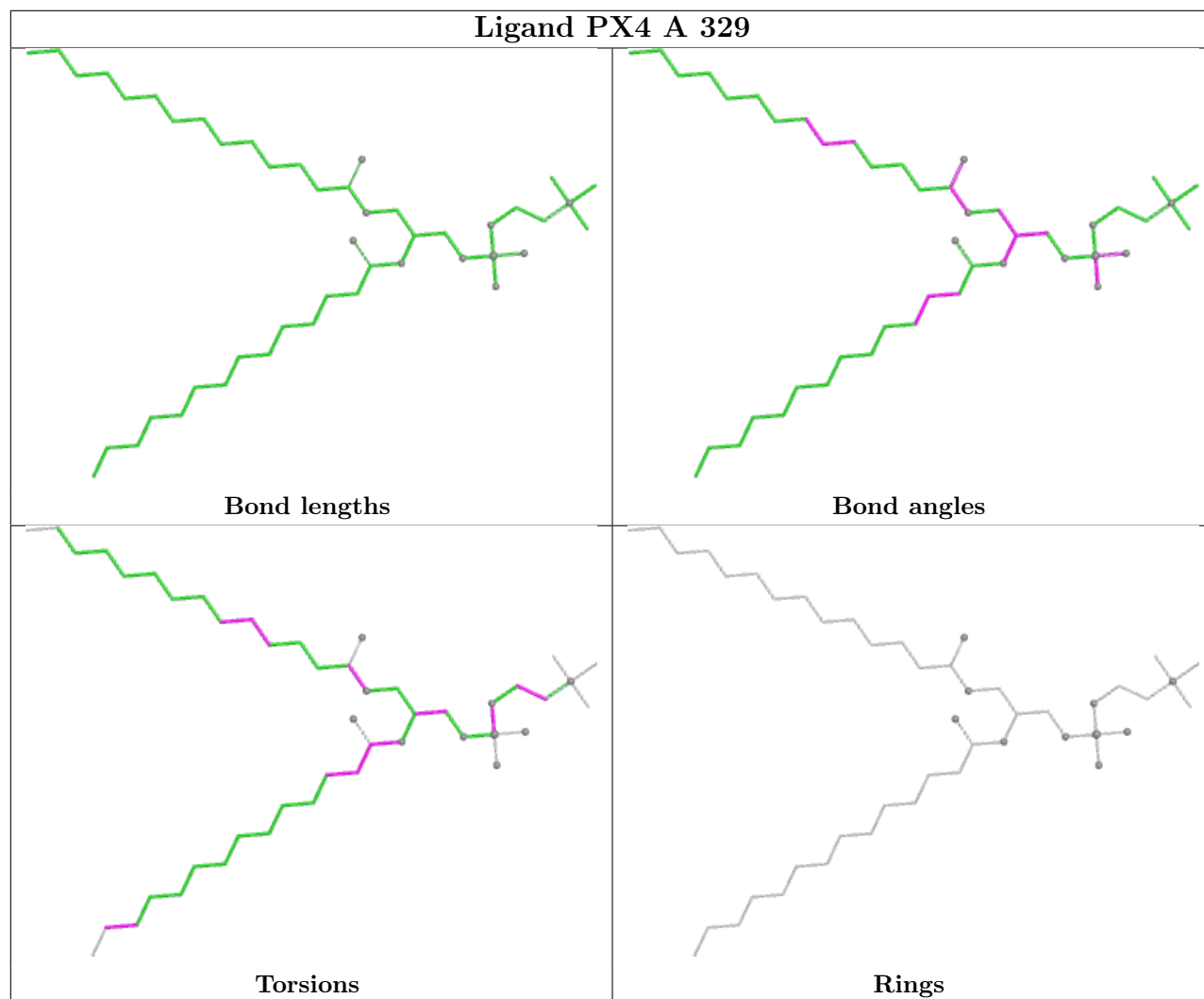


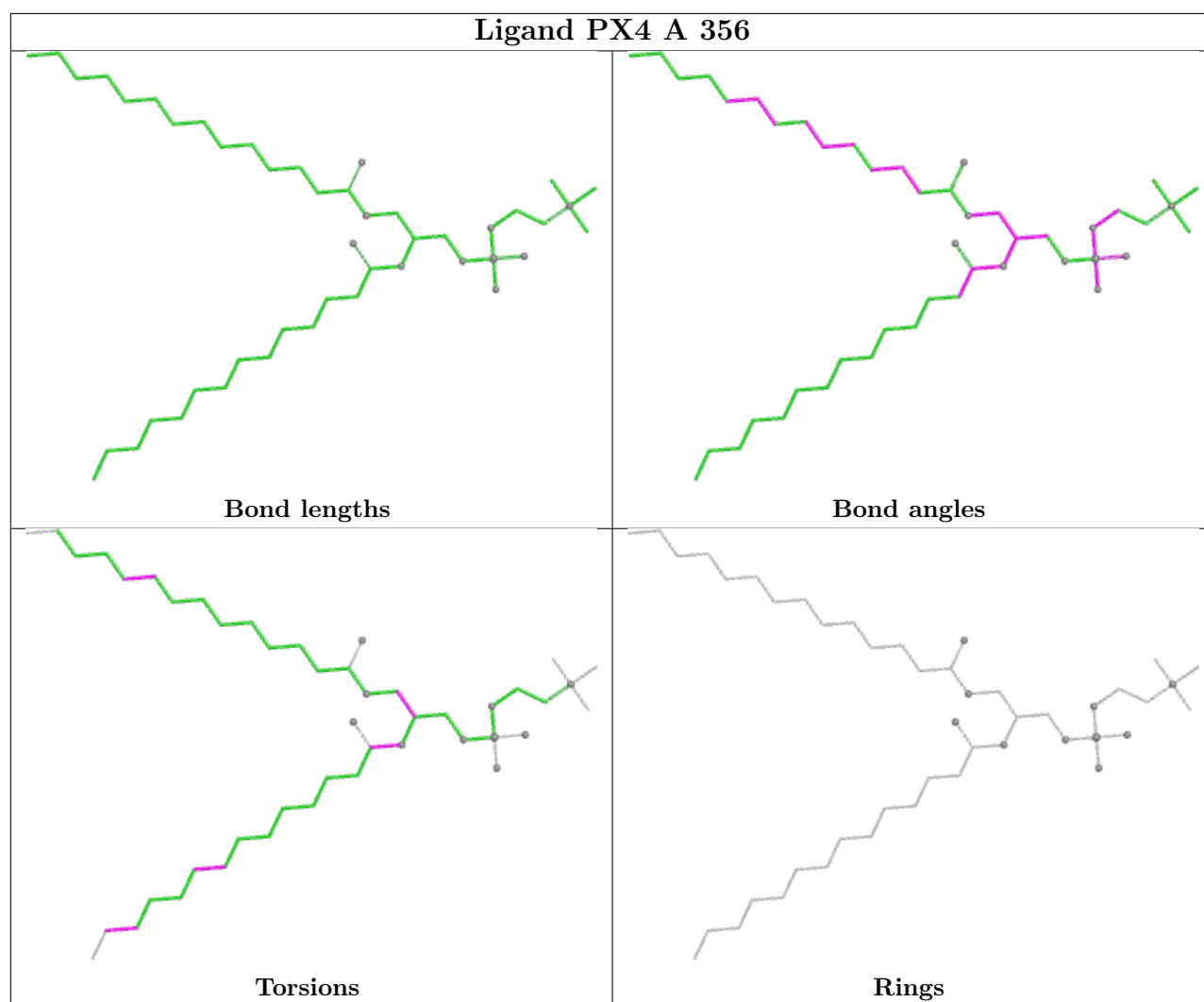


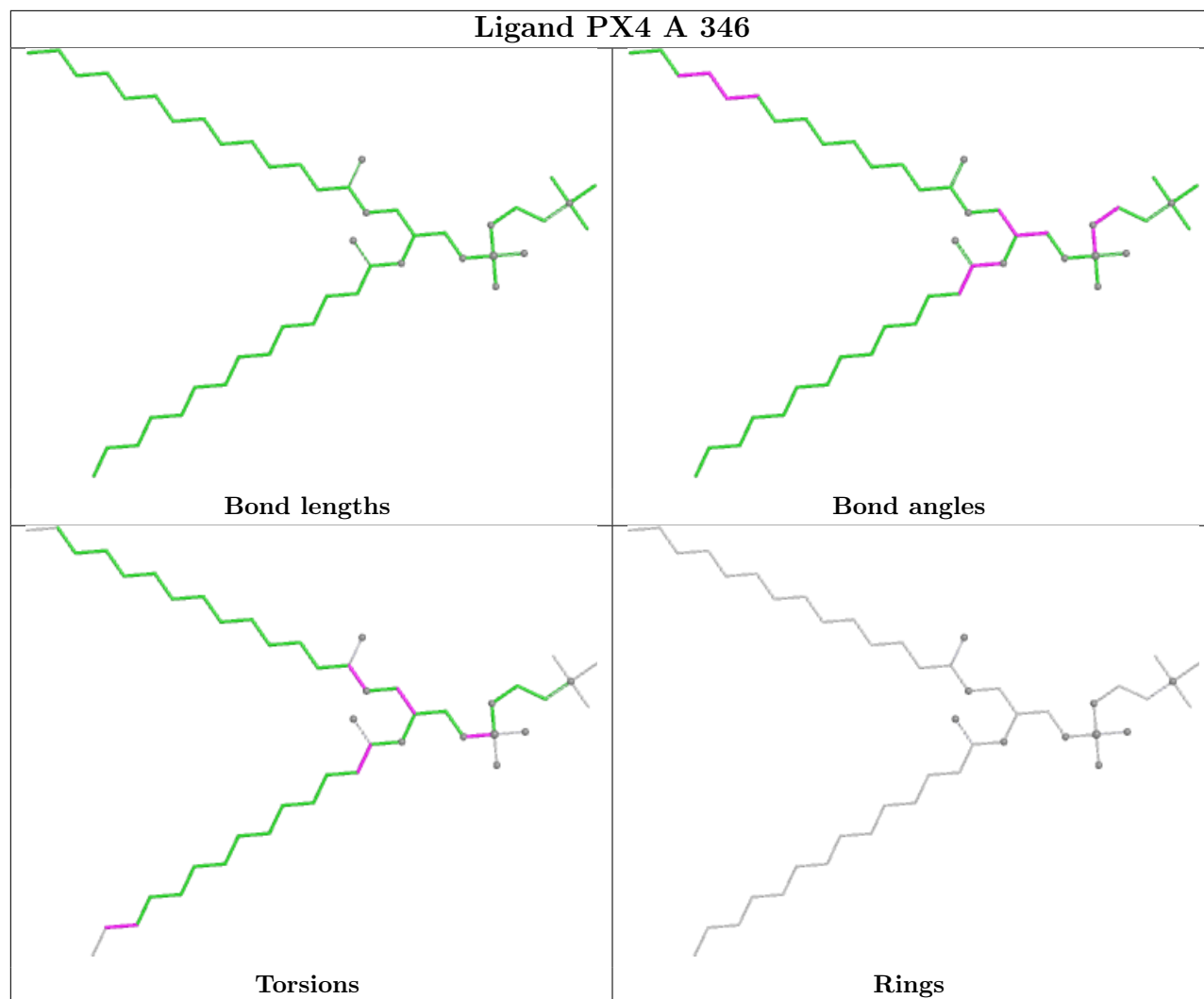


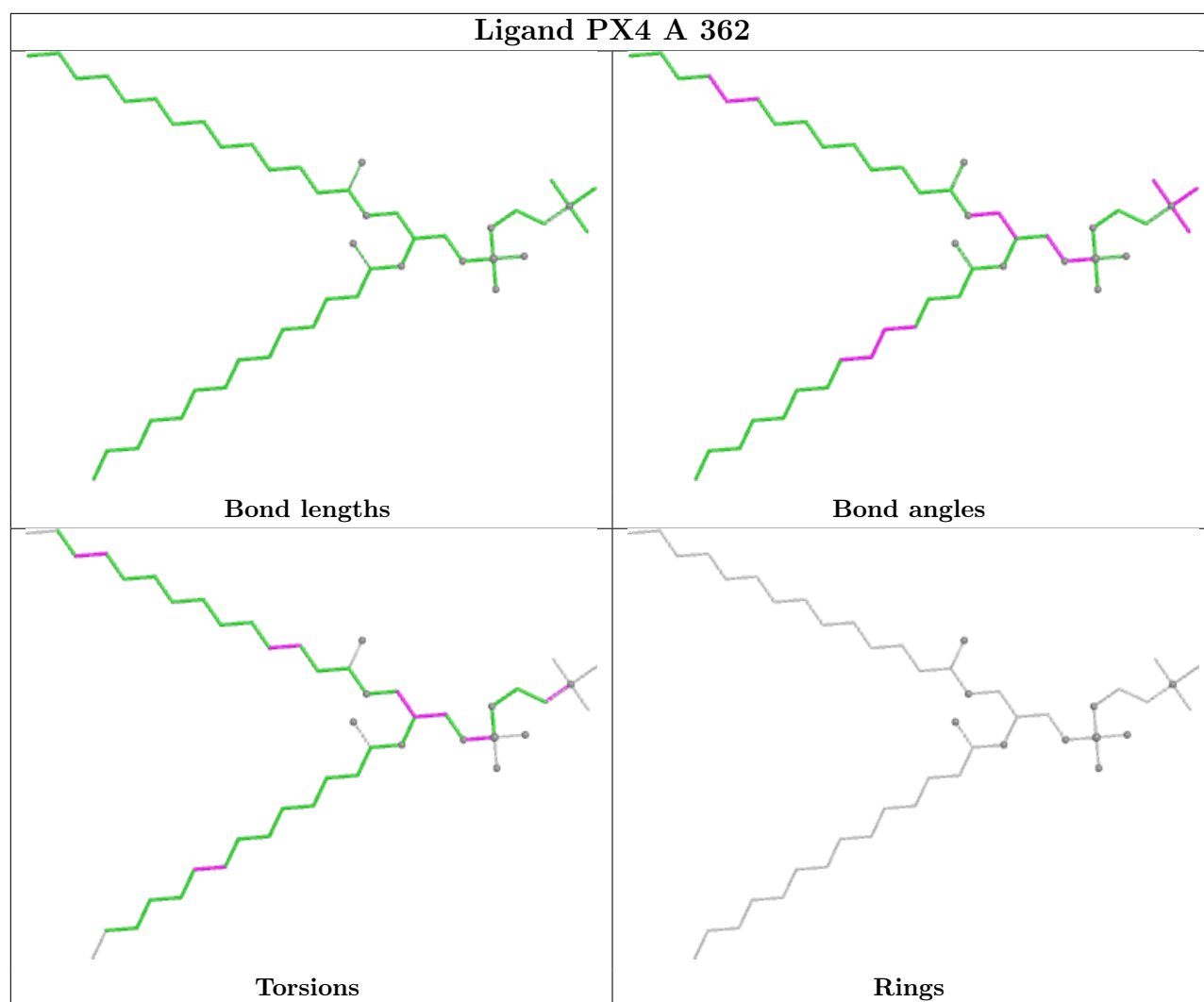


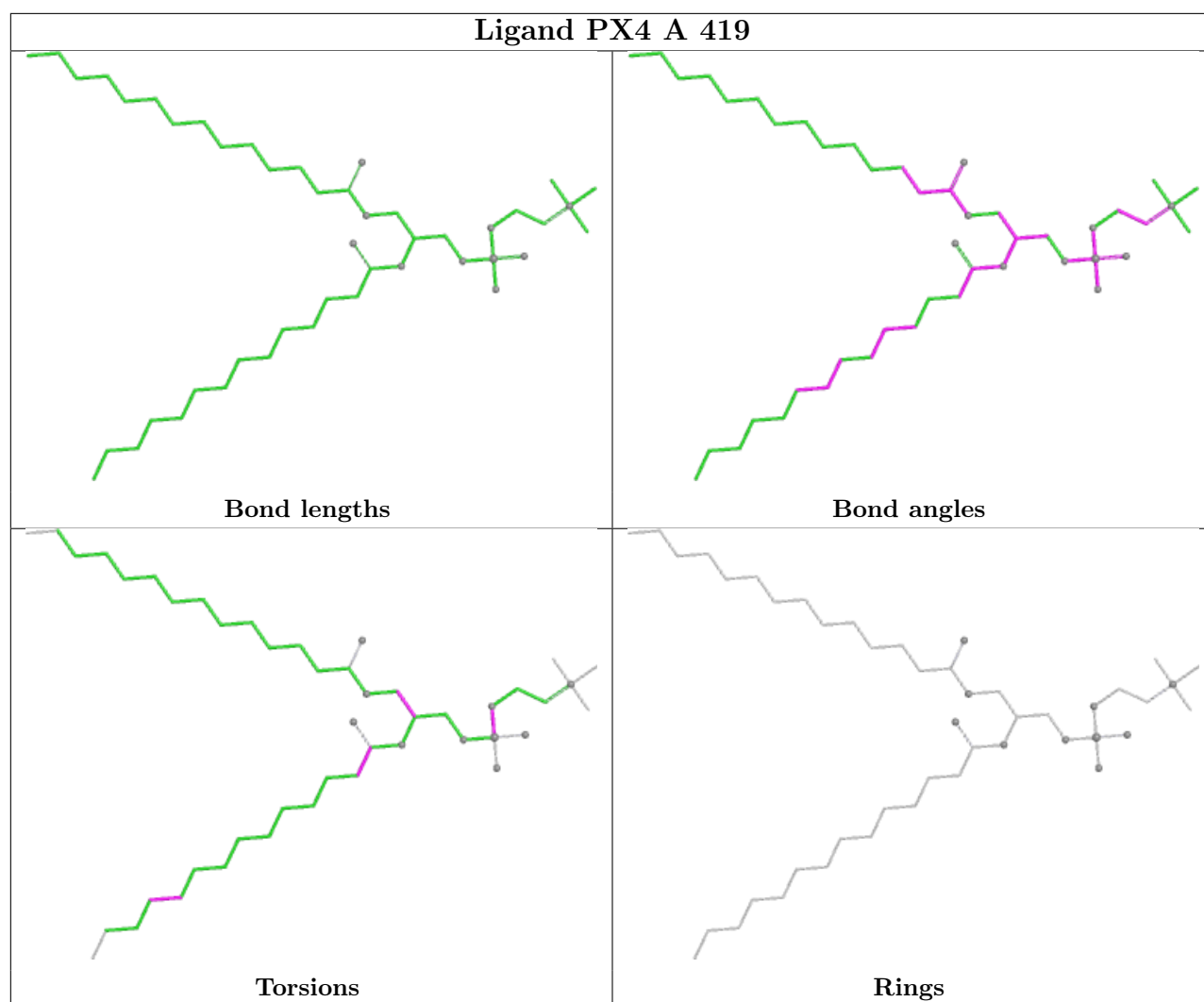


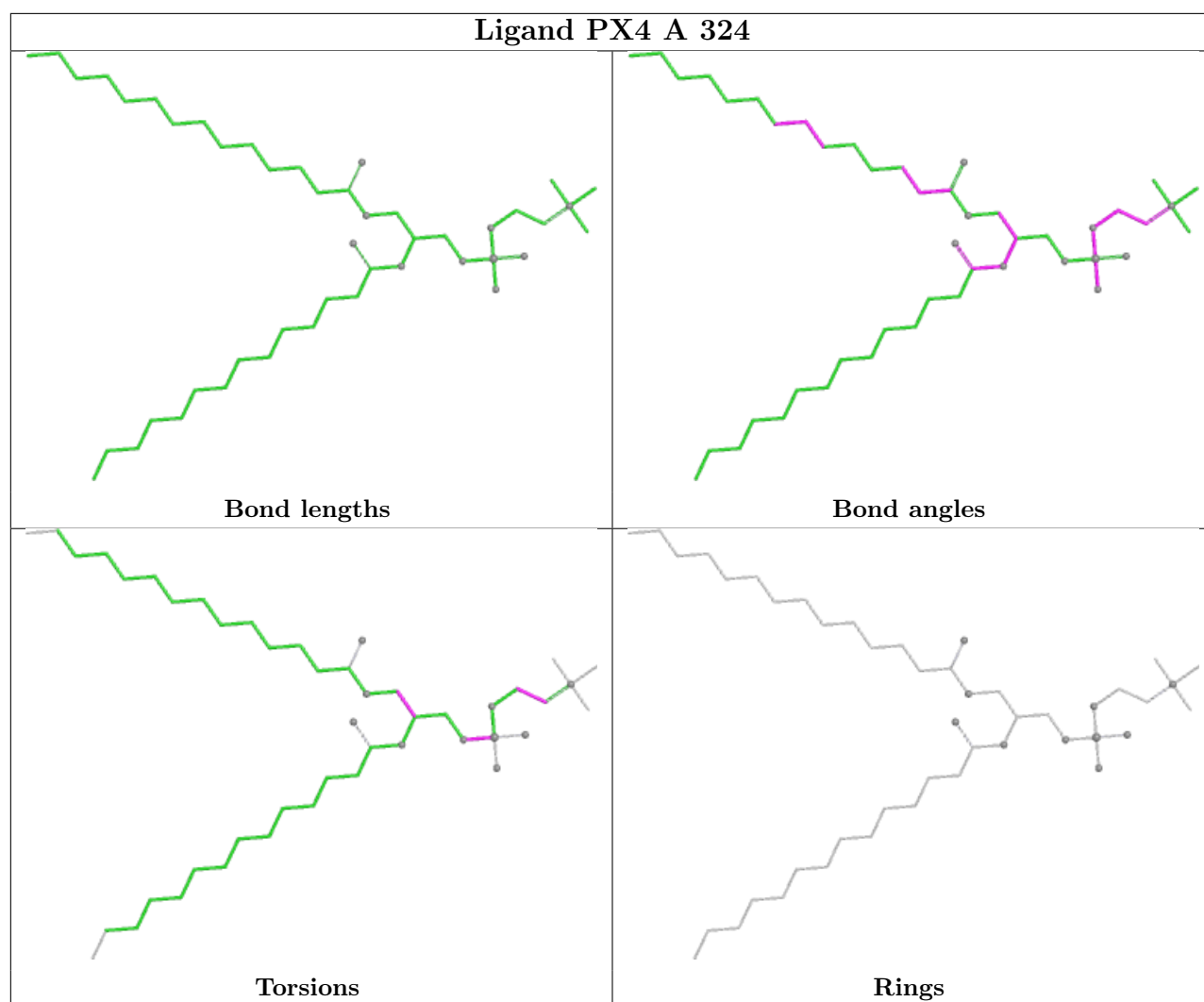


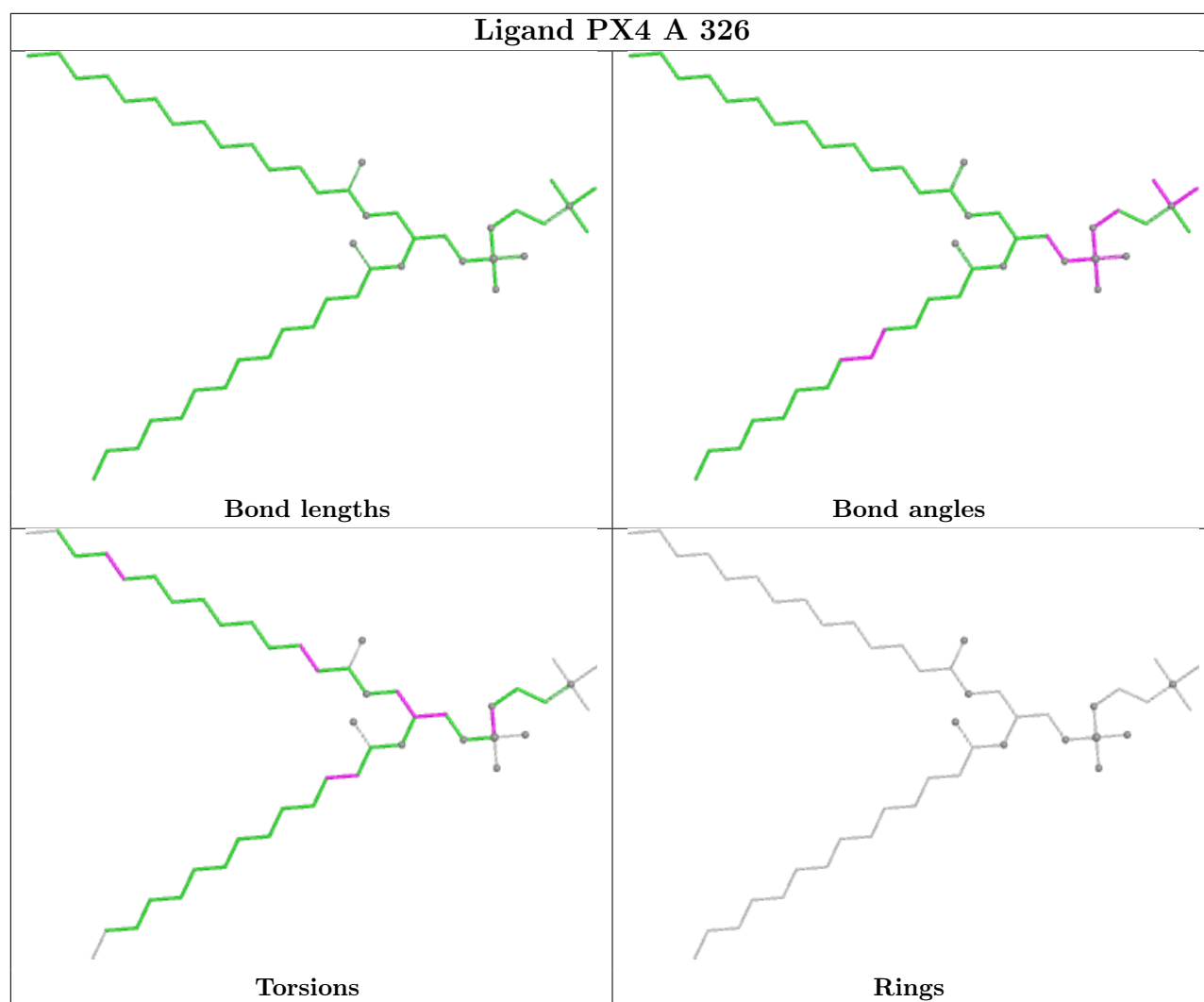


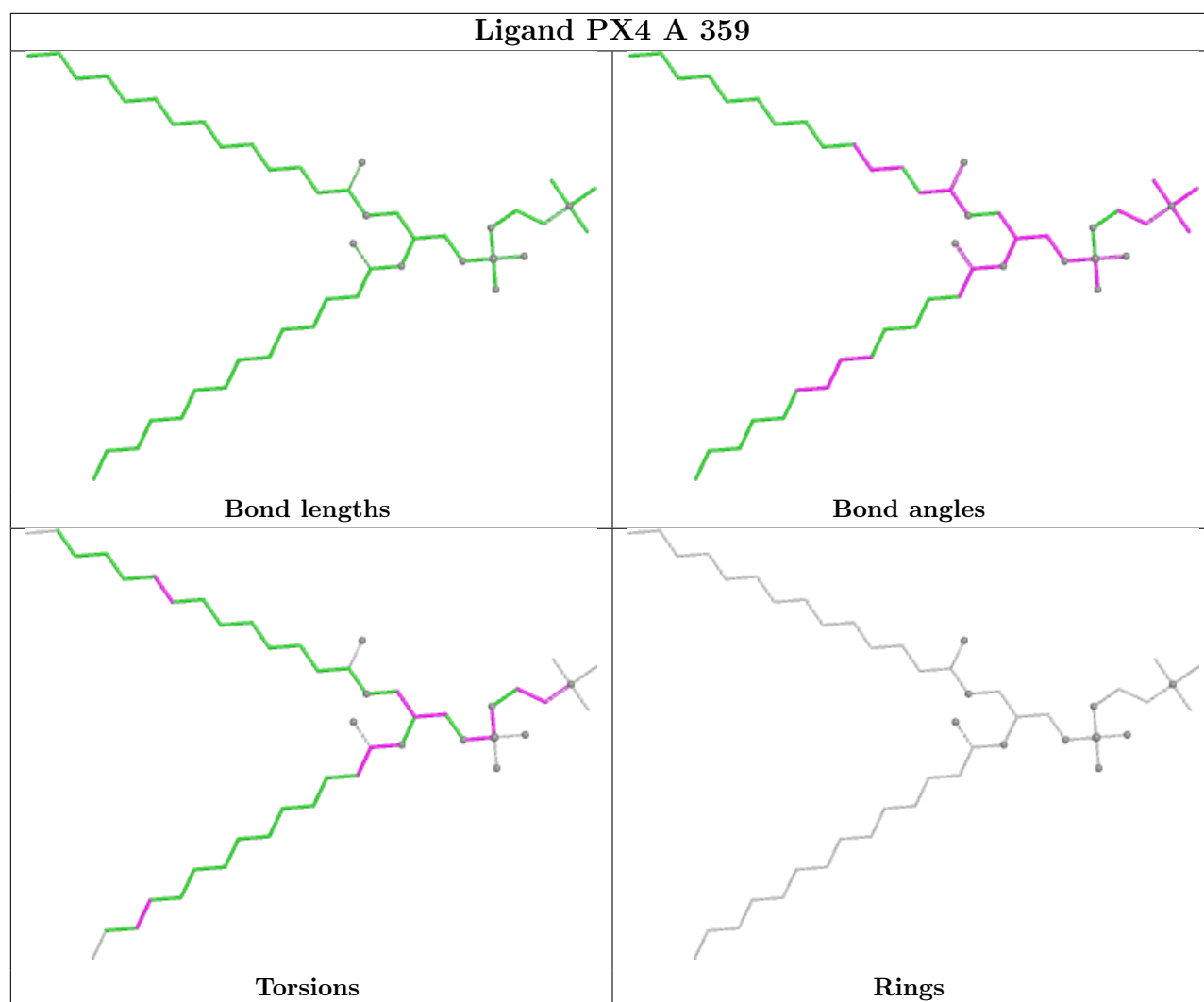


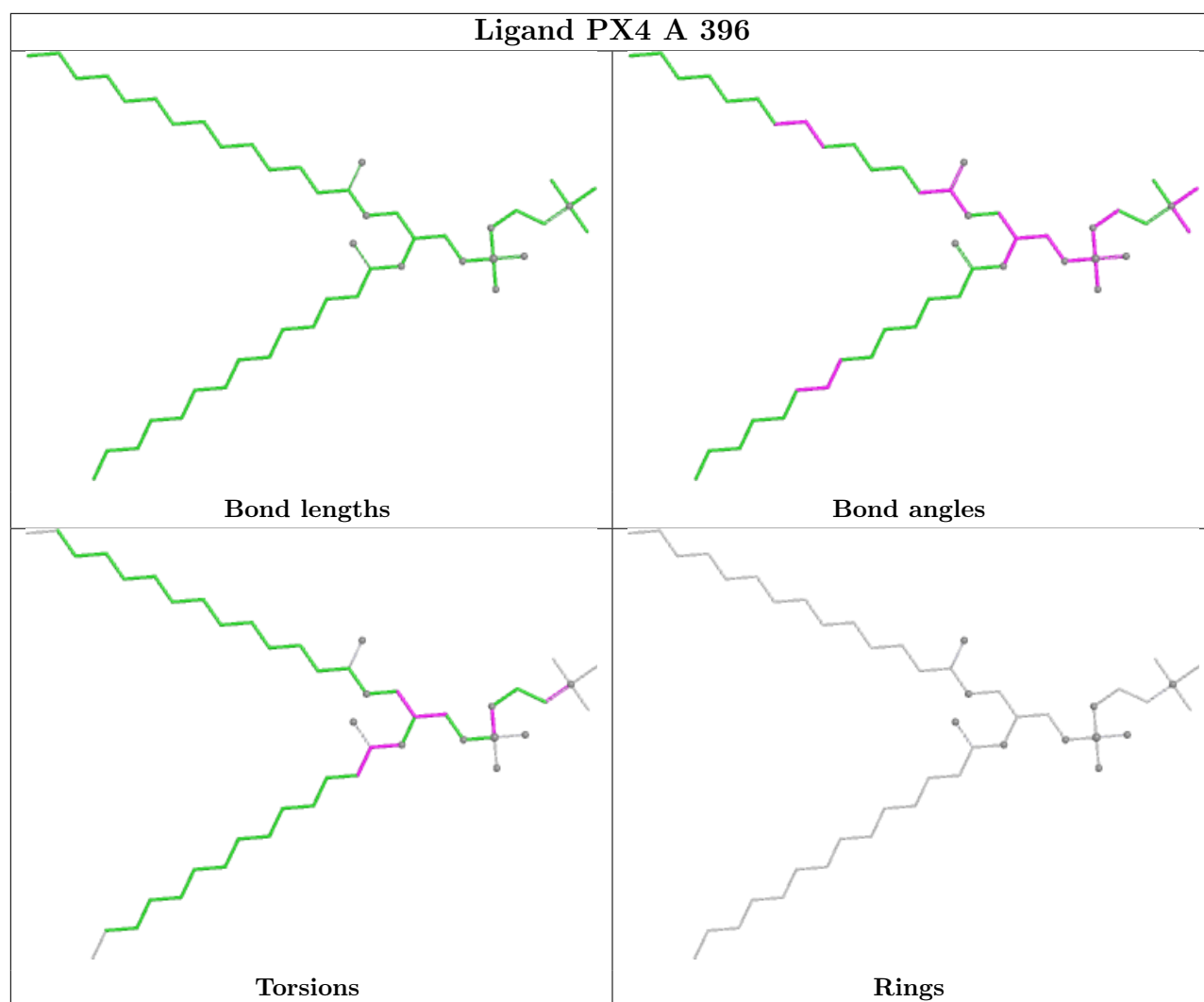


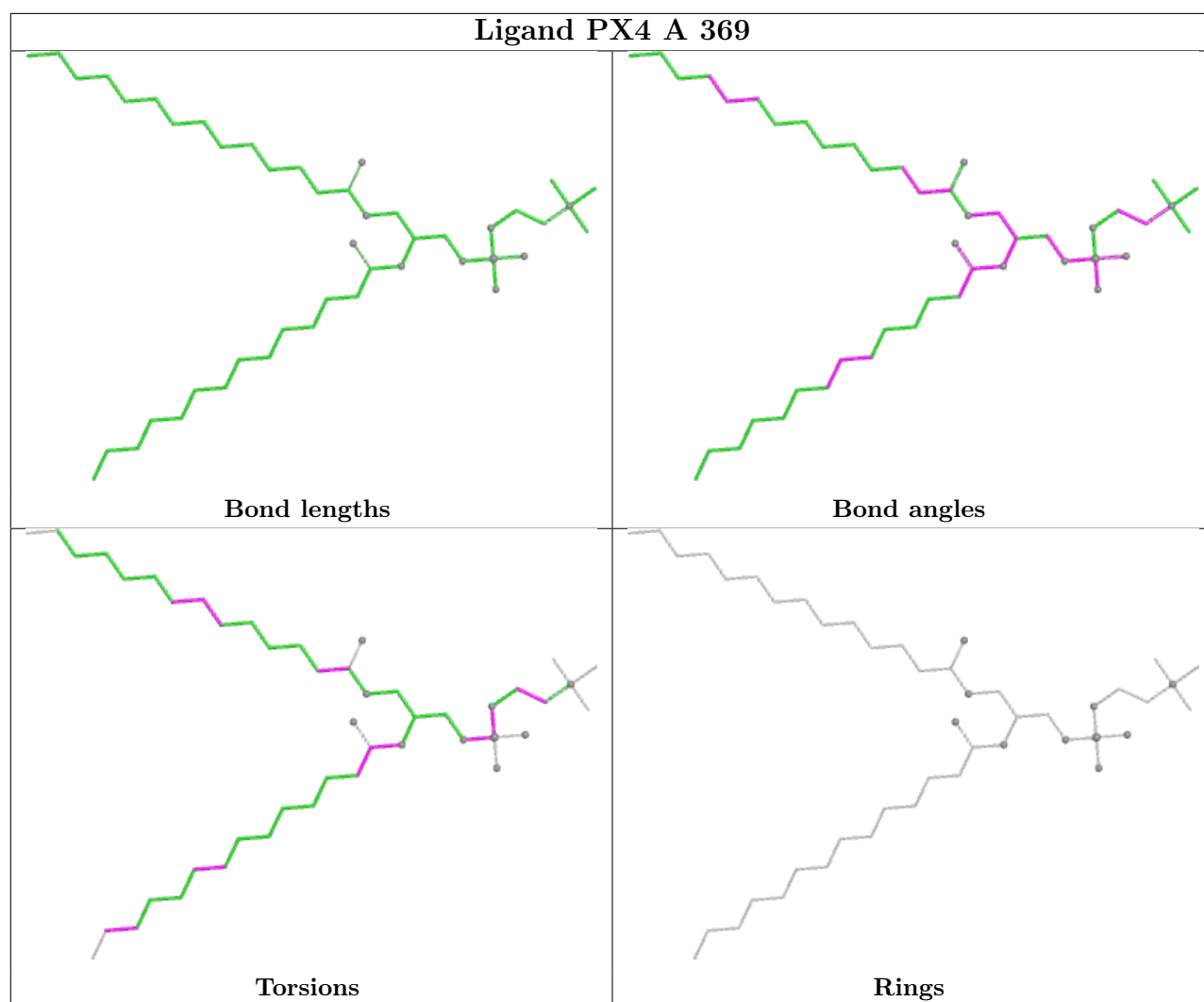


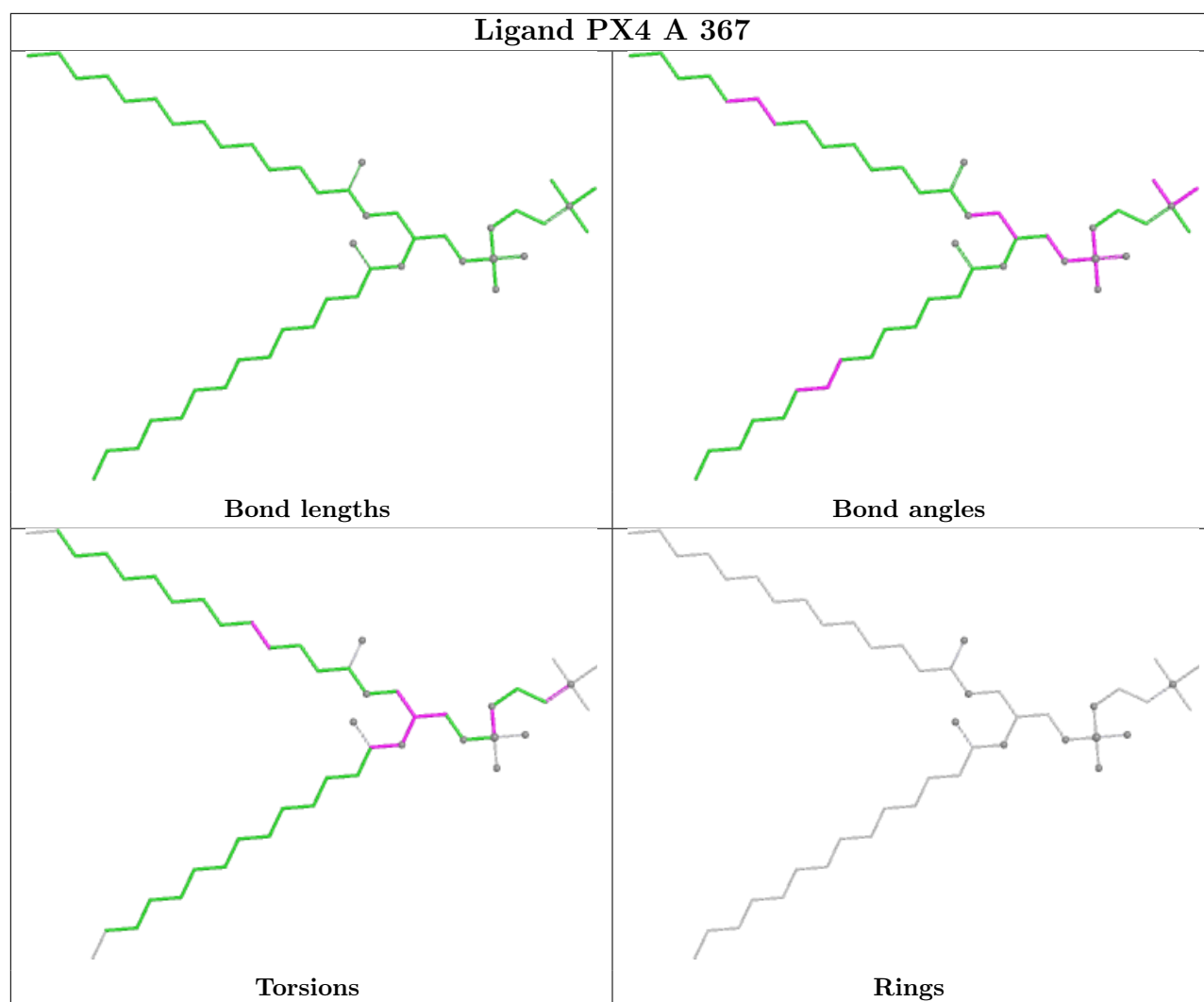


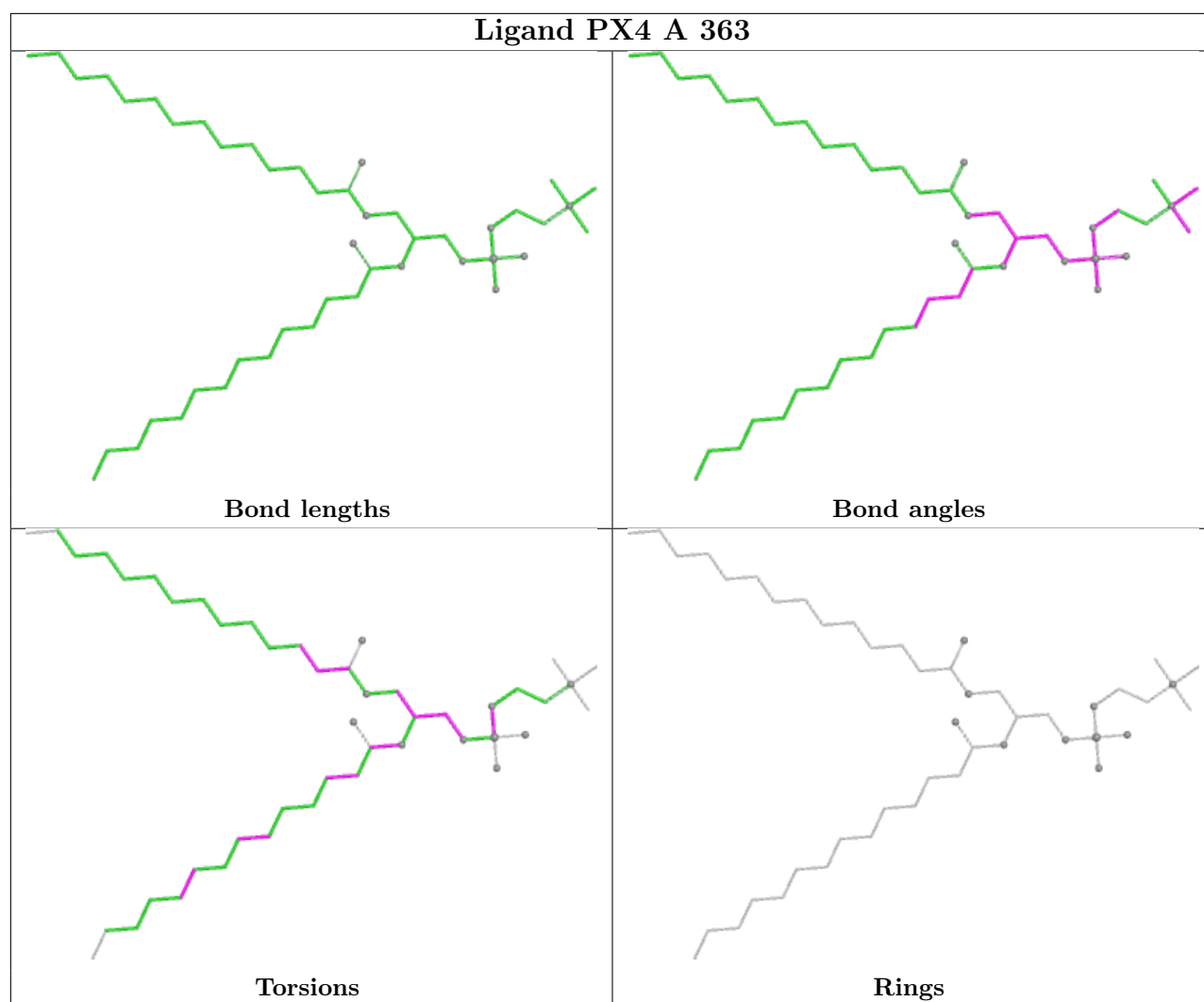


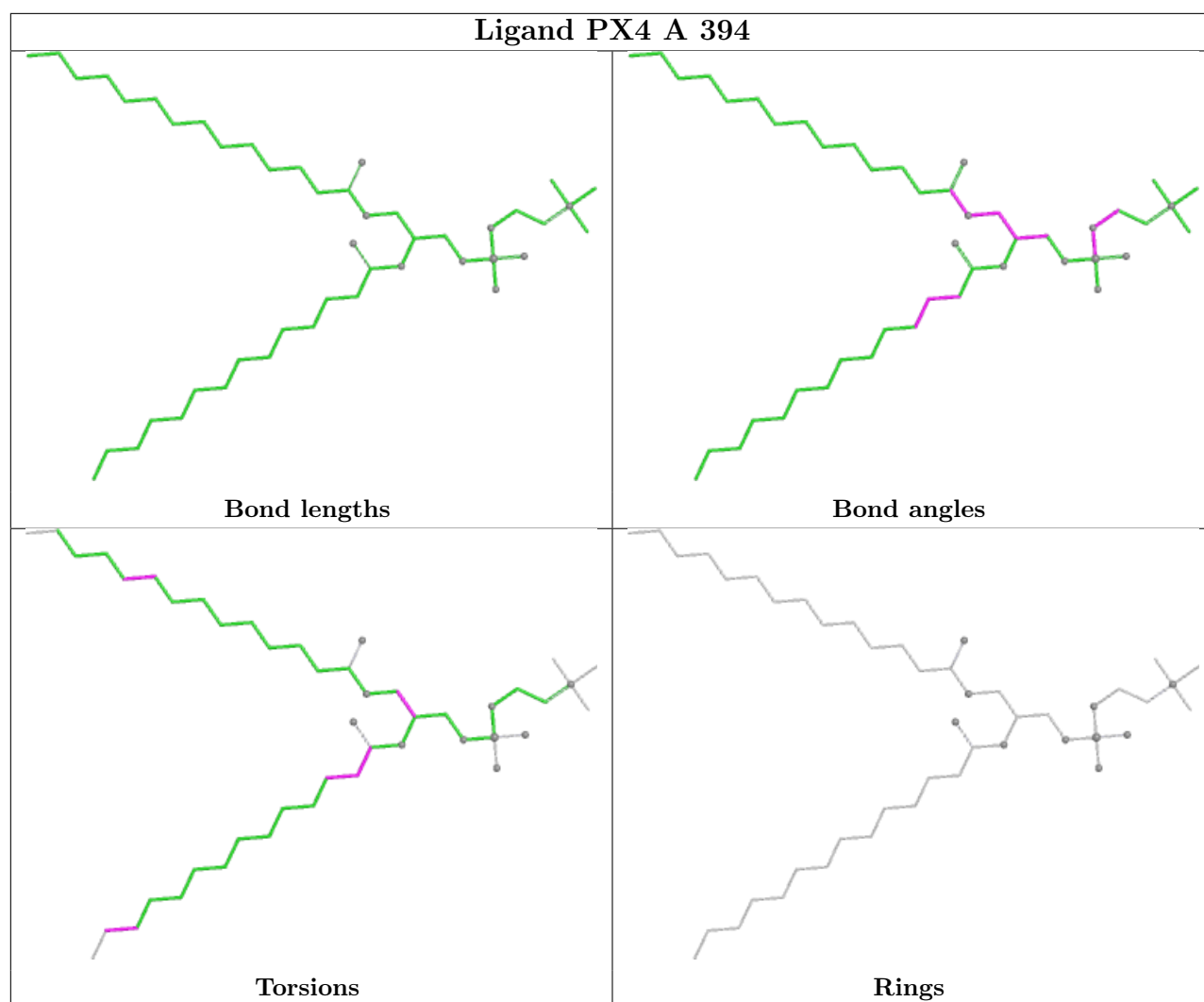


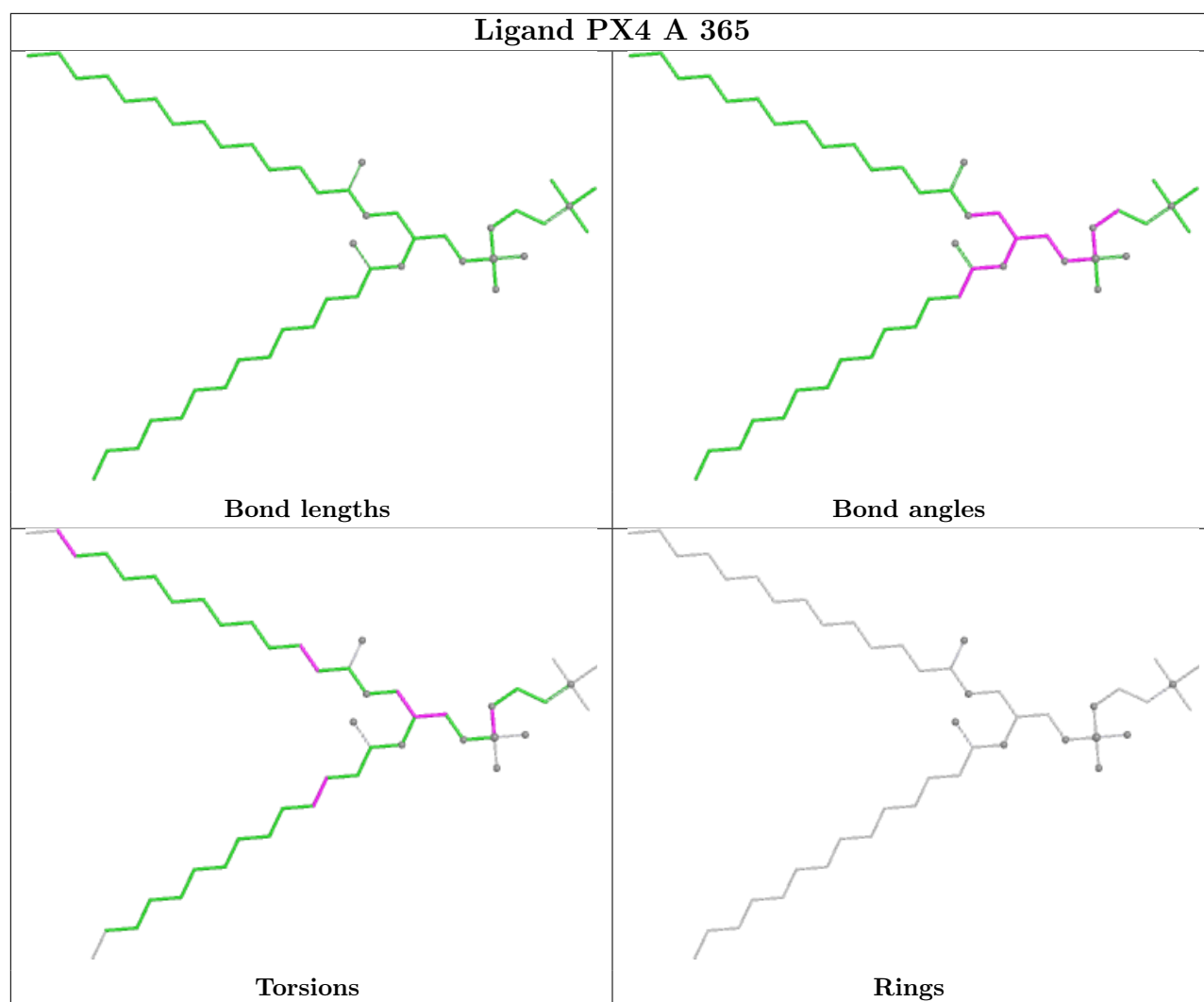


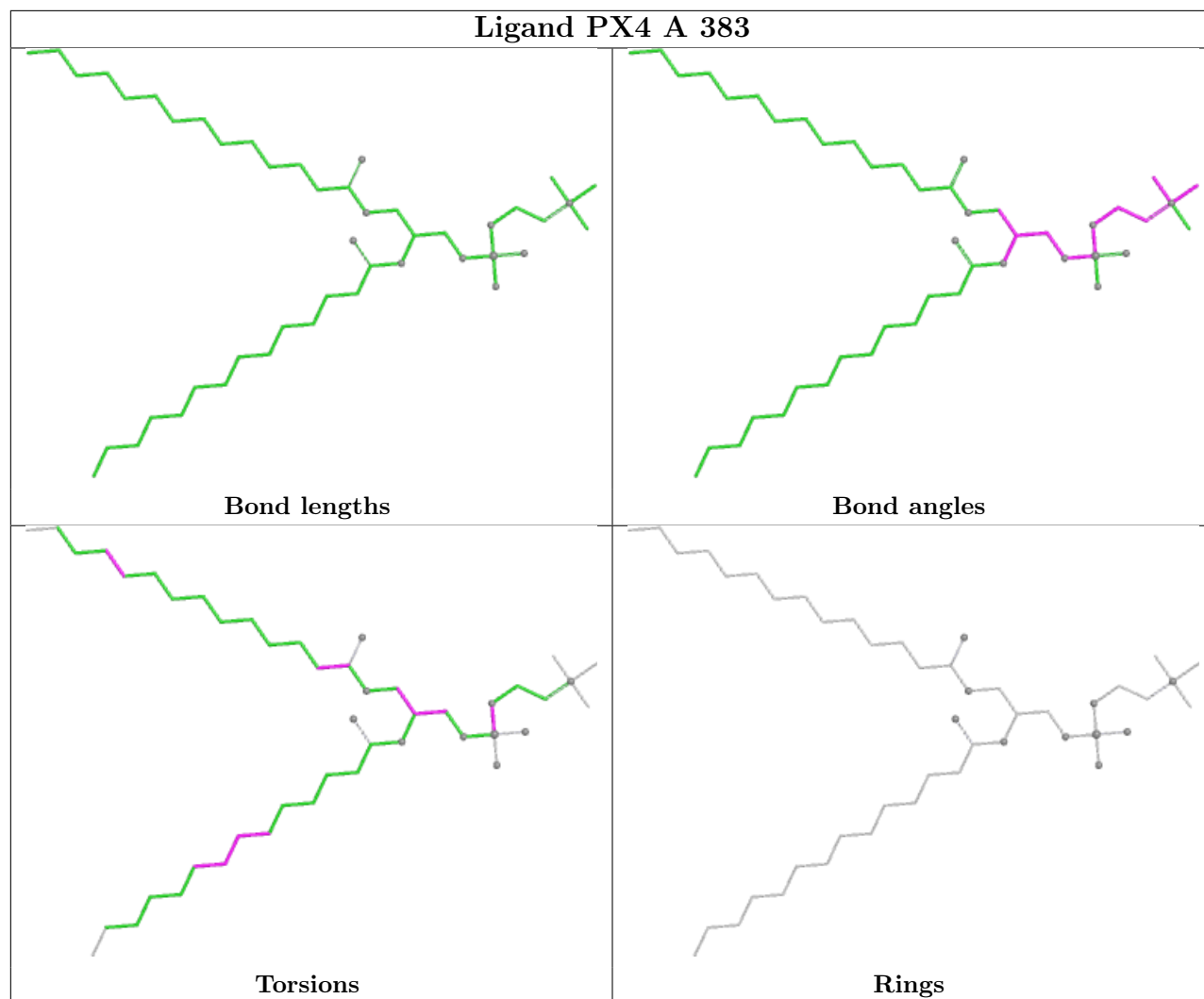


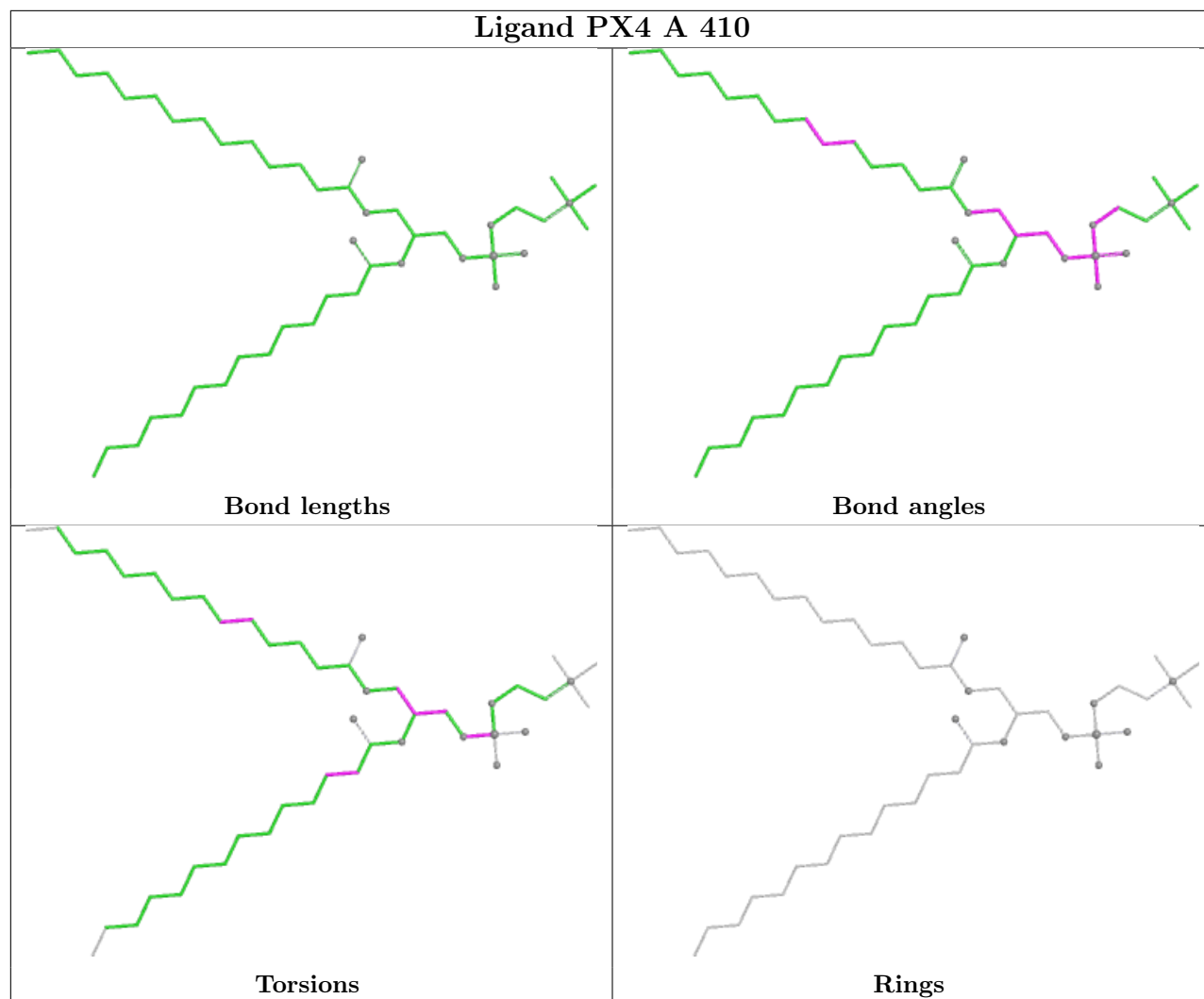


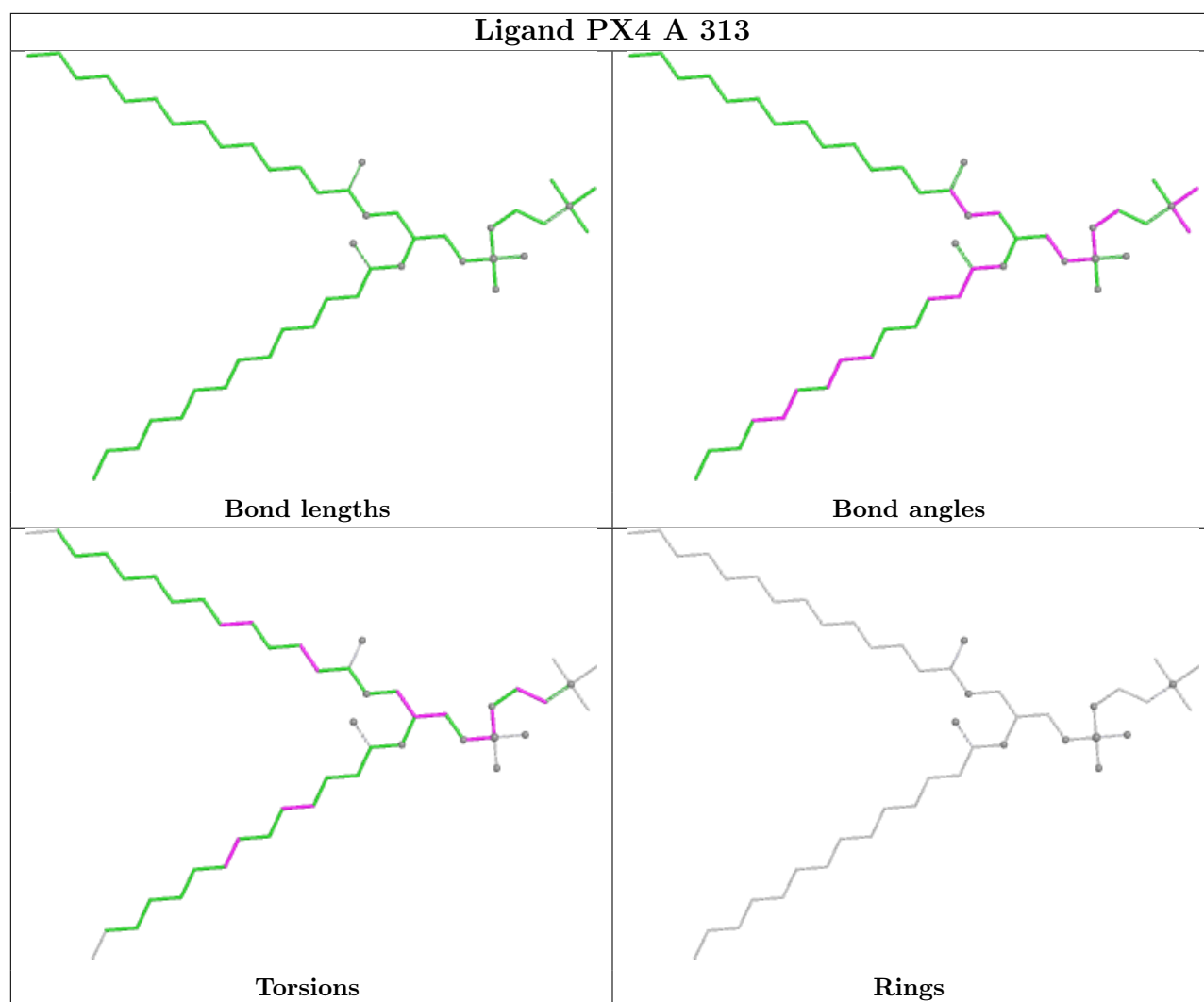


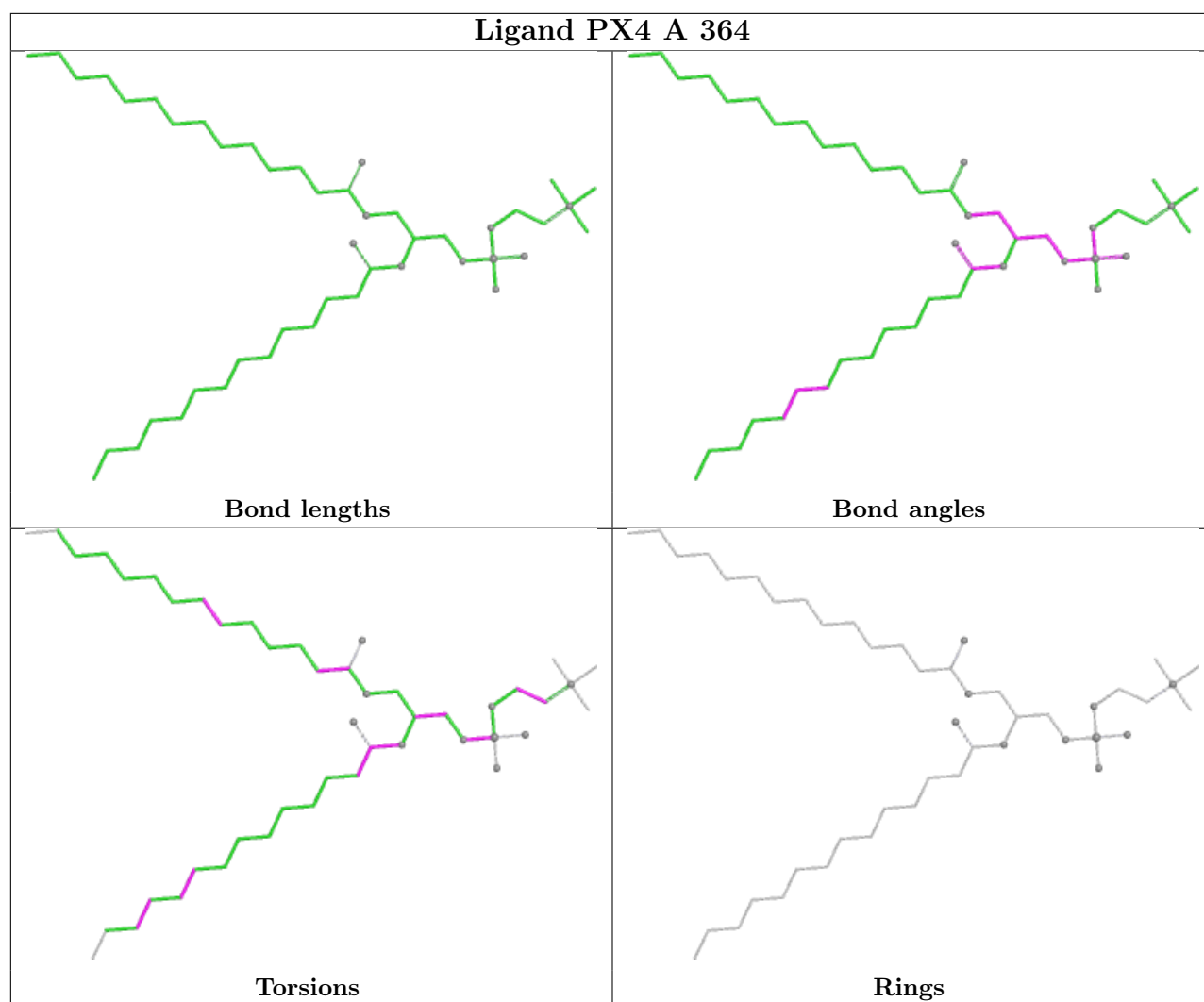


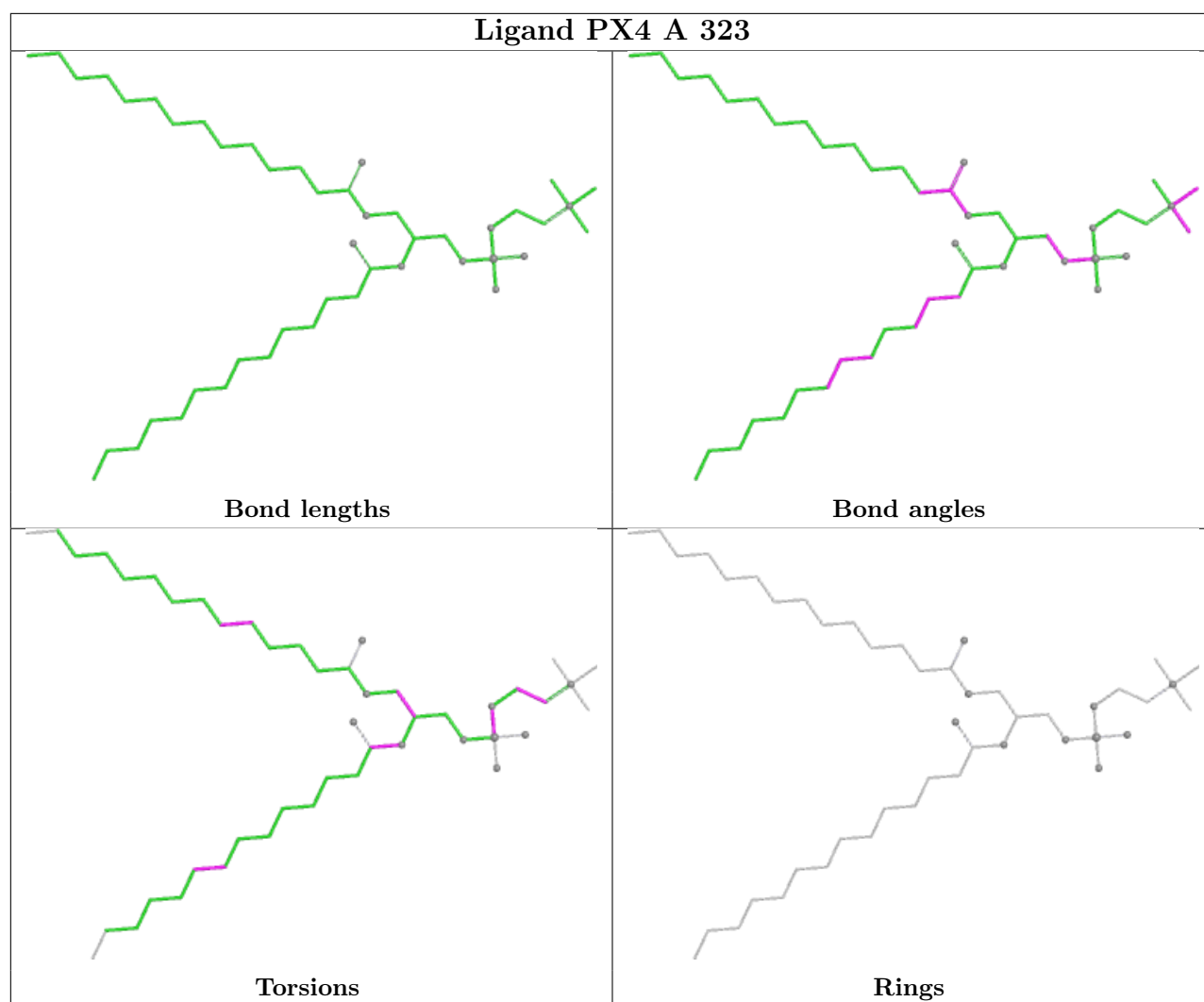


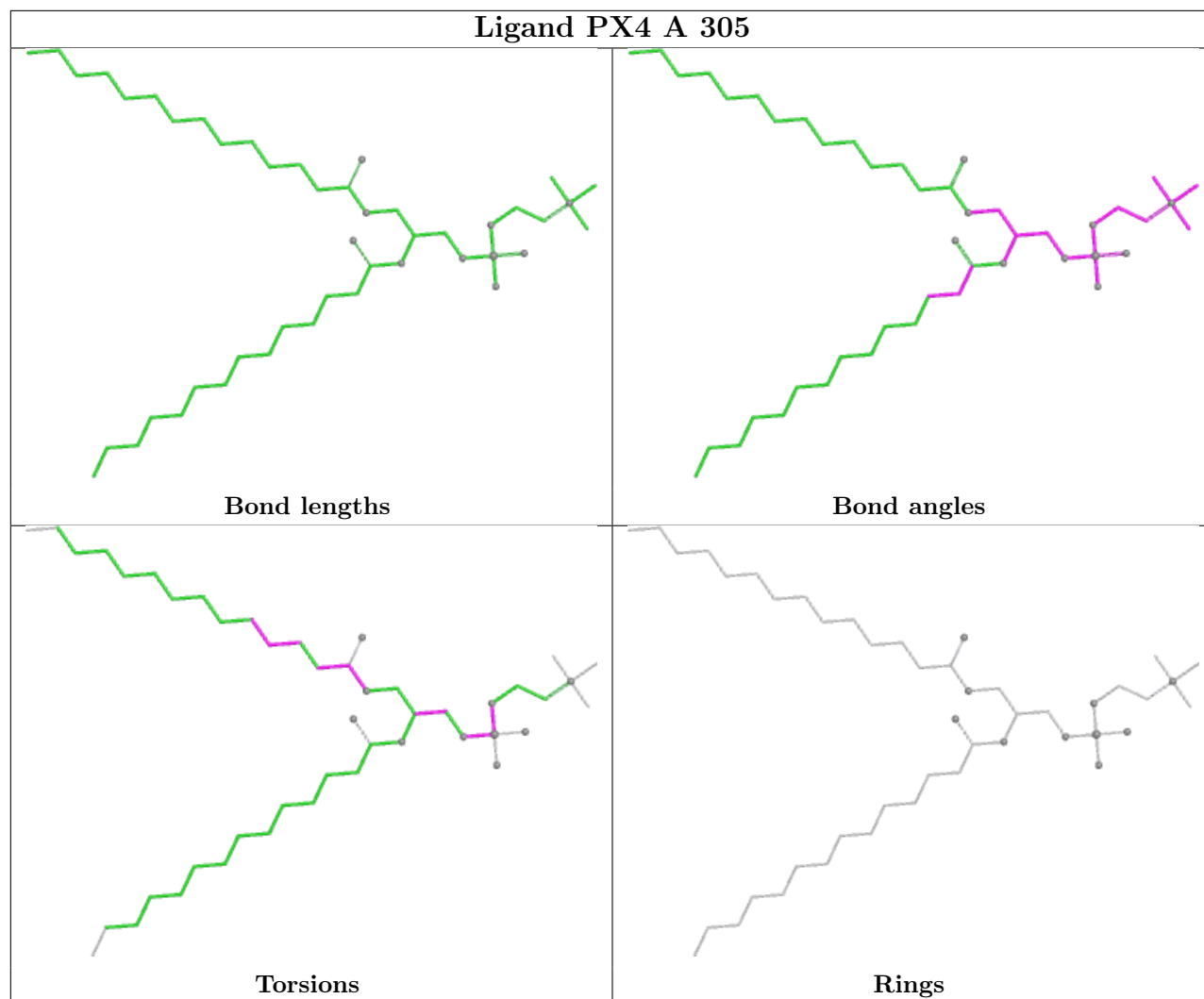


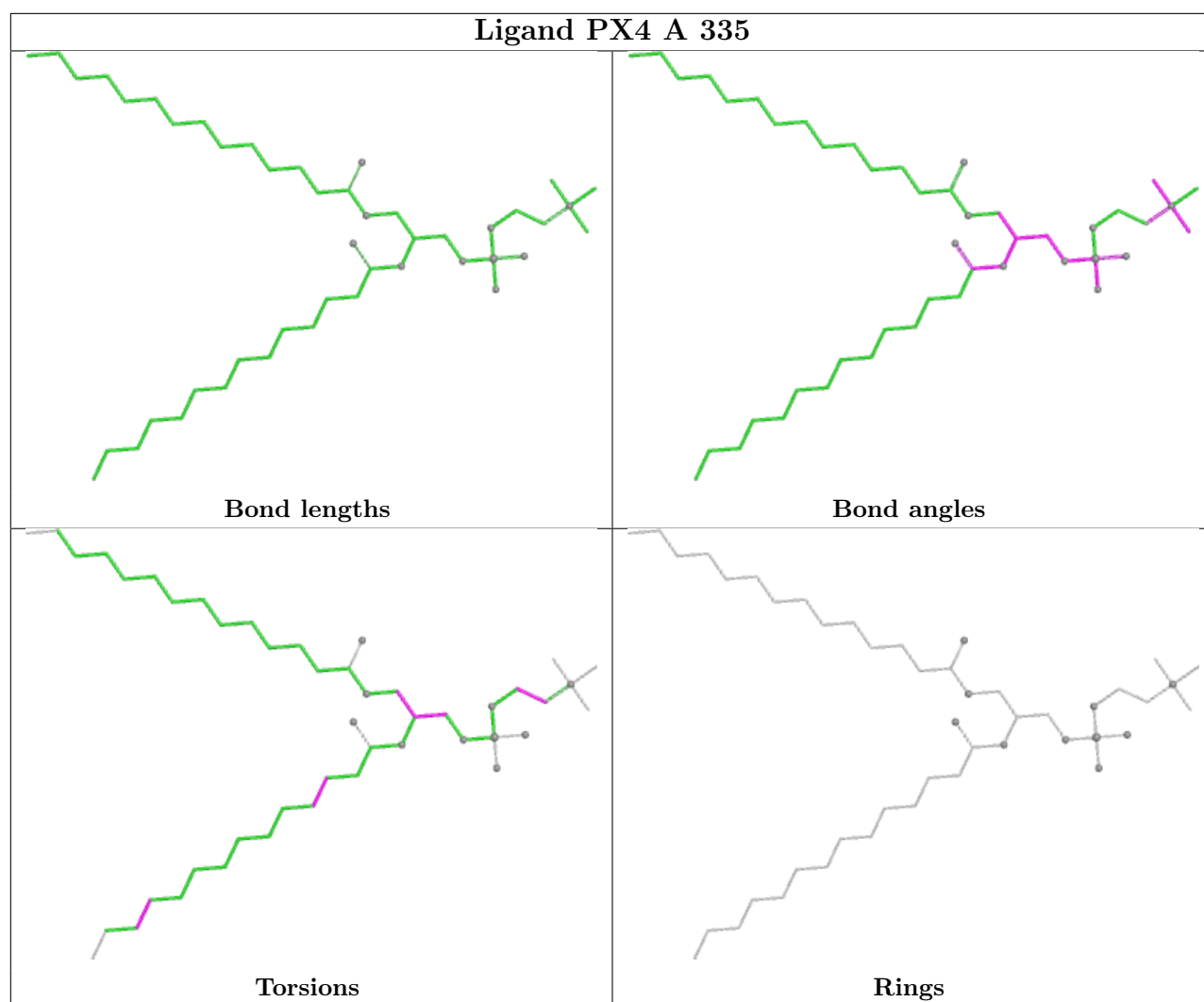


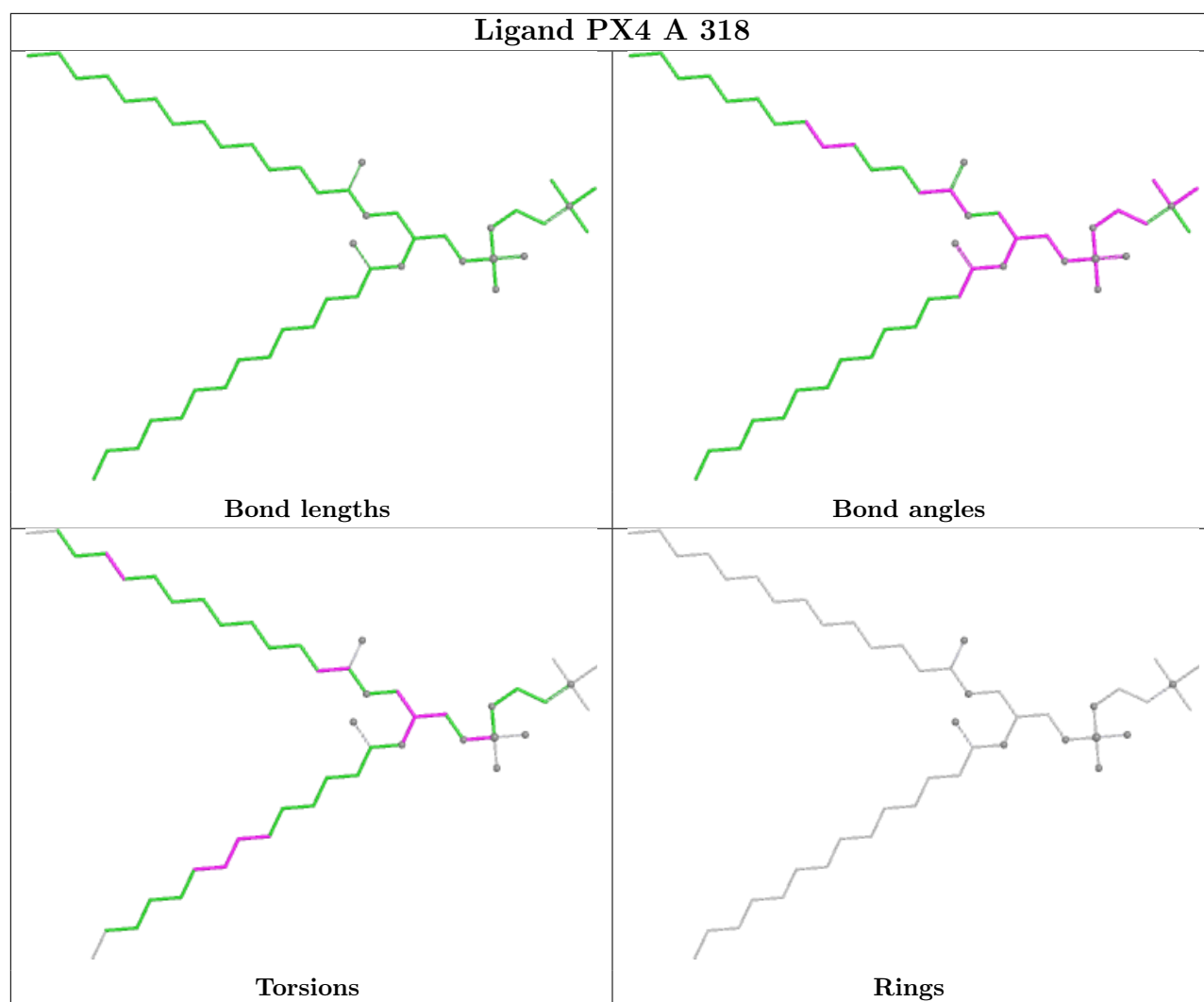


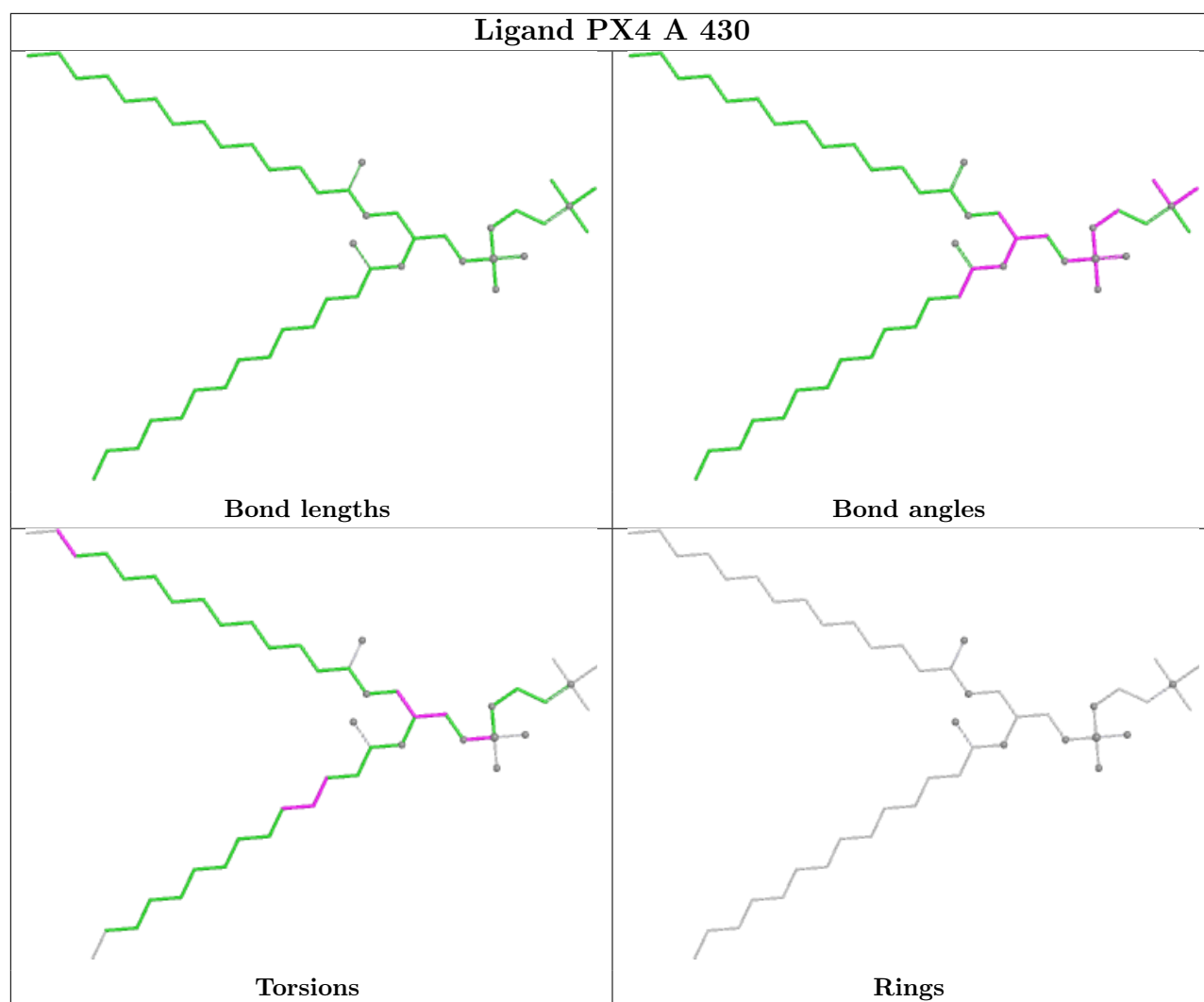


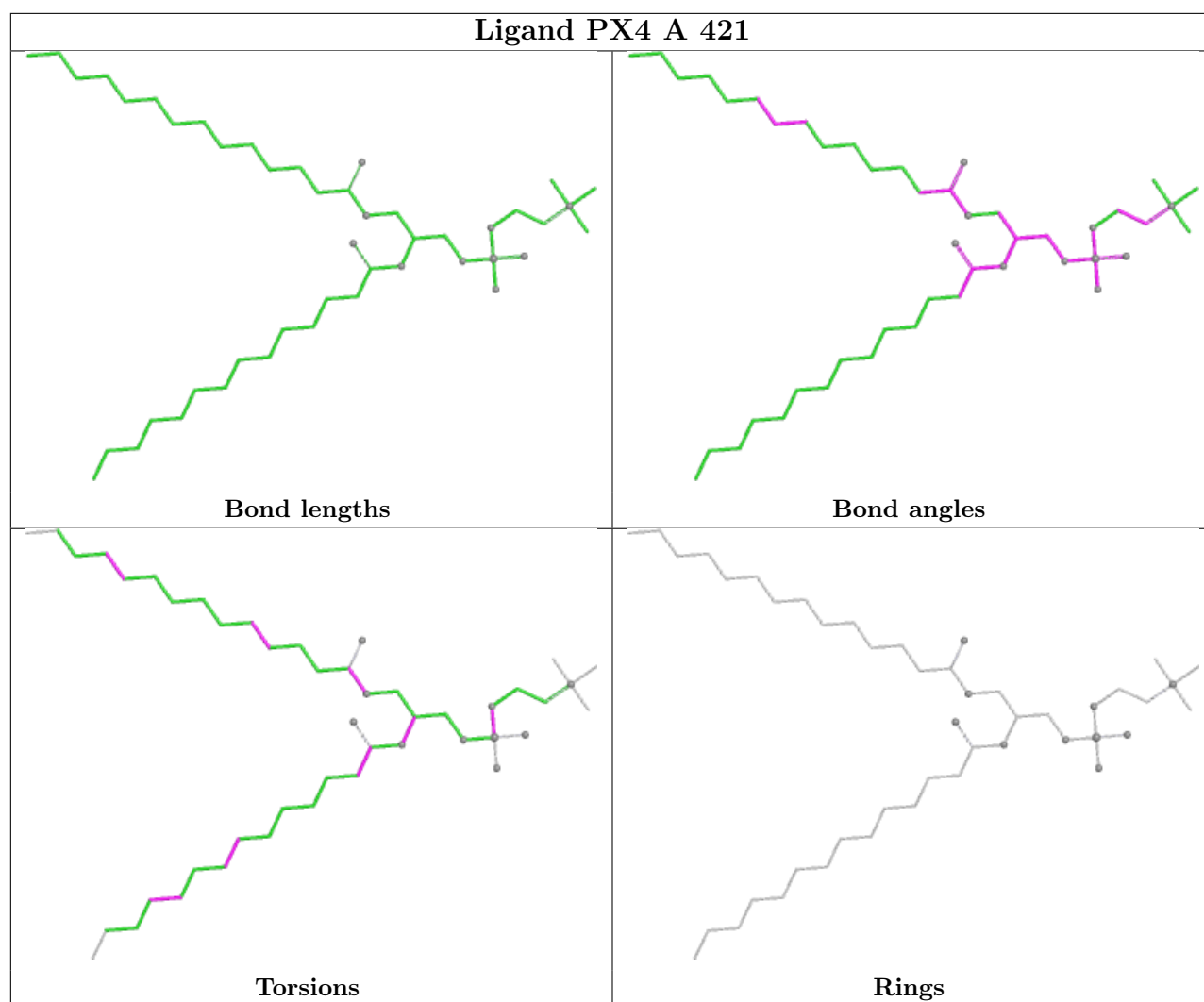


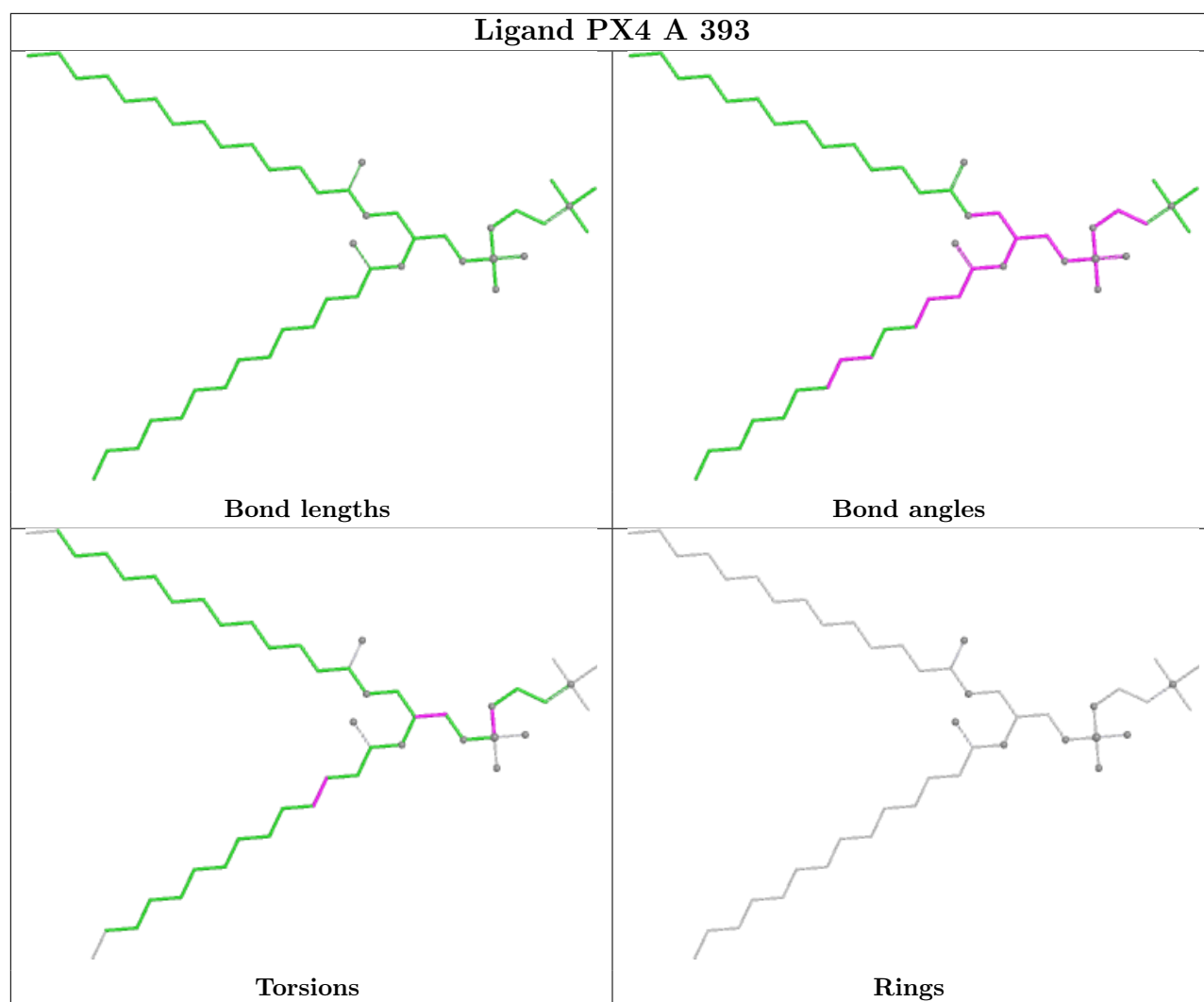


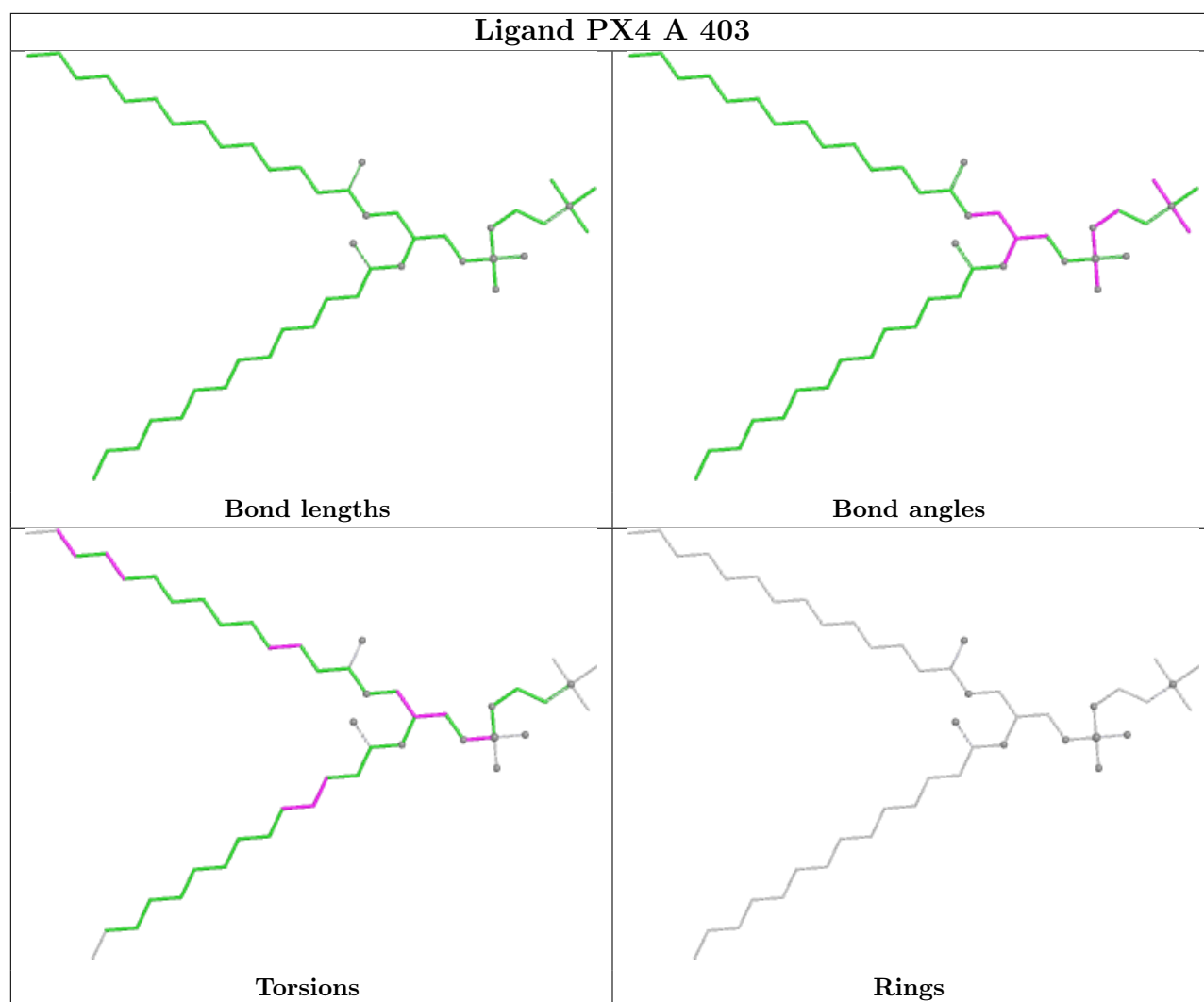


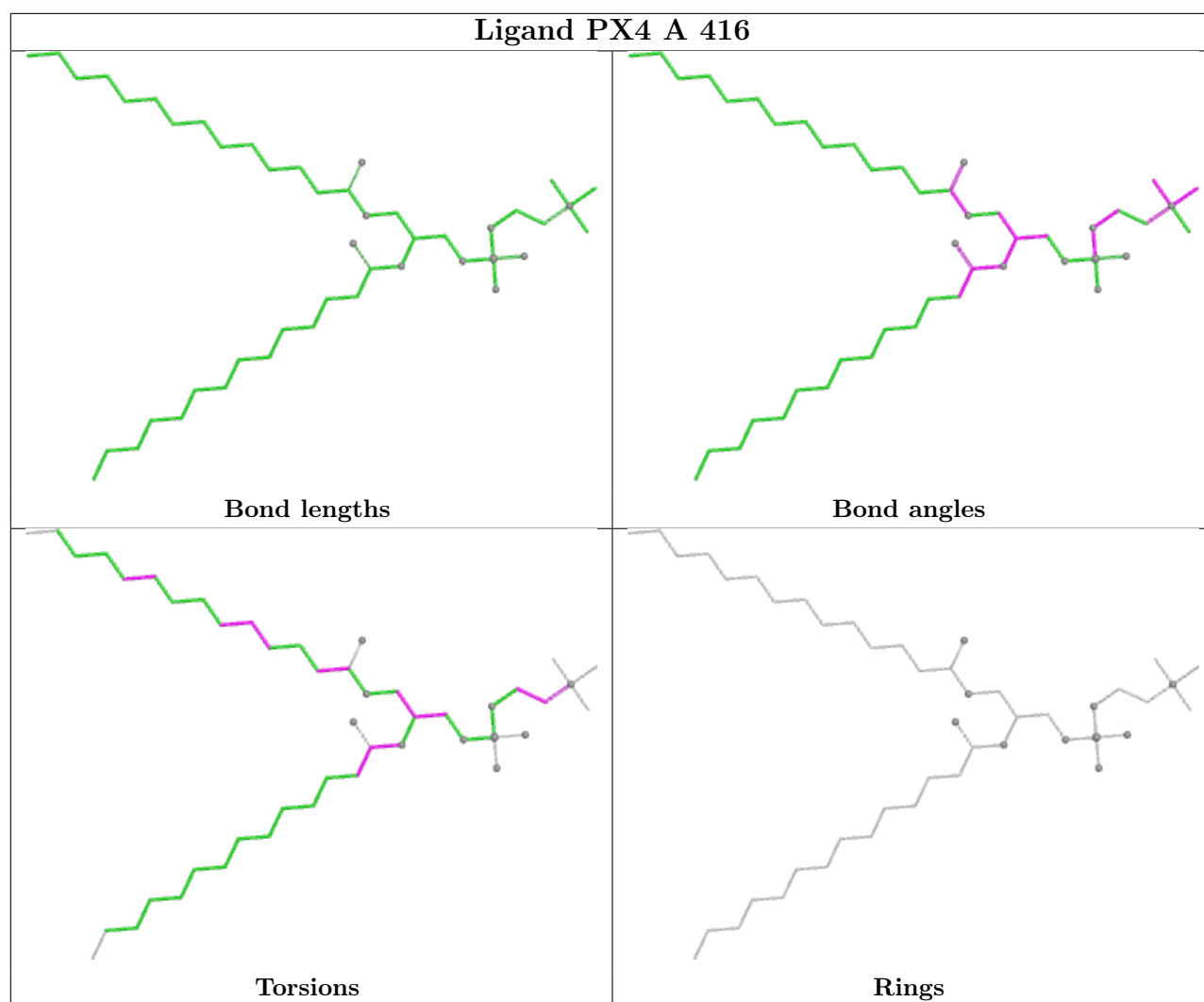


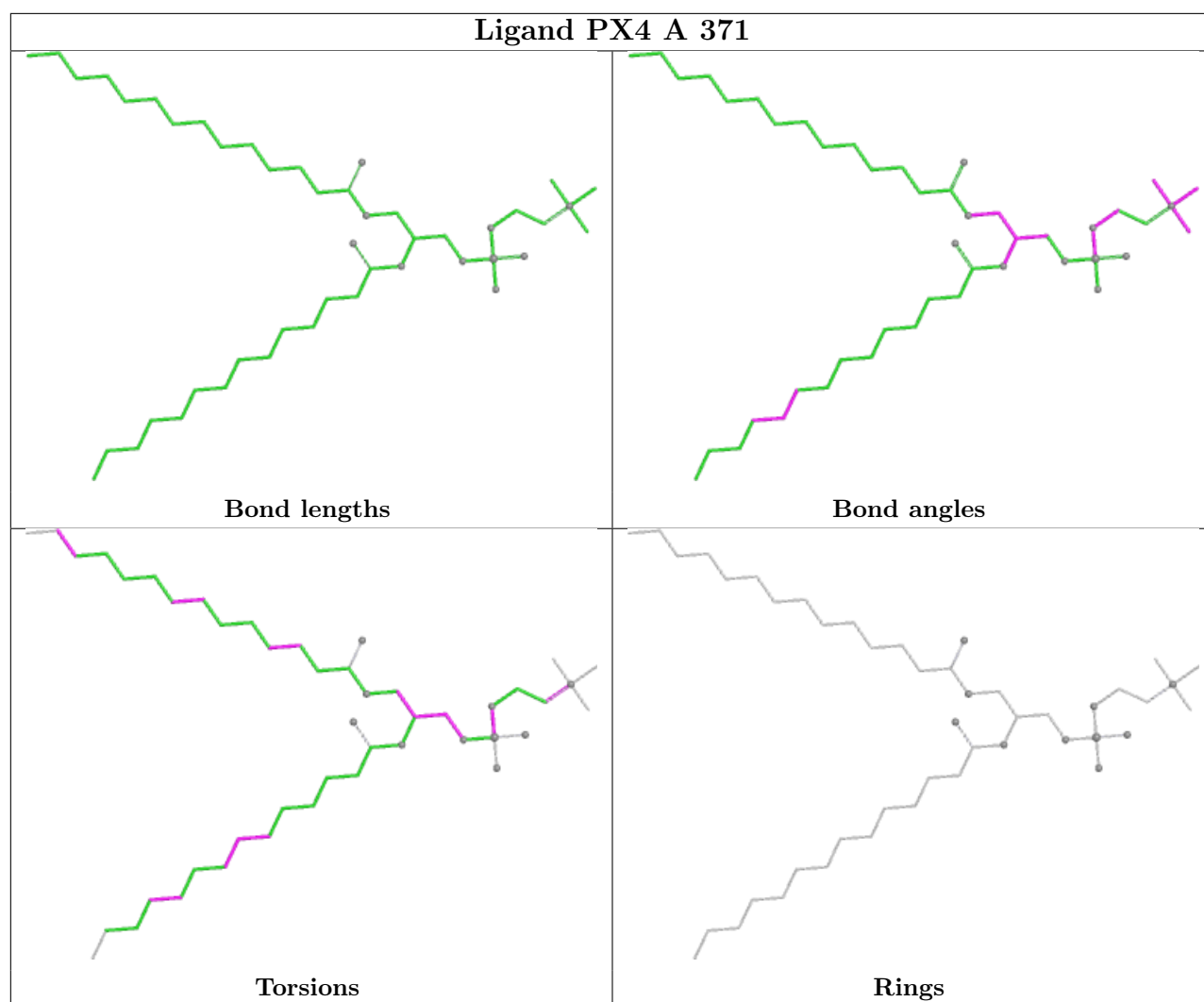


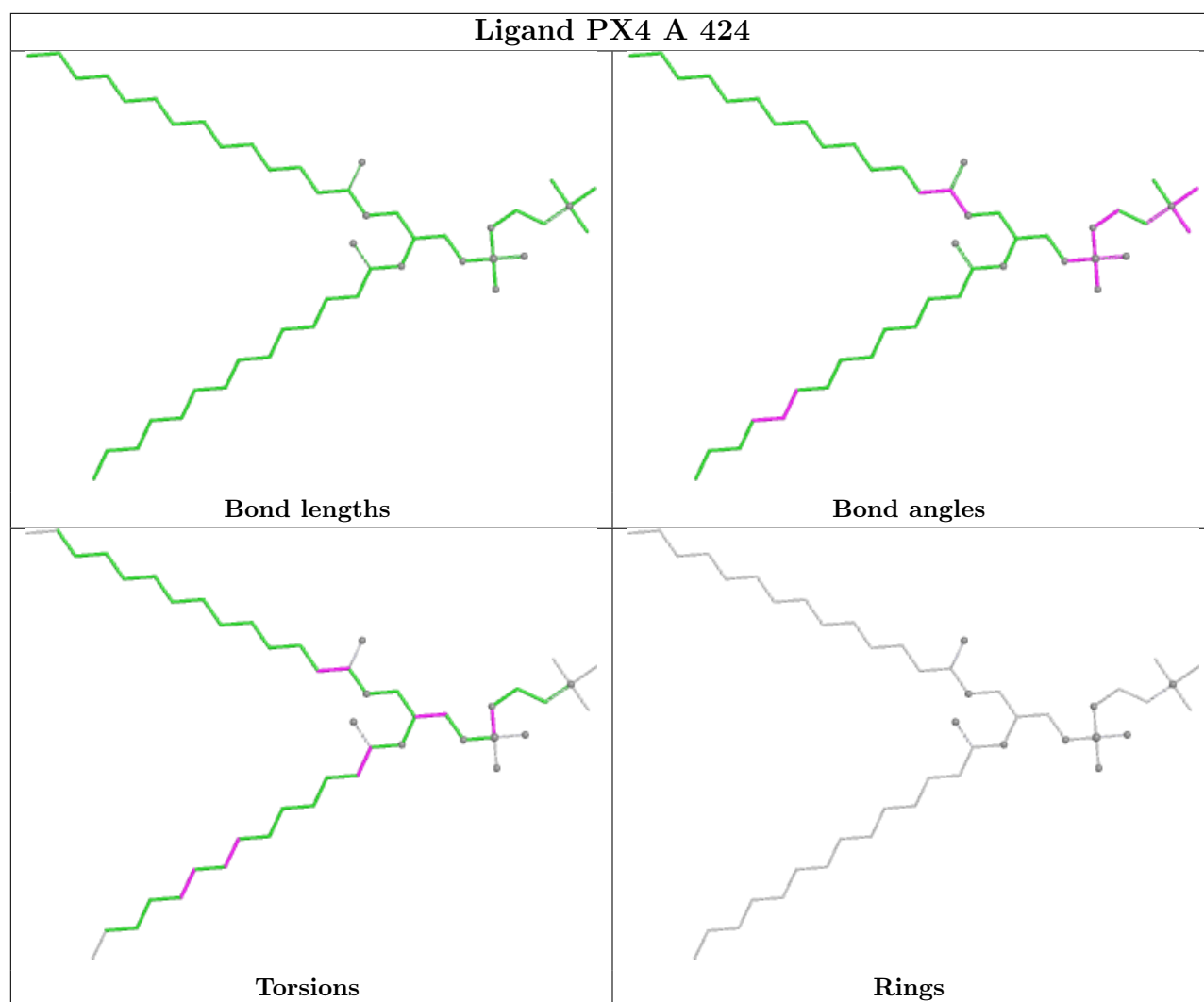


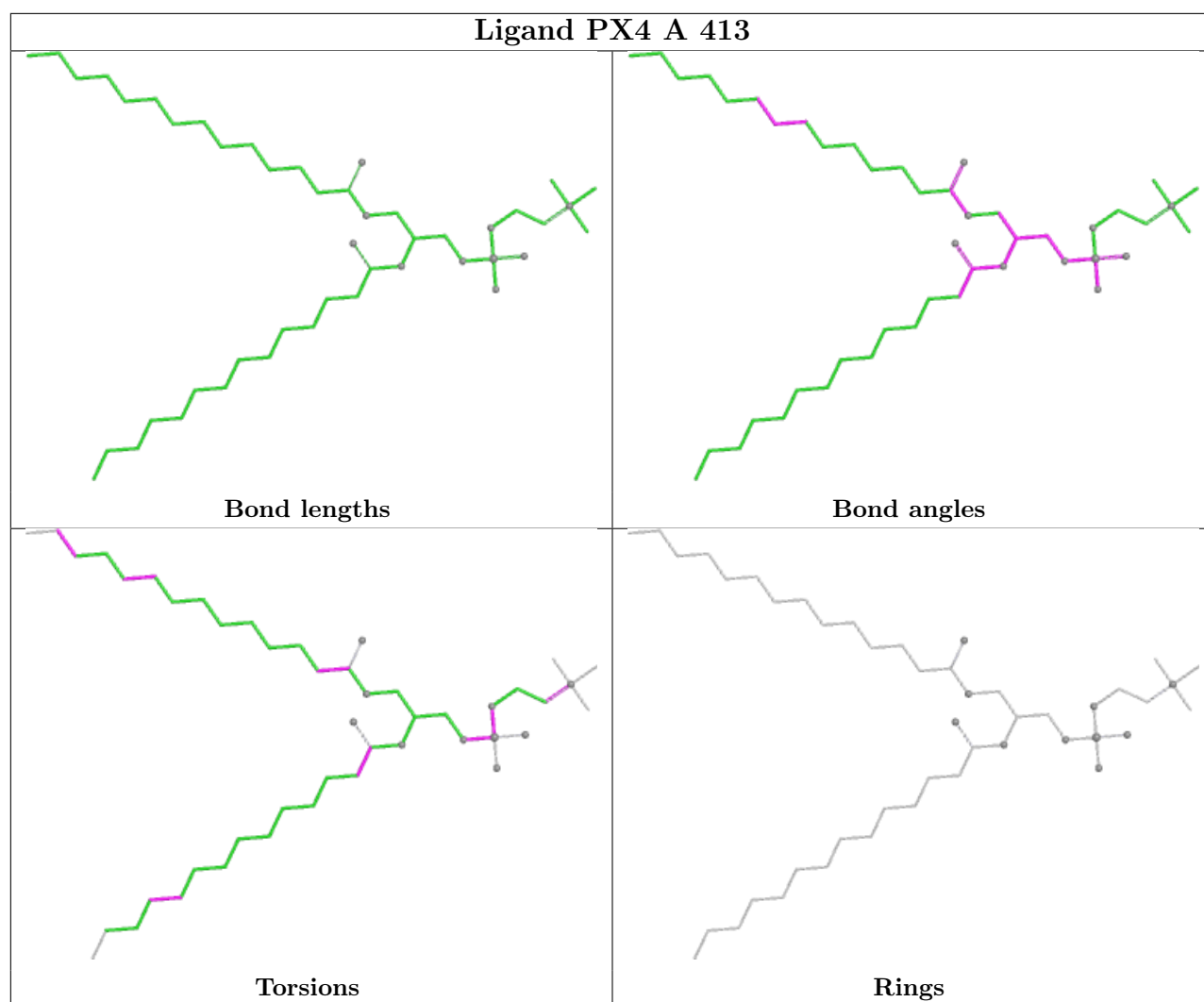


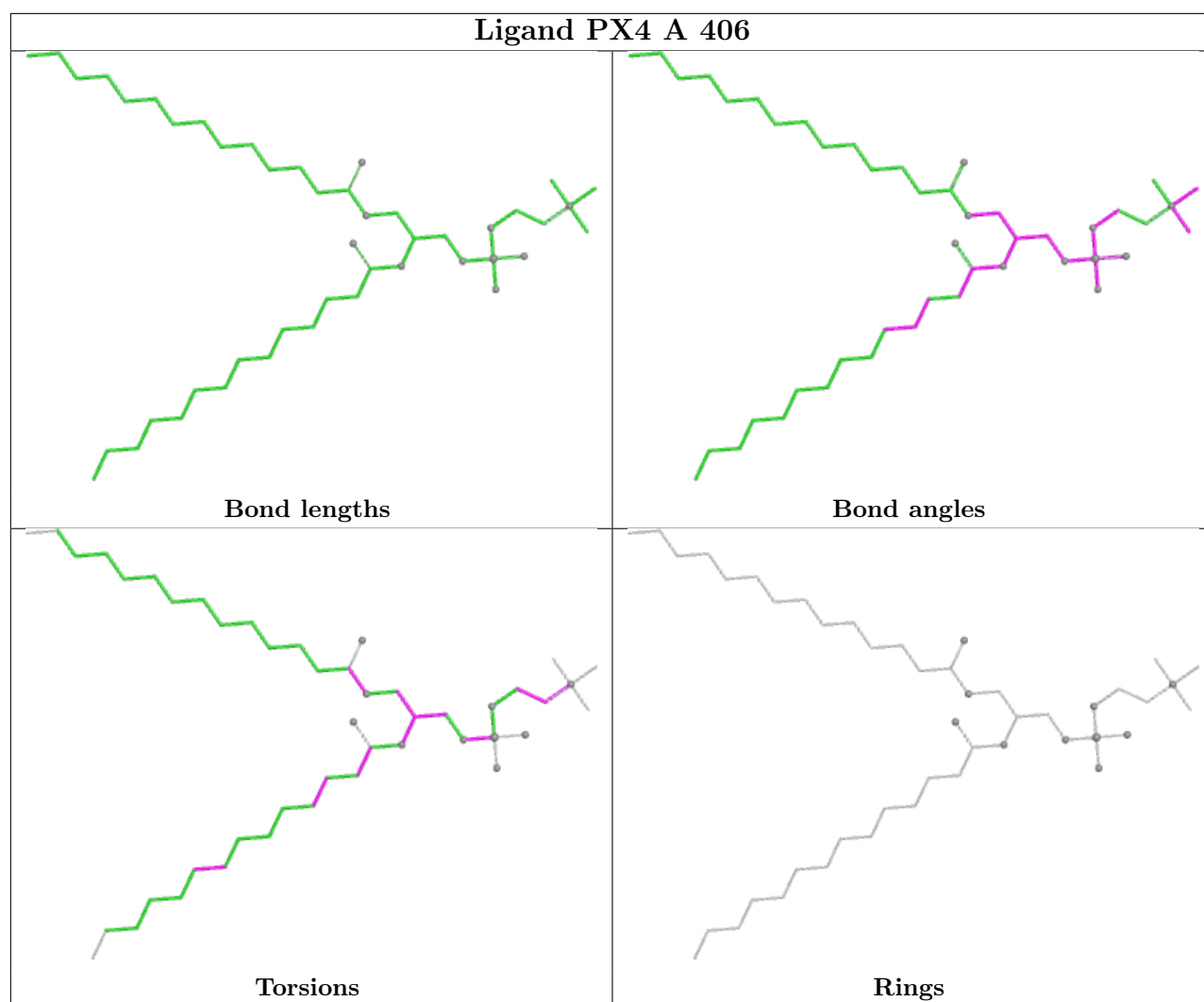


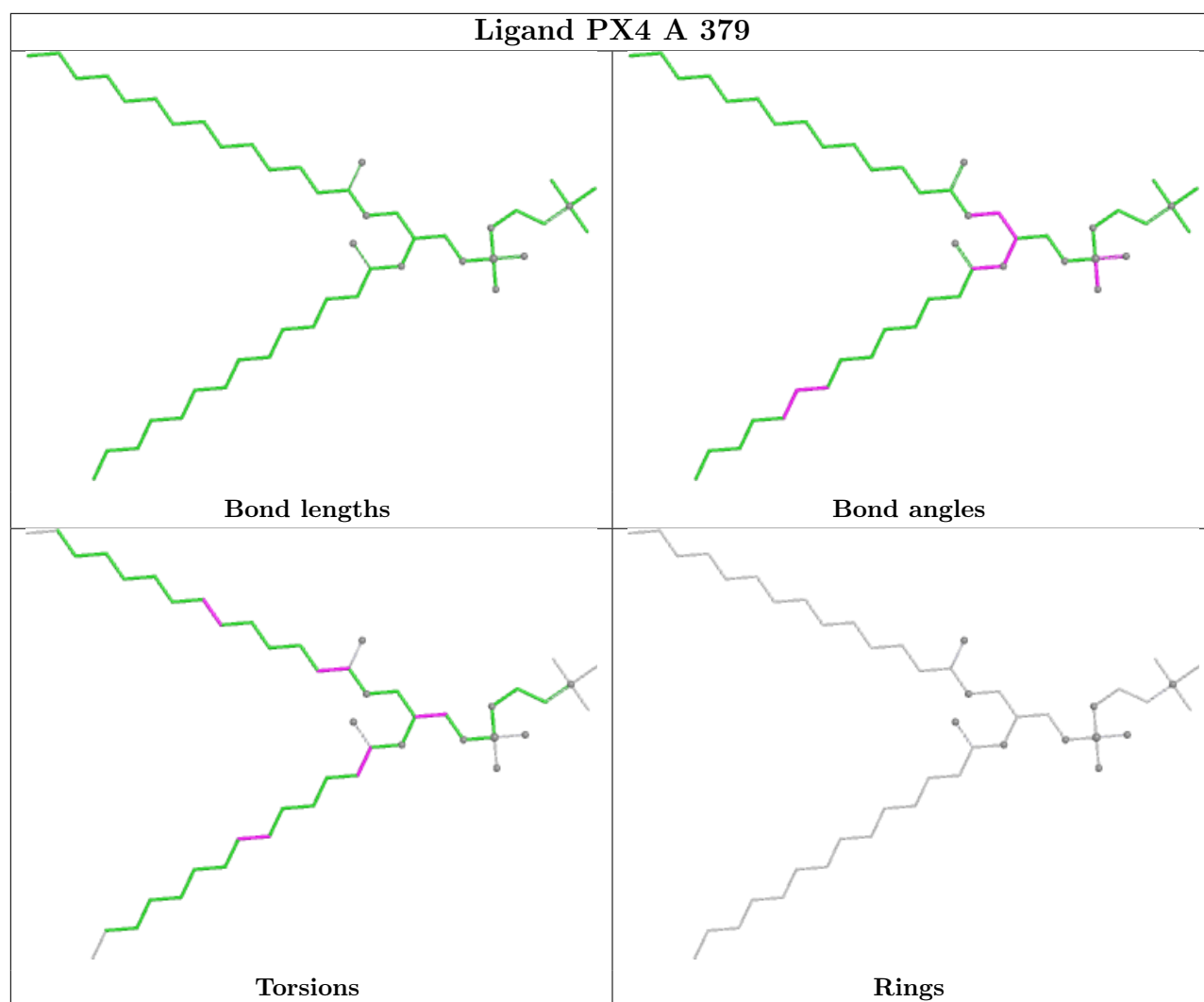


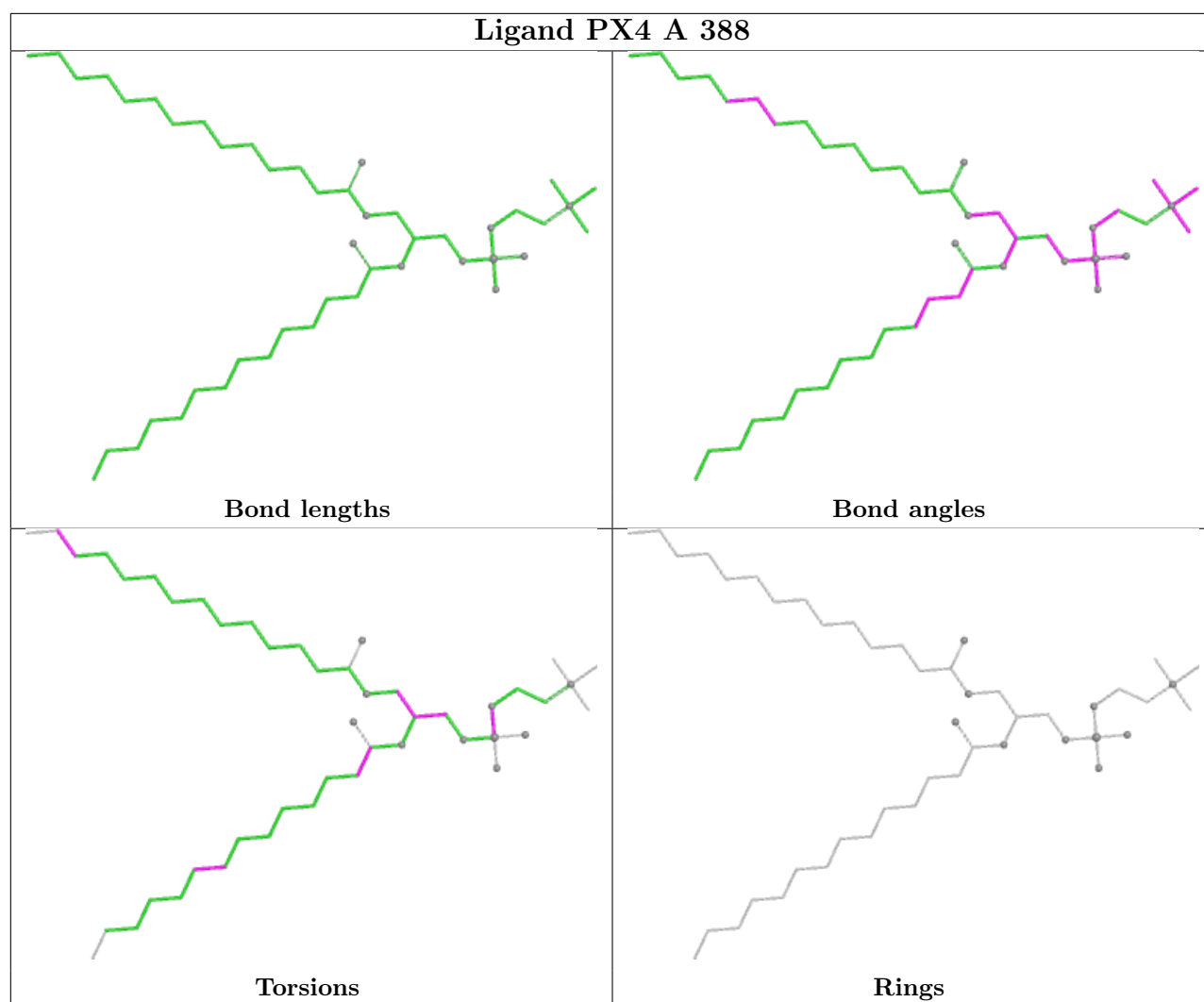


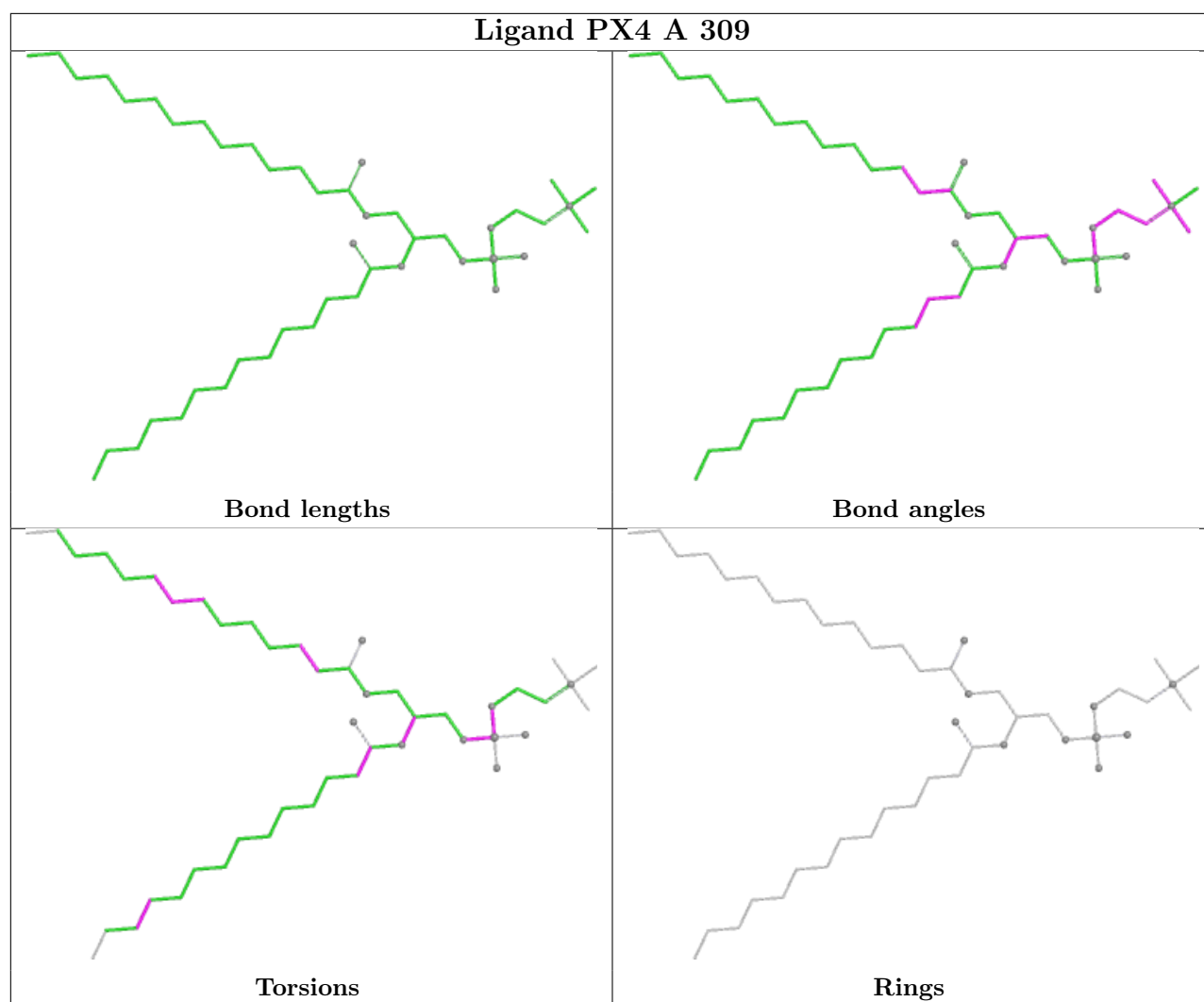


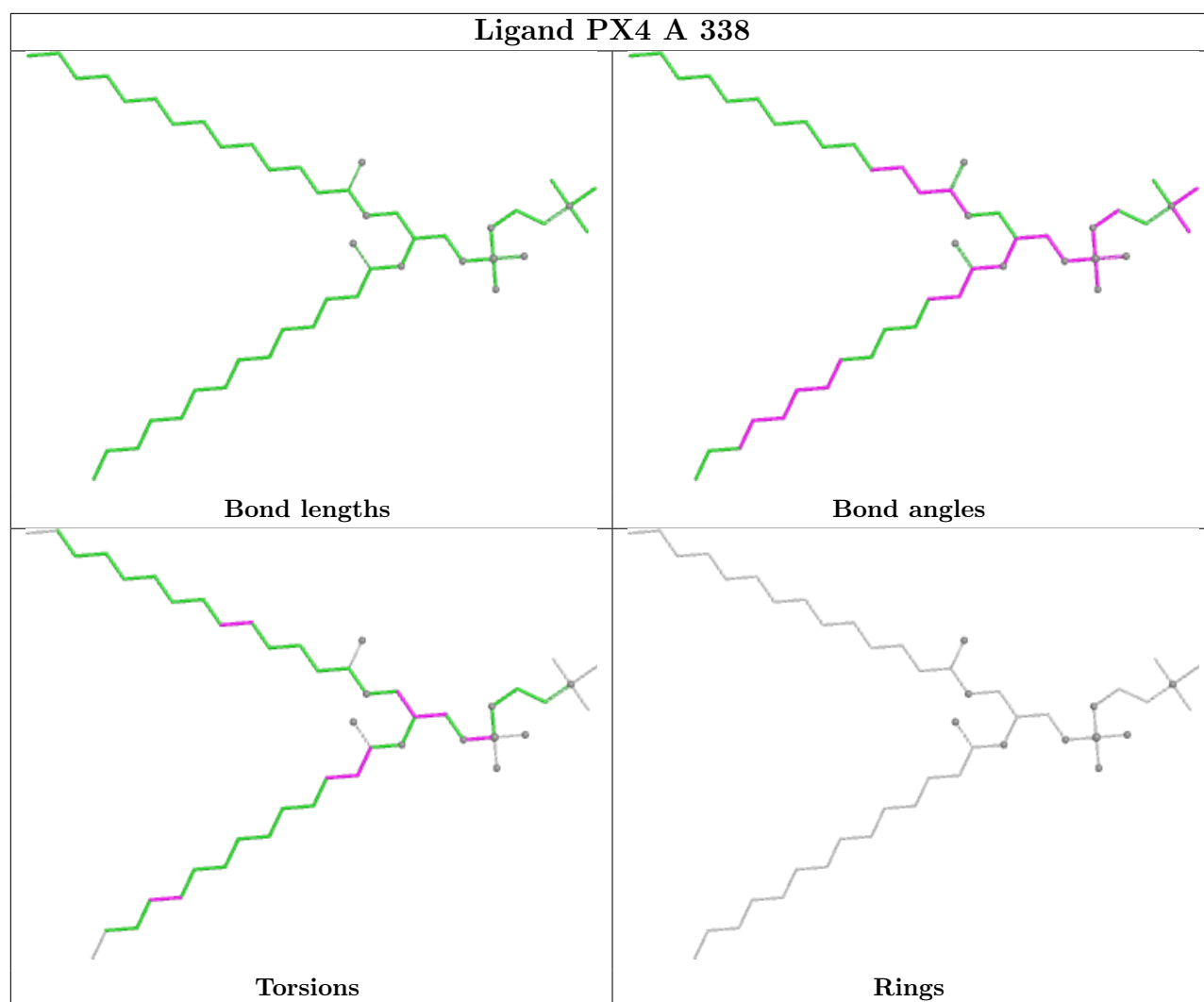


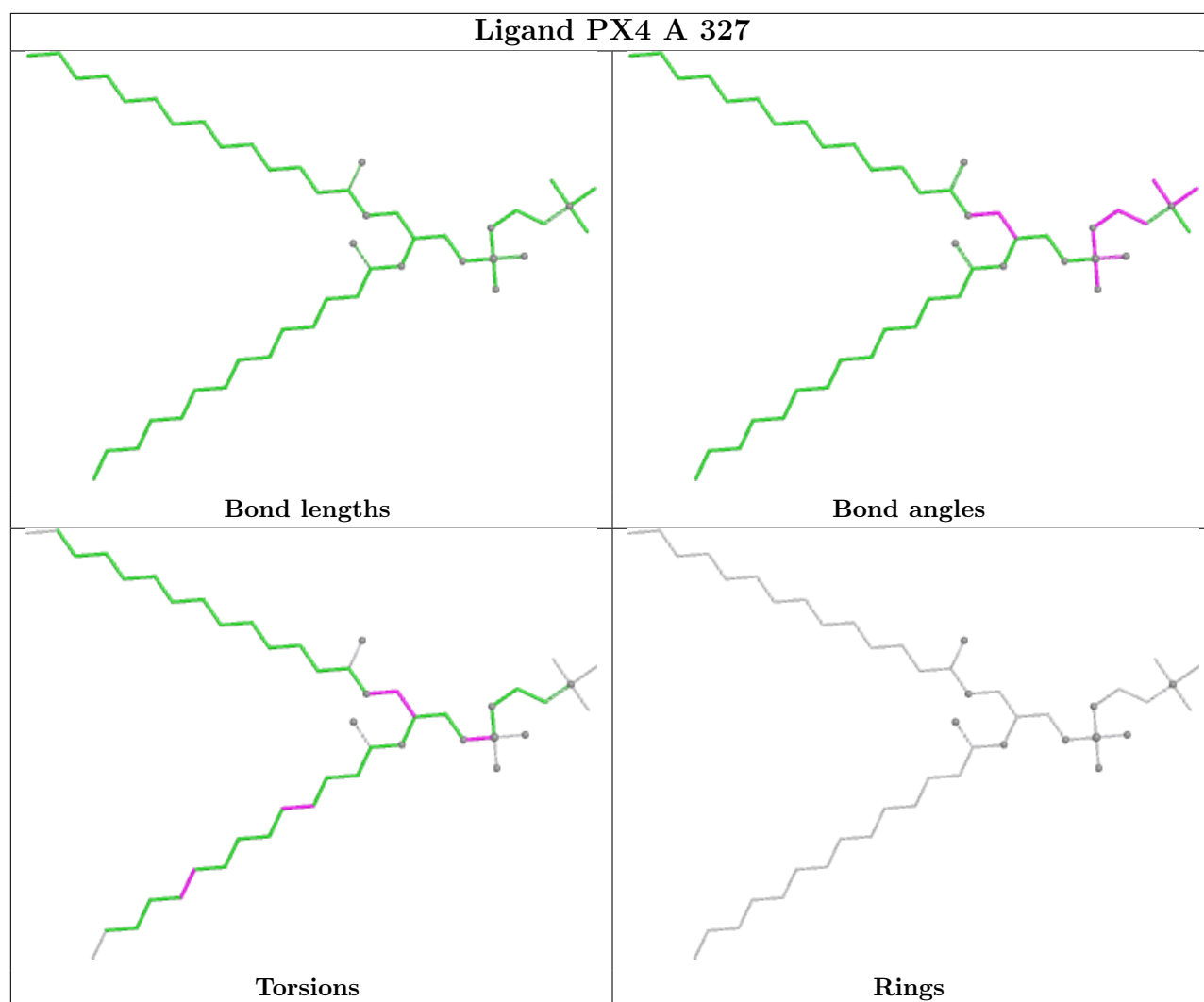


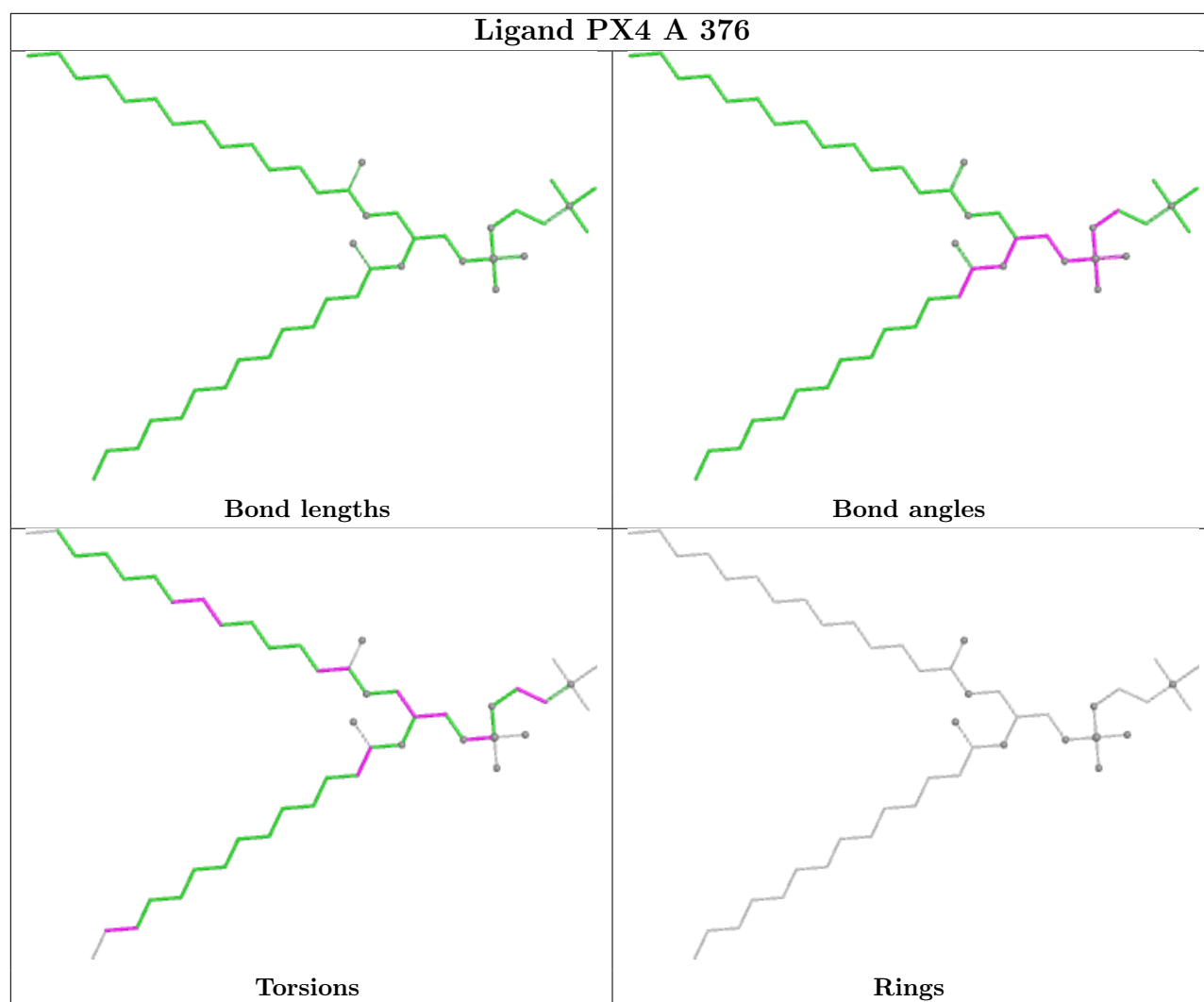


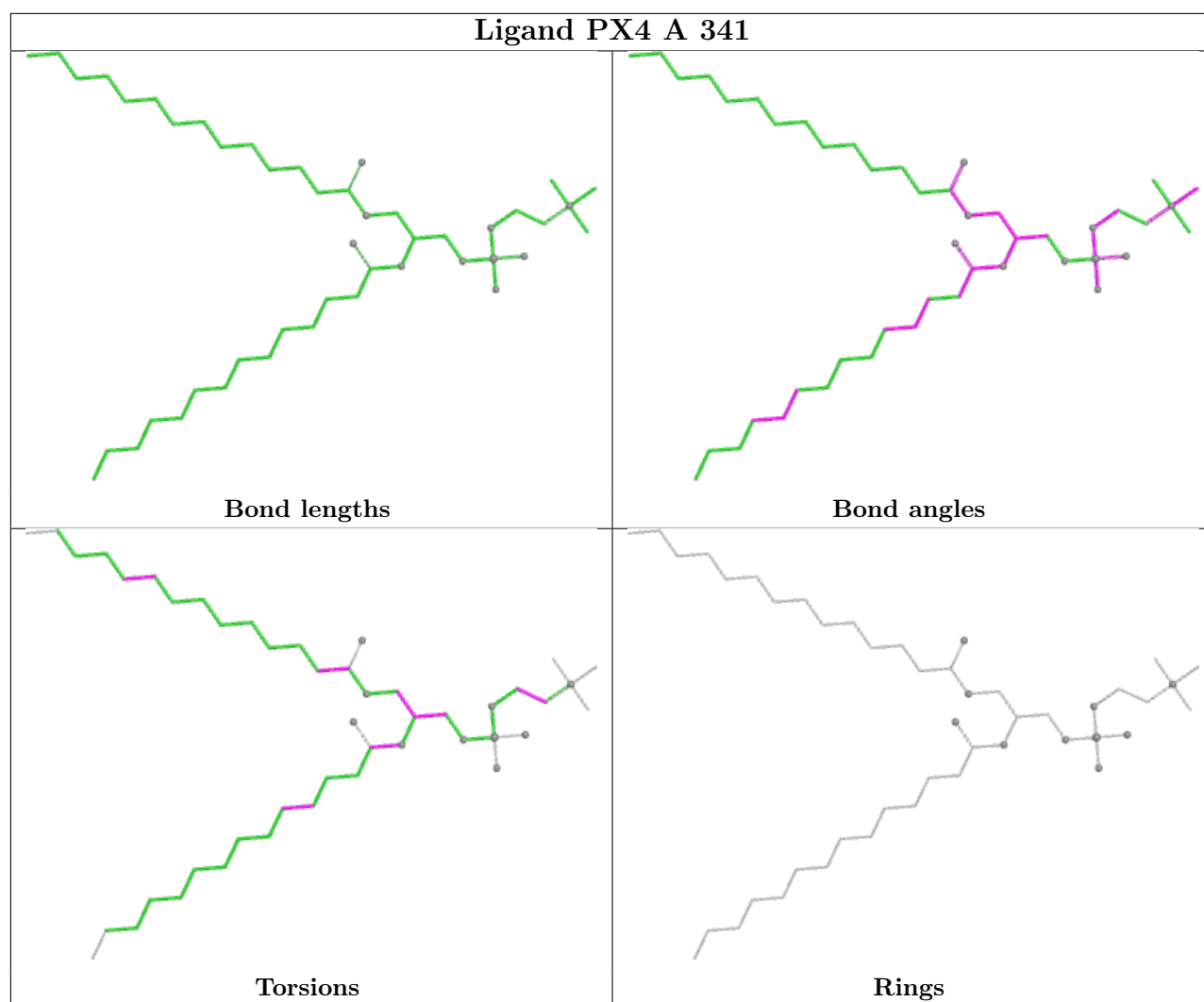


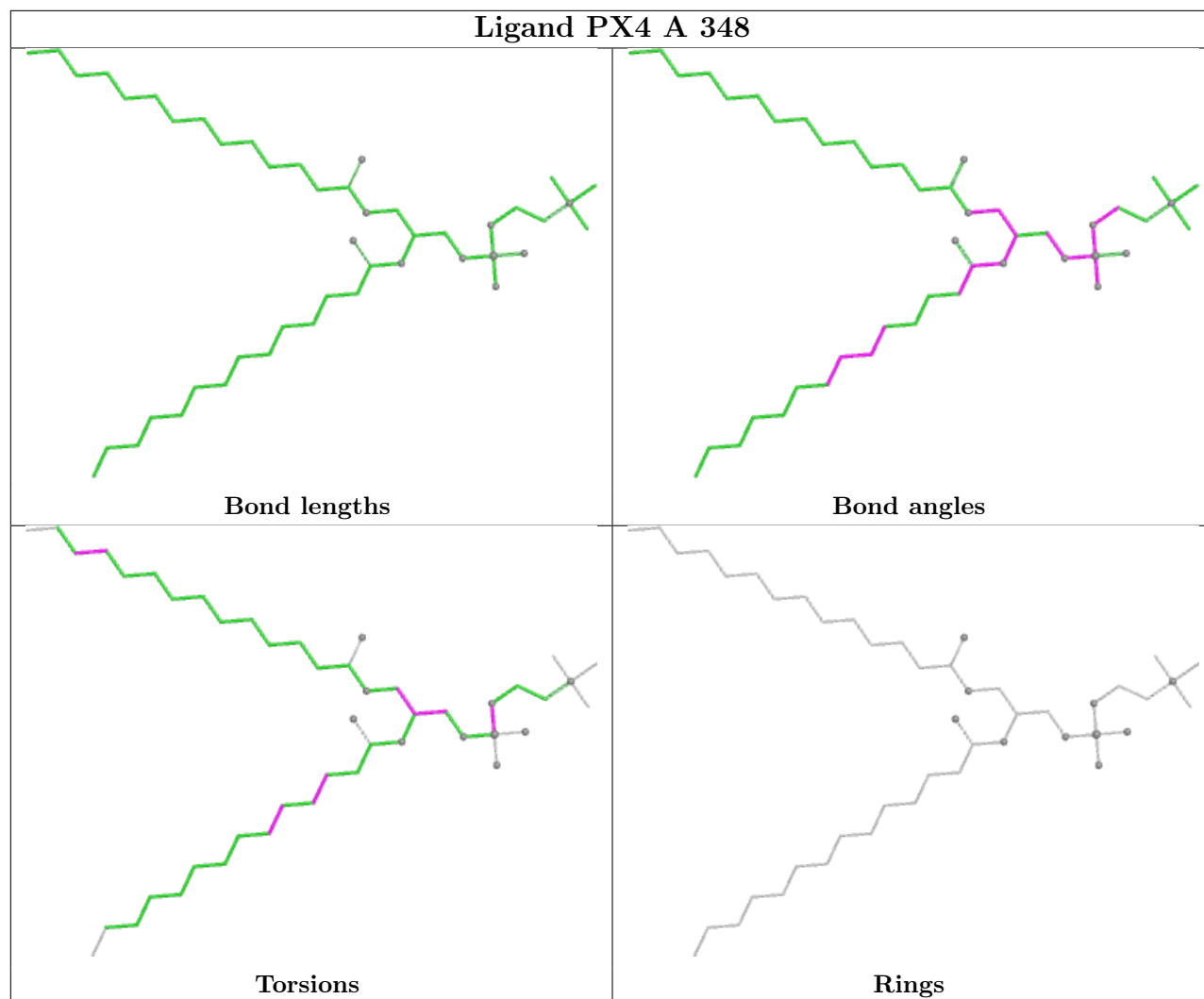


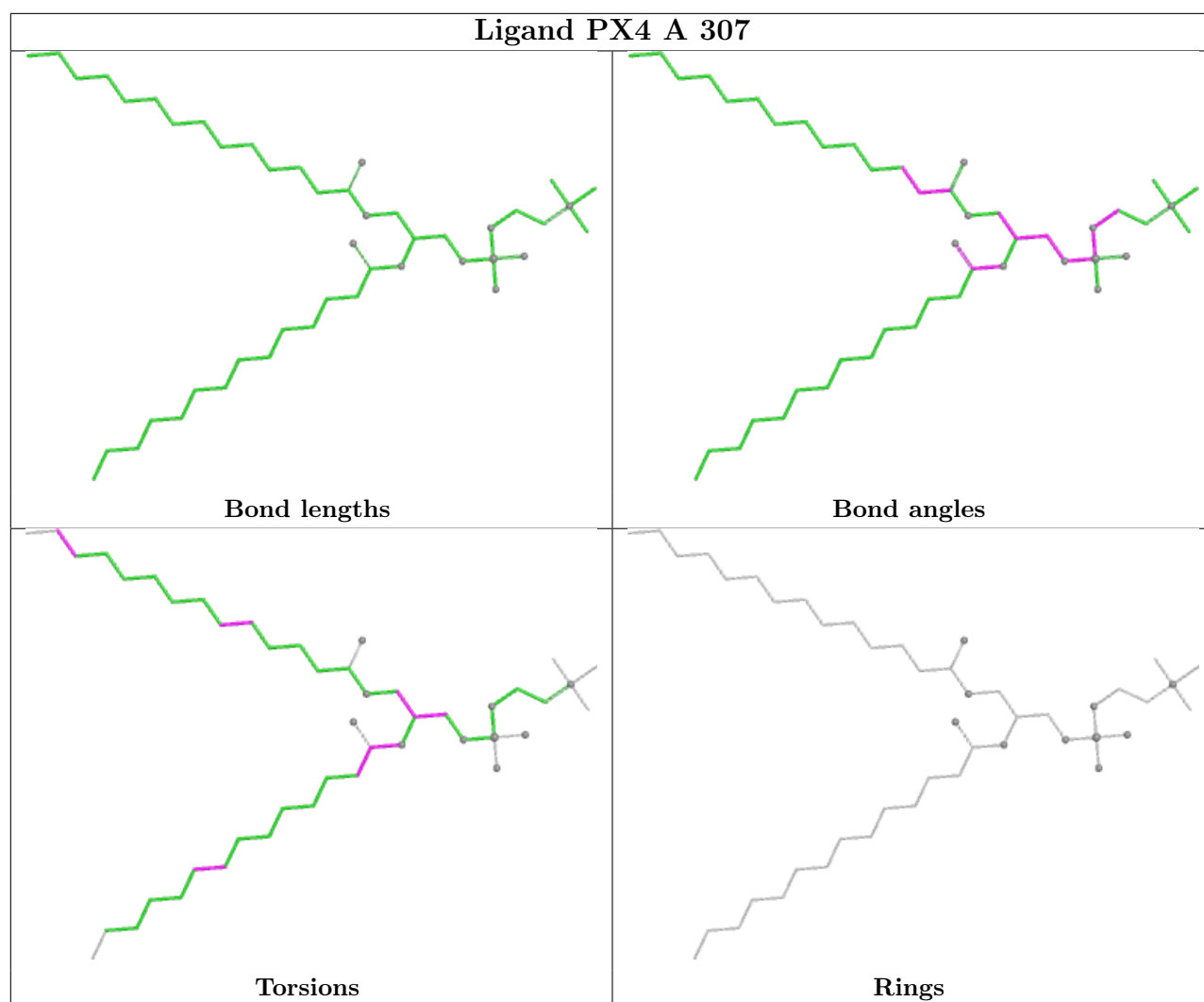


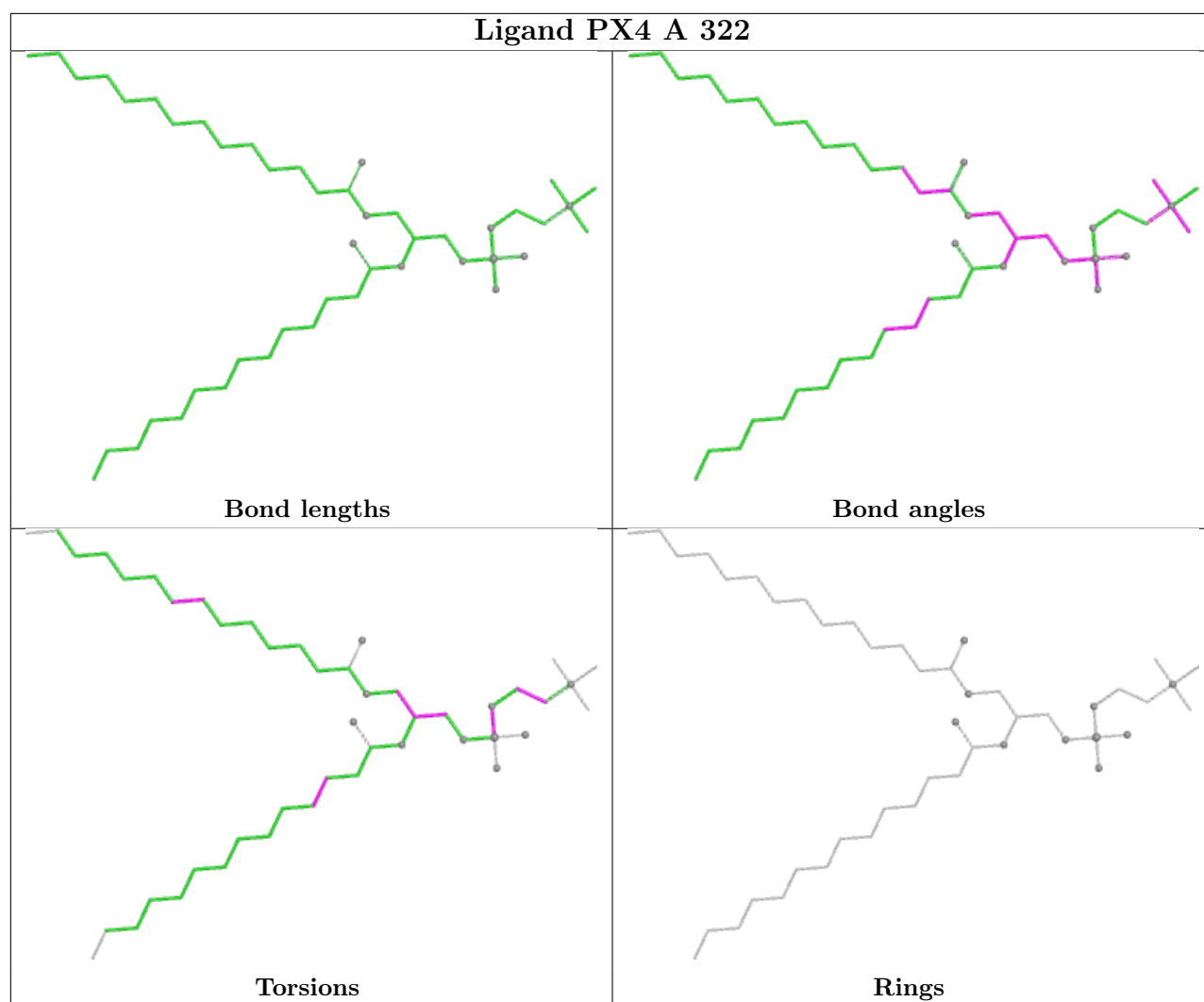


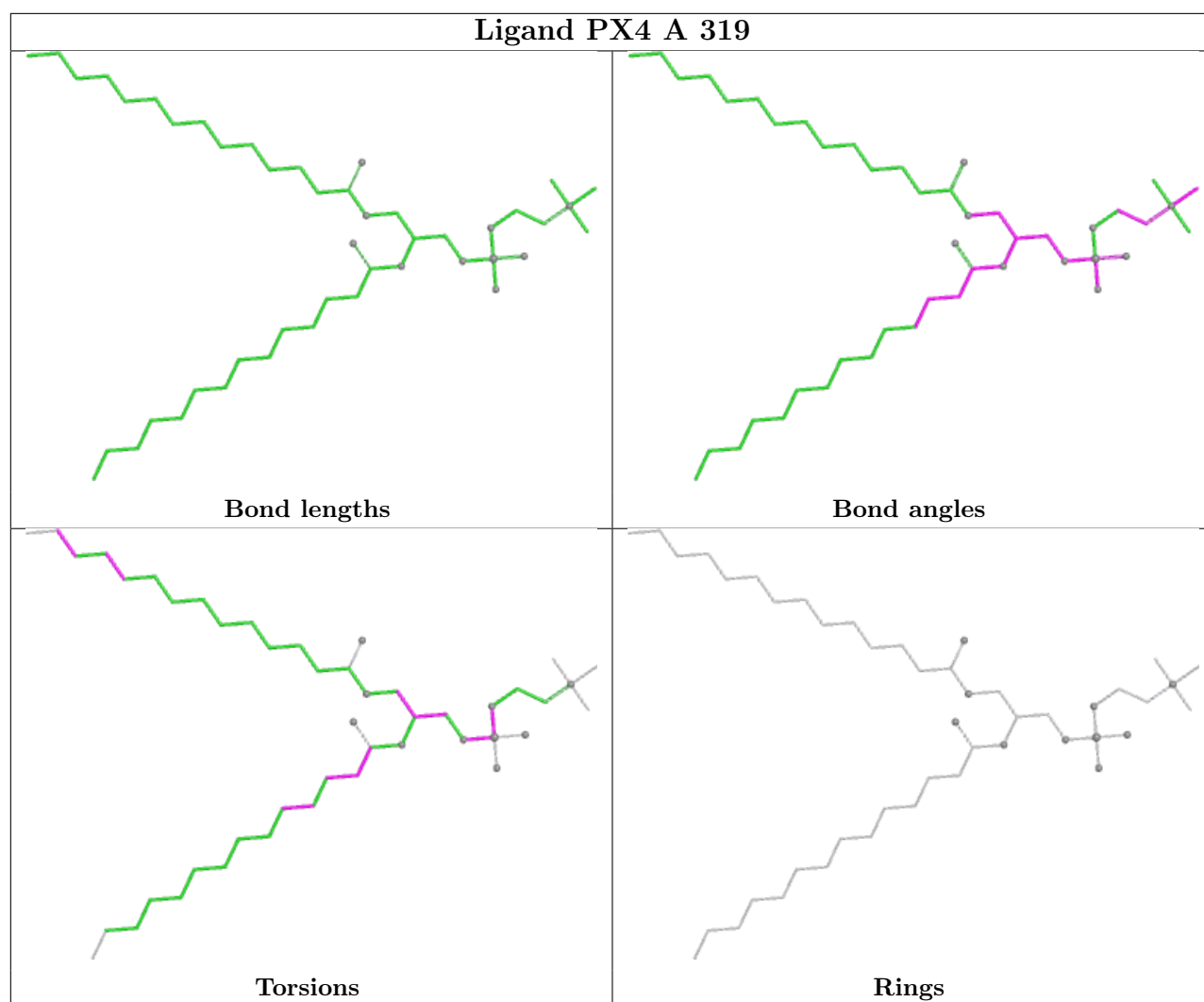


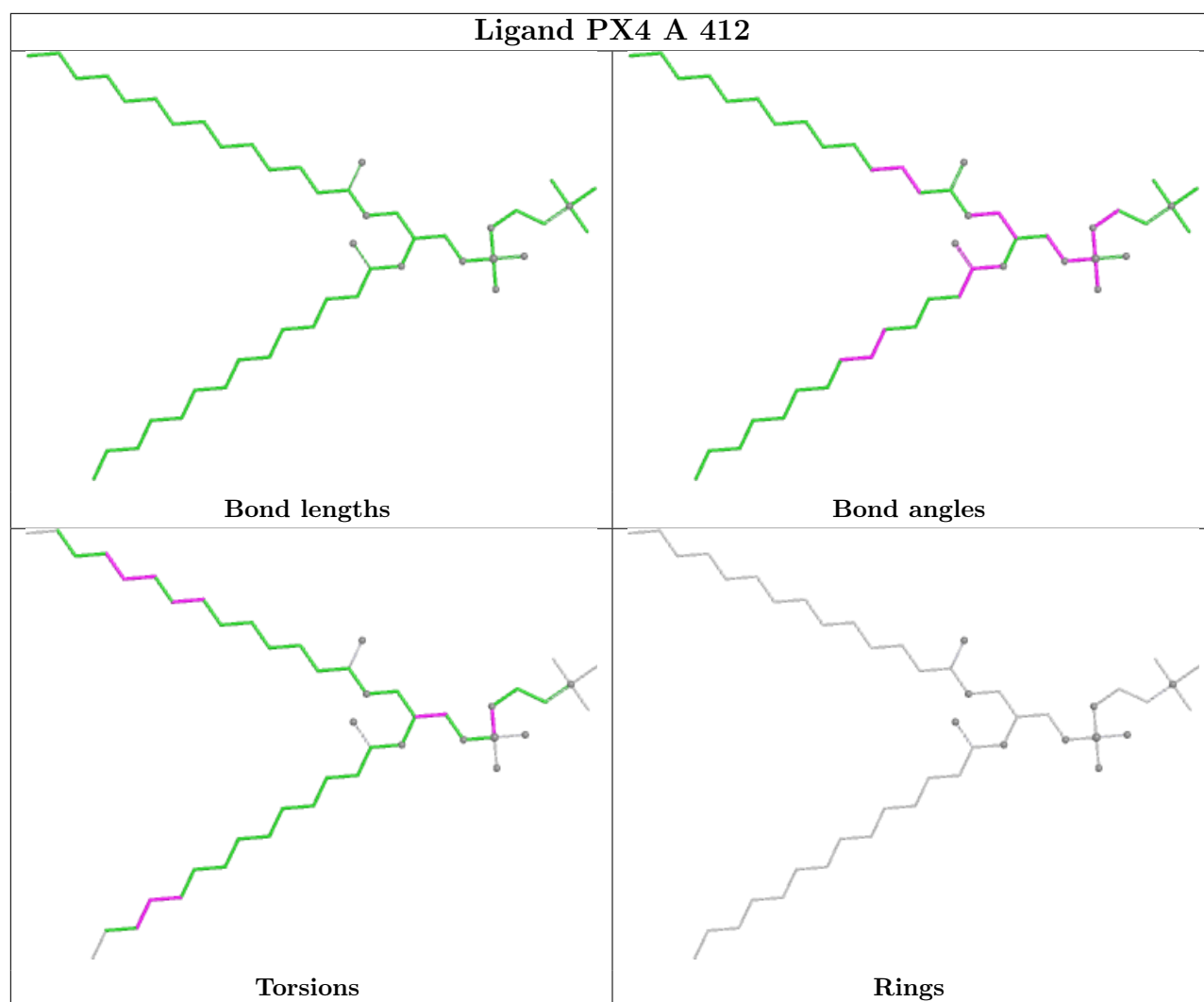


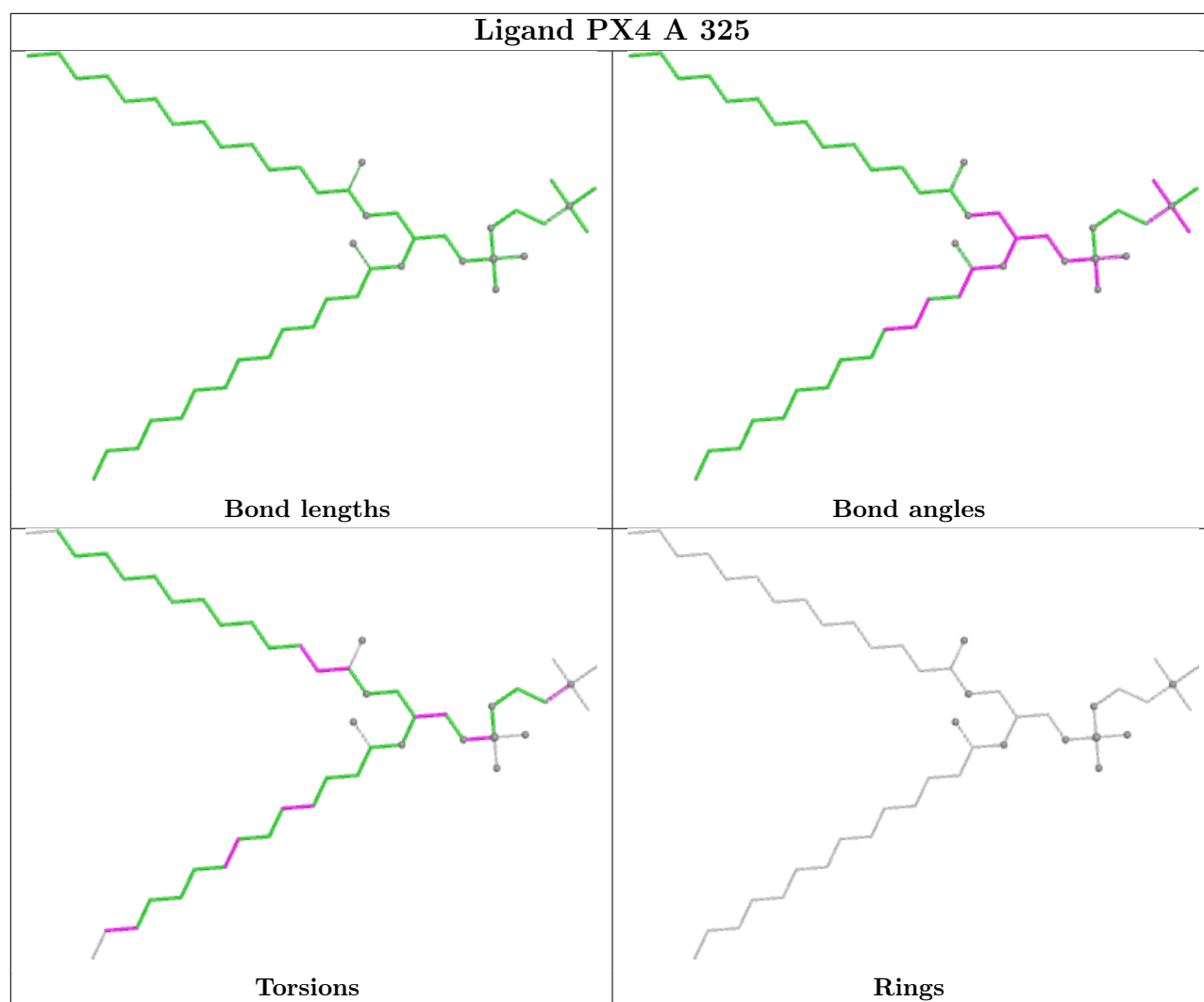


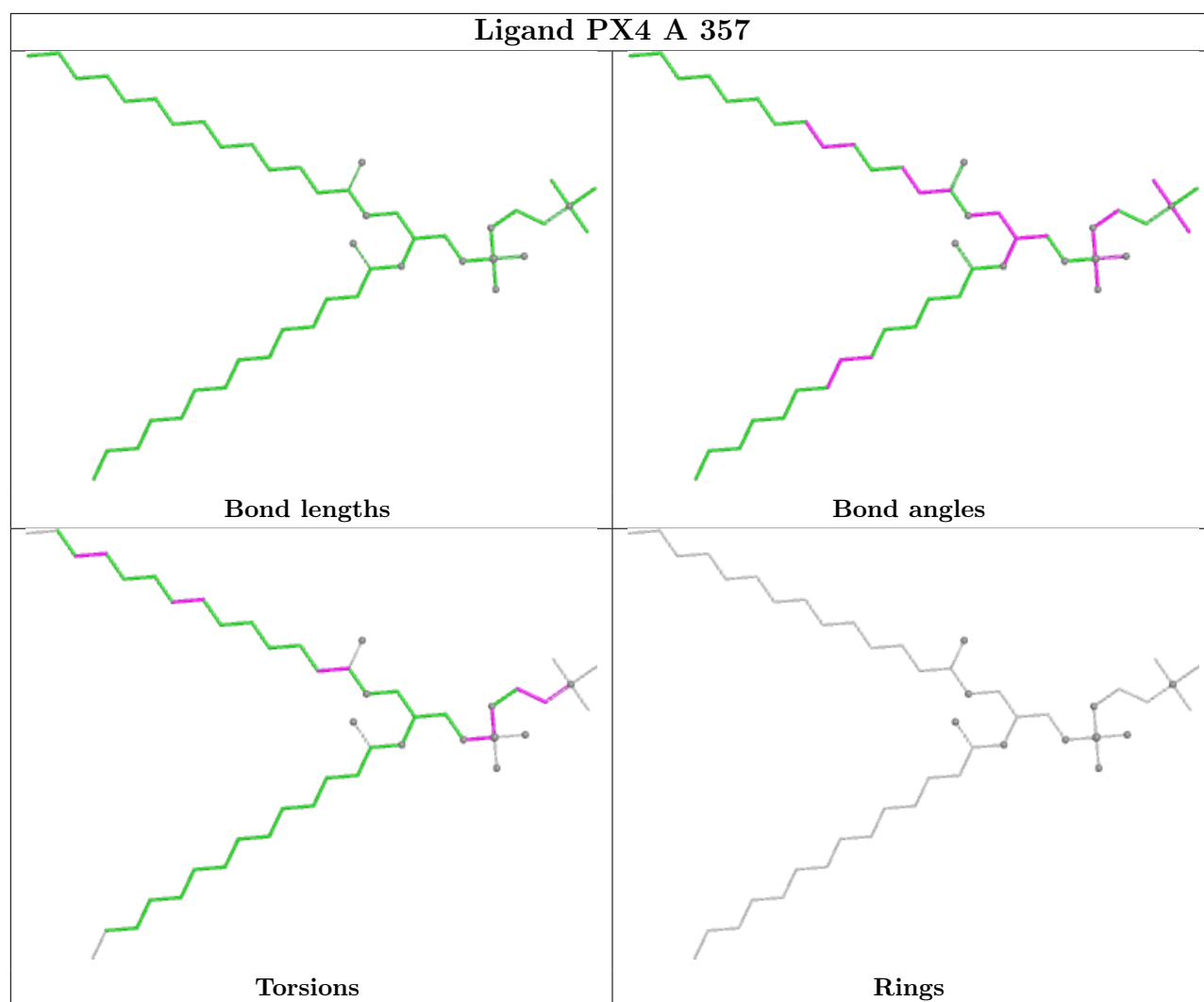


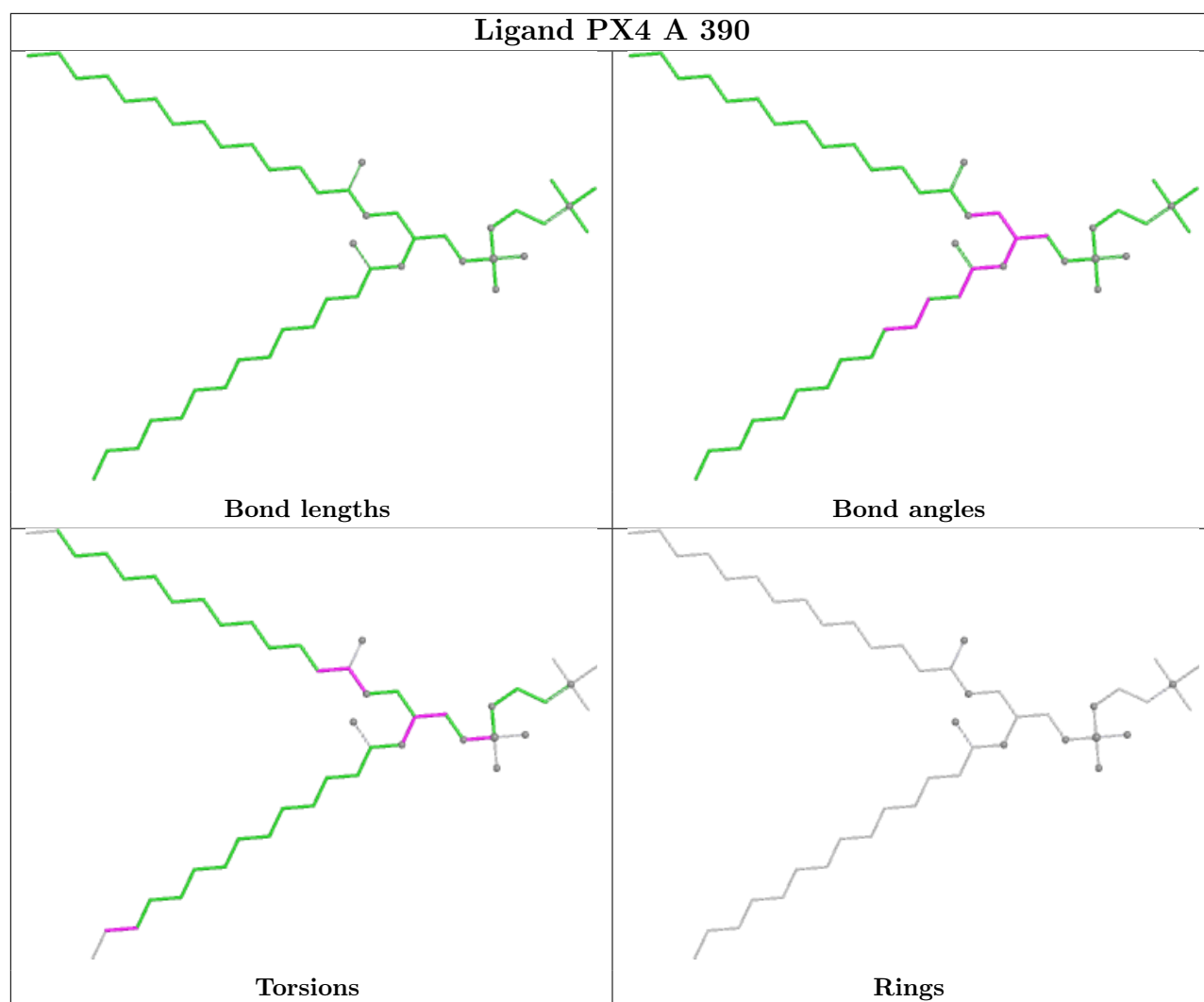


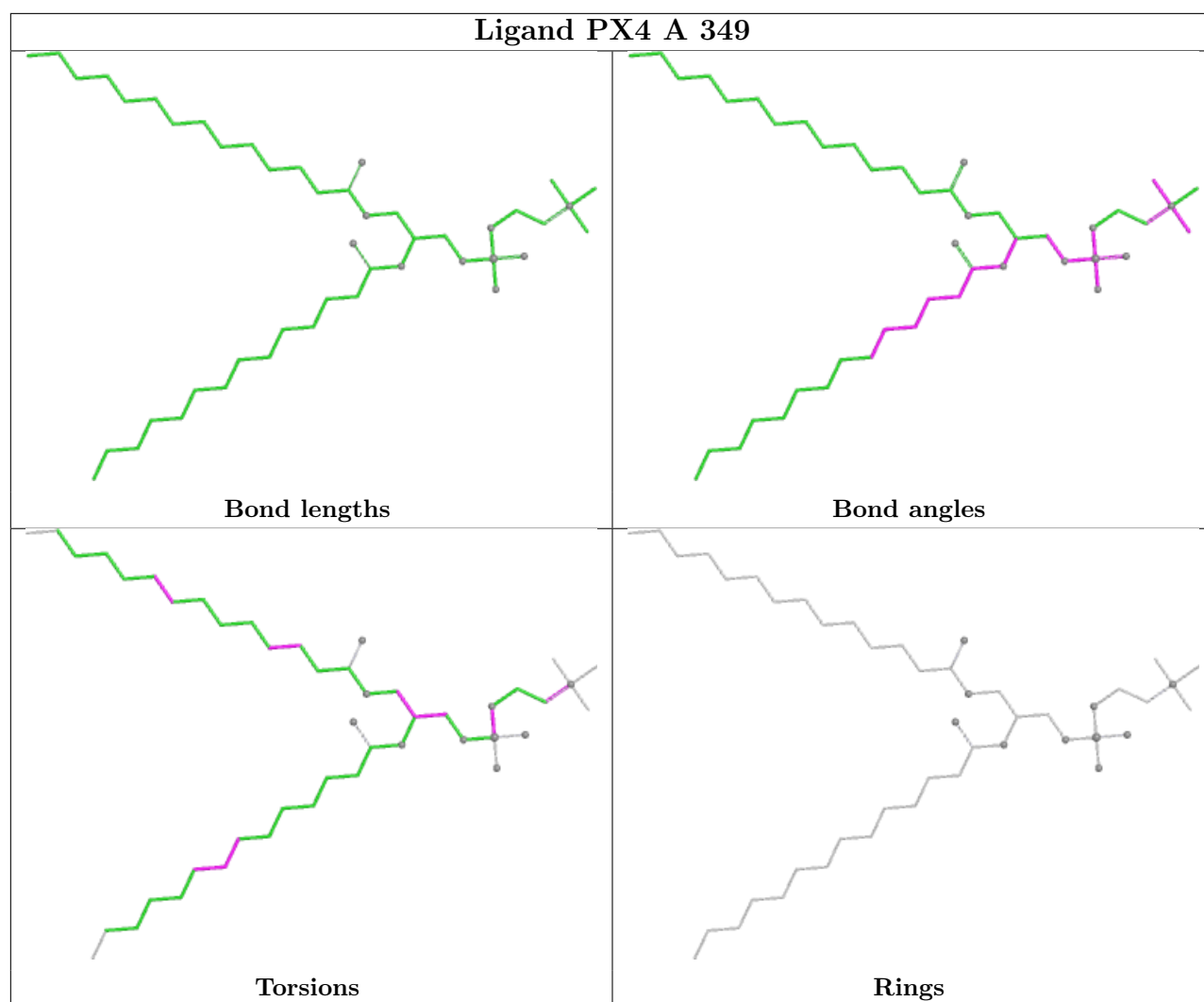




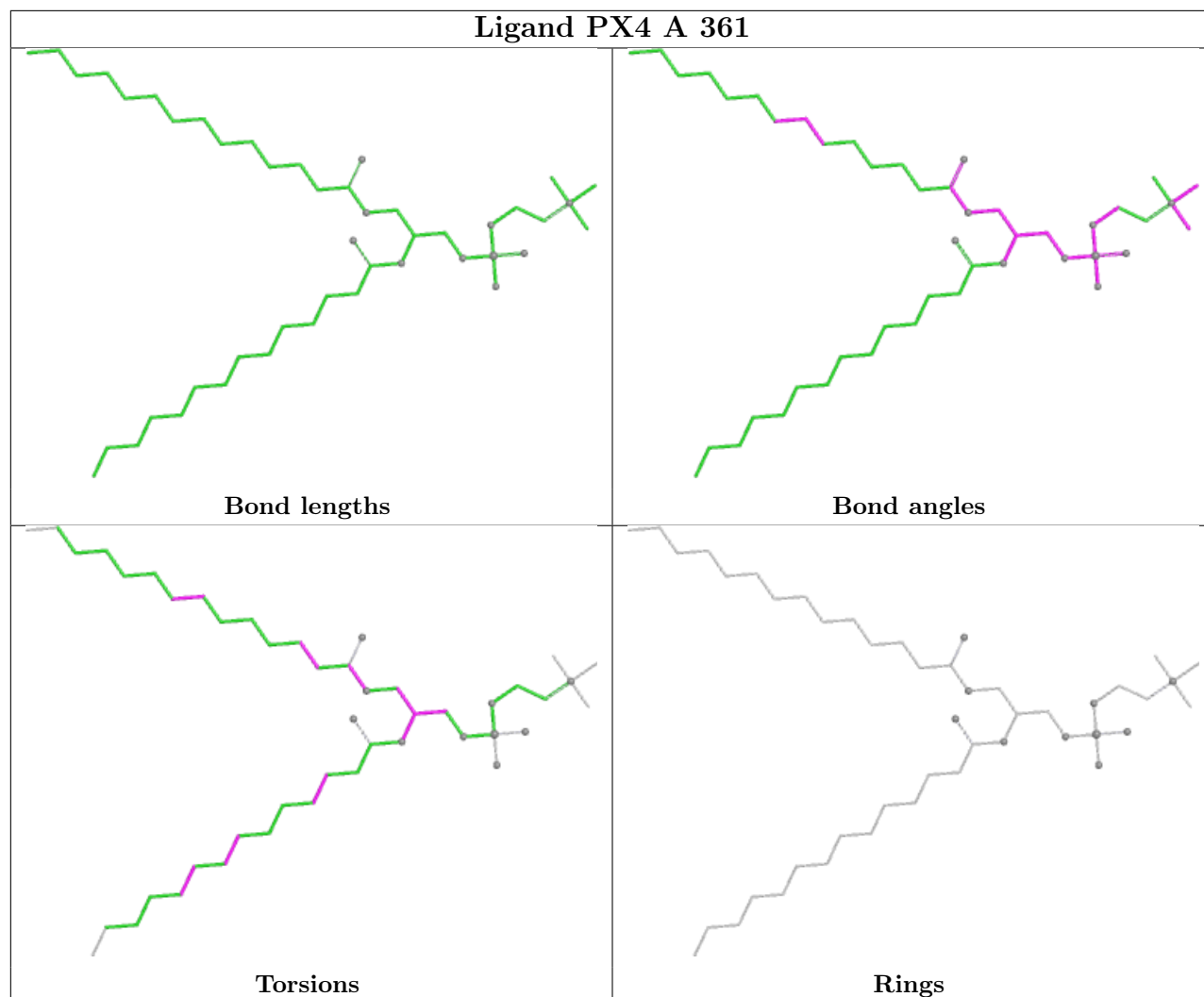




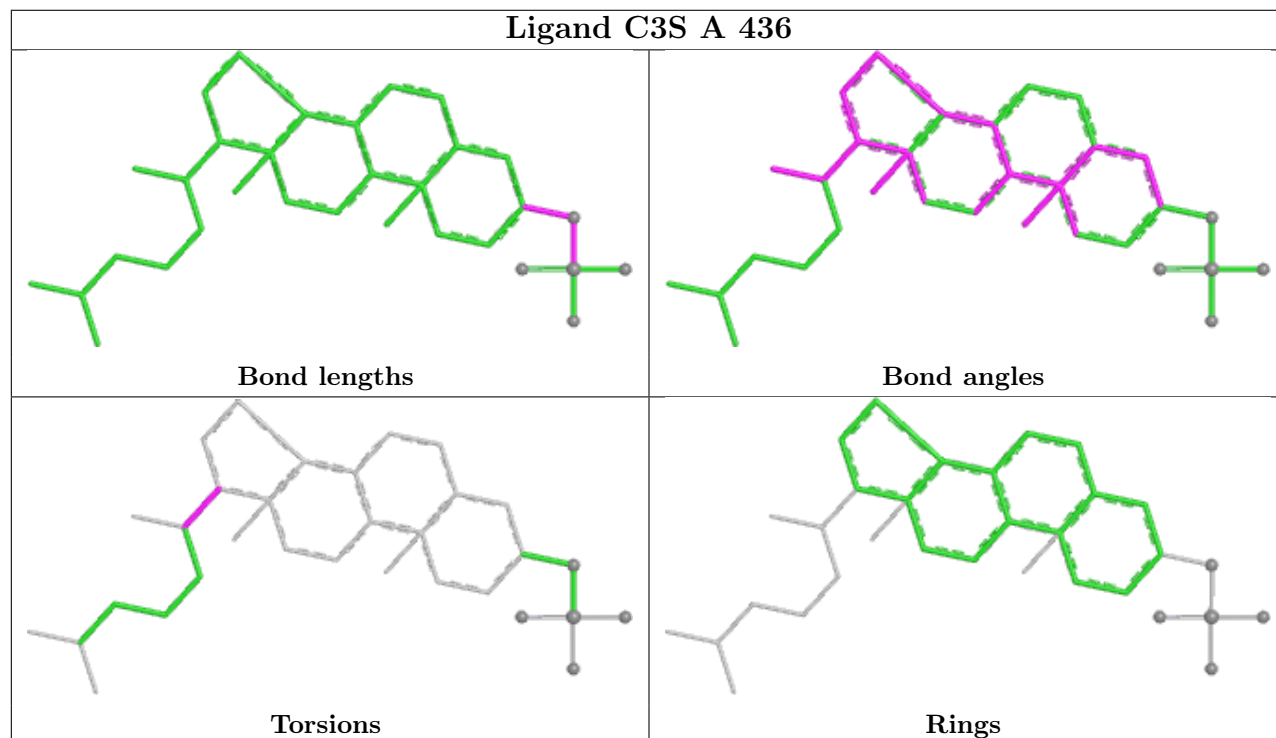




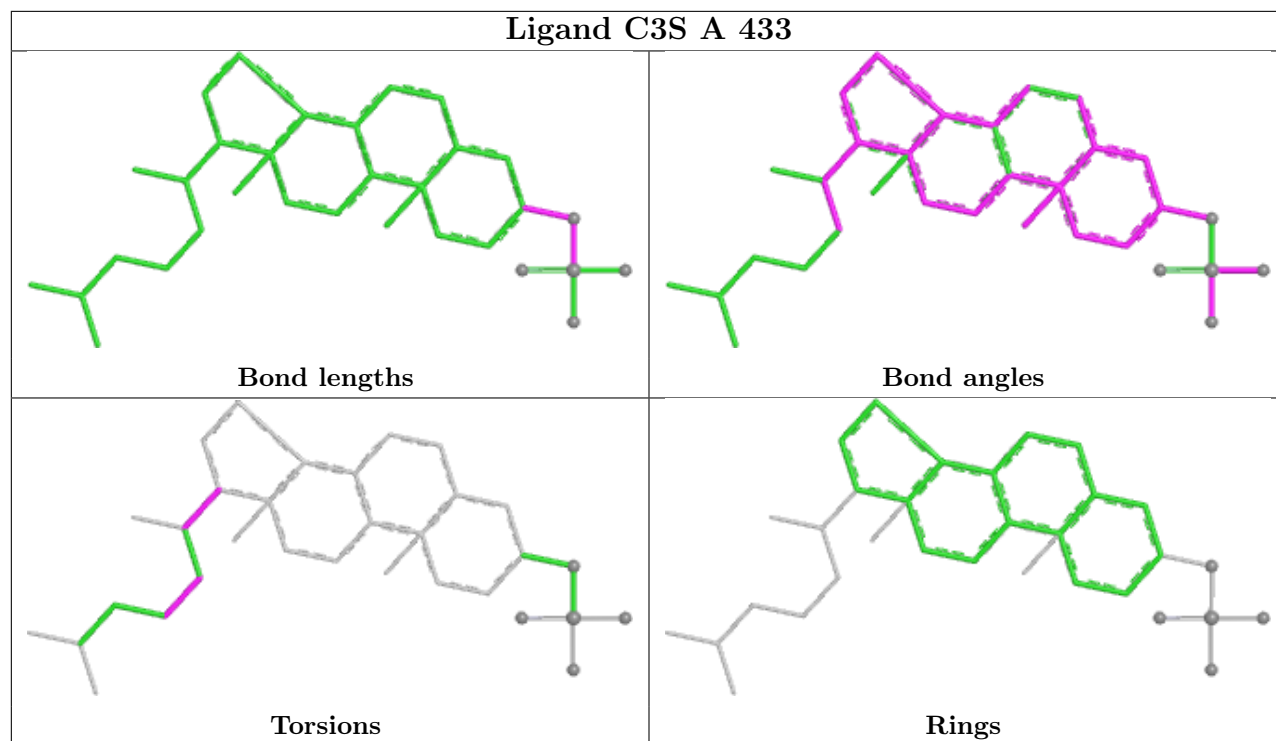
Ligand PX4 A 361



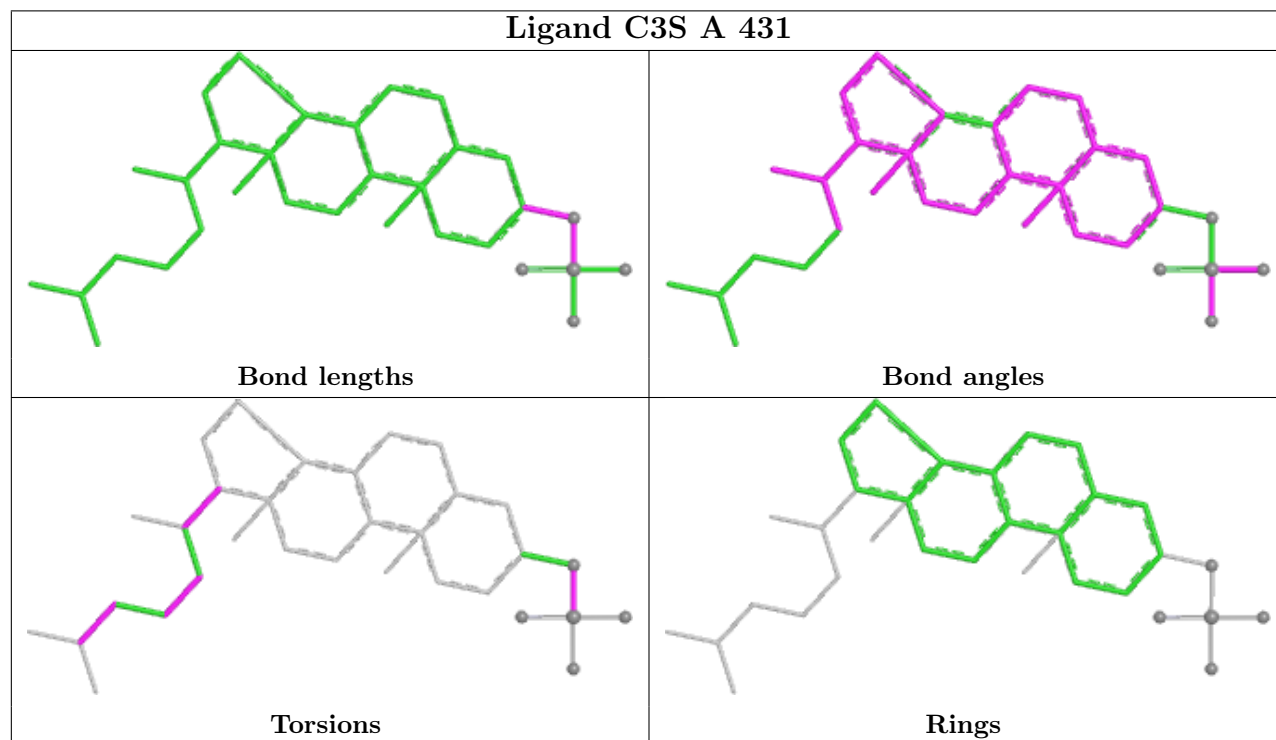
Ligand C3S A 436

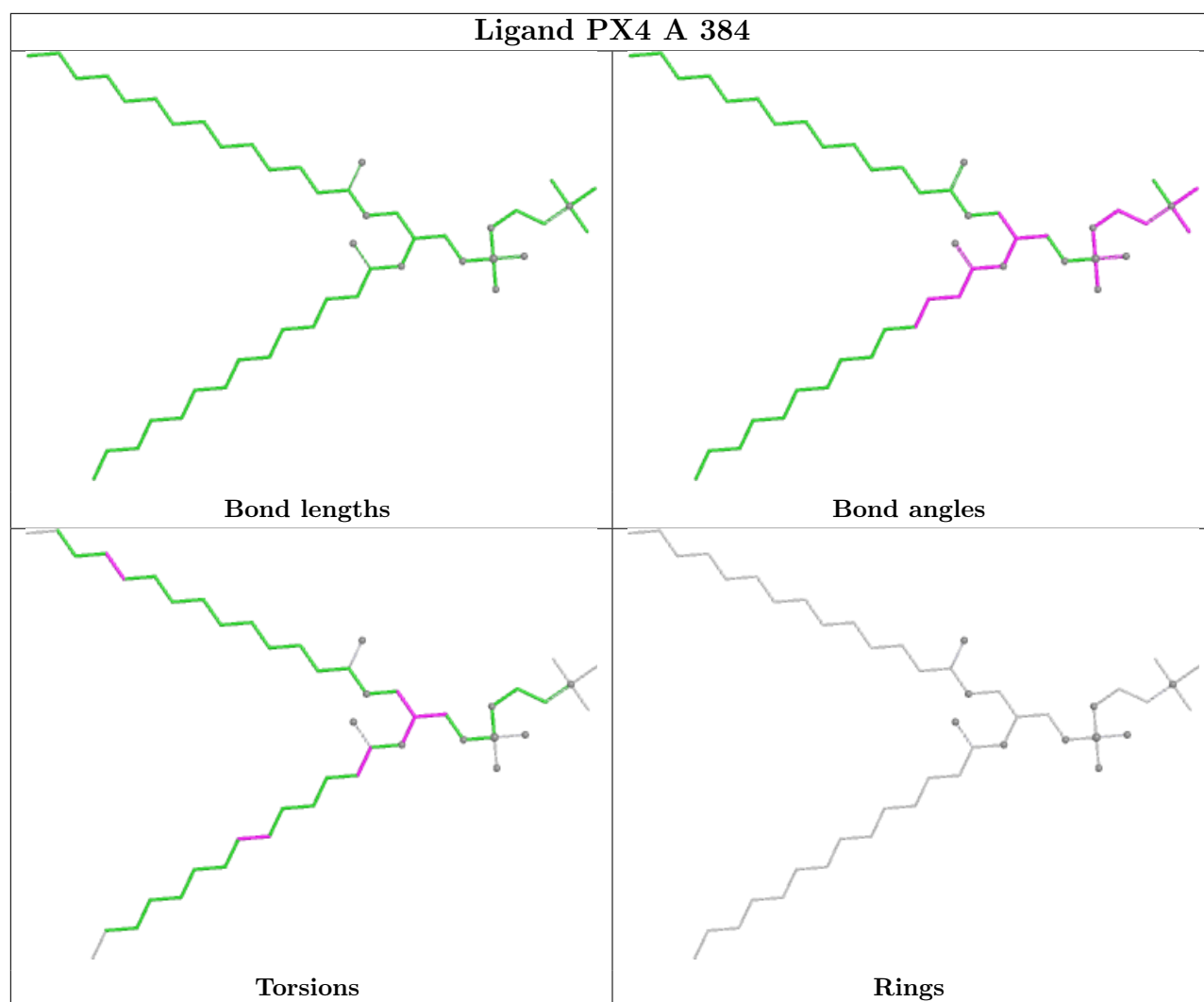


Ligand C3S A 433



Ligand C3S A 431





6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	797
Number of shifts mapped to atoms	797
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	188	0.12 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

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

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

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

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 24%, i.e. 797 atoms were assigned a chemical shift out of a possible 3323. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	436/1237 (35%)	248/507 (49%)	0/496 (0%)	188/234 (80%)
Sidechain	348/1761 (20%)	298/1143 (26%)	46/548 (8%)	4/70 (6%)
Aromatic	13/325 (4%)	9/161 (6%)	0/151 (0%)	4/13 (31%)
Overall	797/3323 (24%)	555/1811 (31%)	46/1195 (4%)	196/317 (62%)

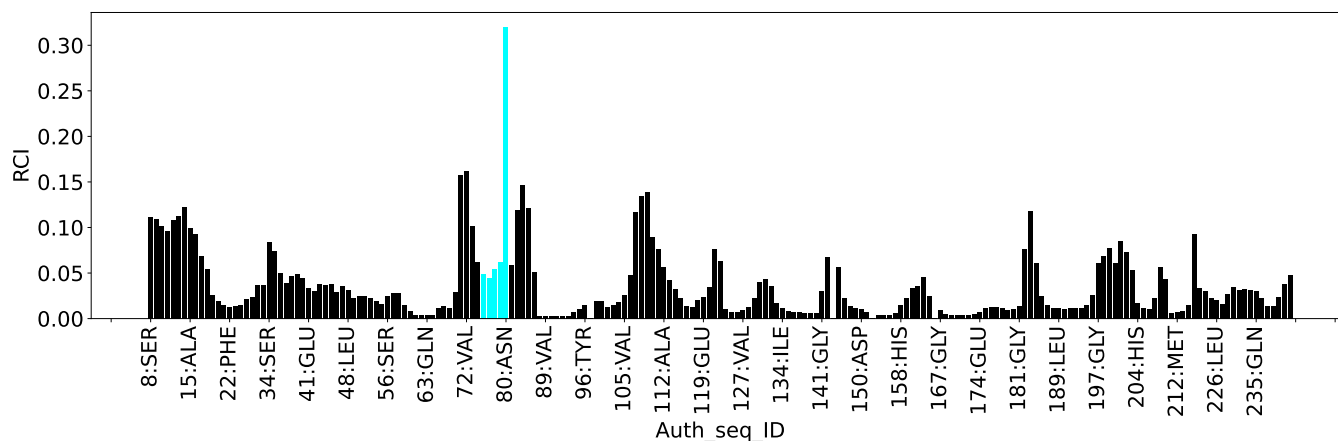
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

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

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

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

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

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

9 Distance violation analysis ⓘ

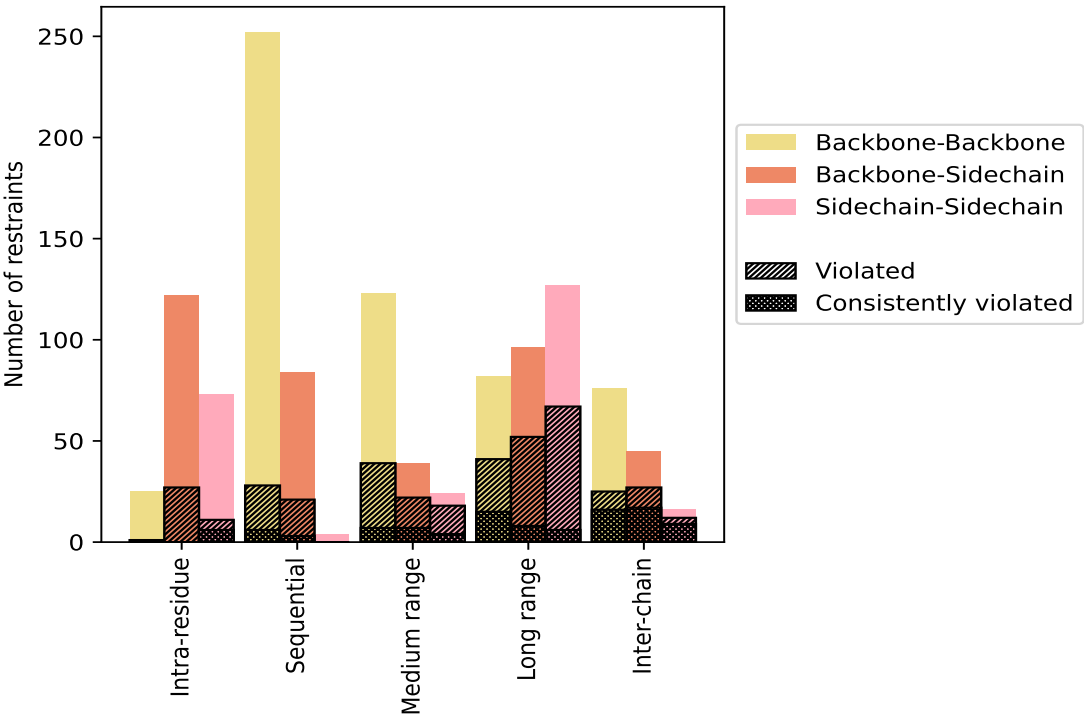
9.1 Summary of distance violations ⓘ

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

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

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

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



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

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

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

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

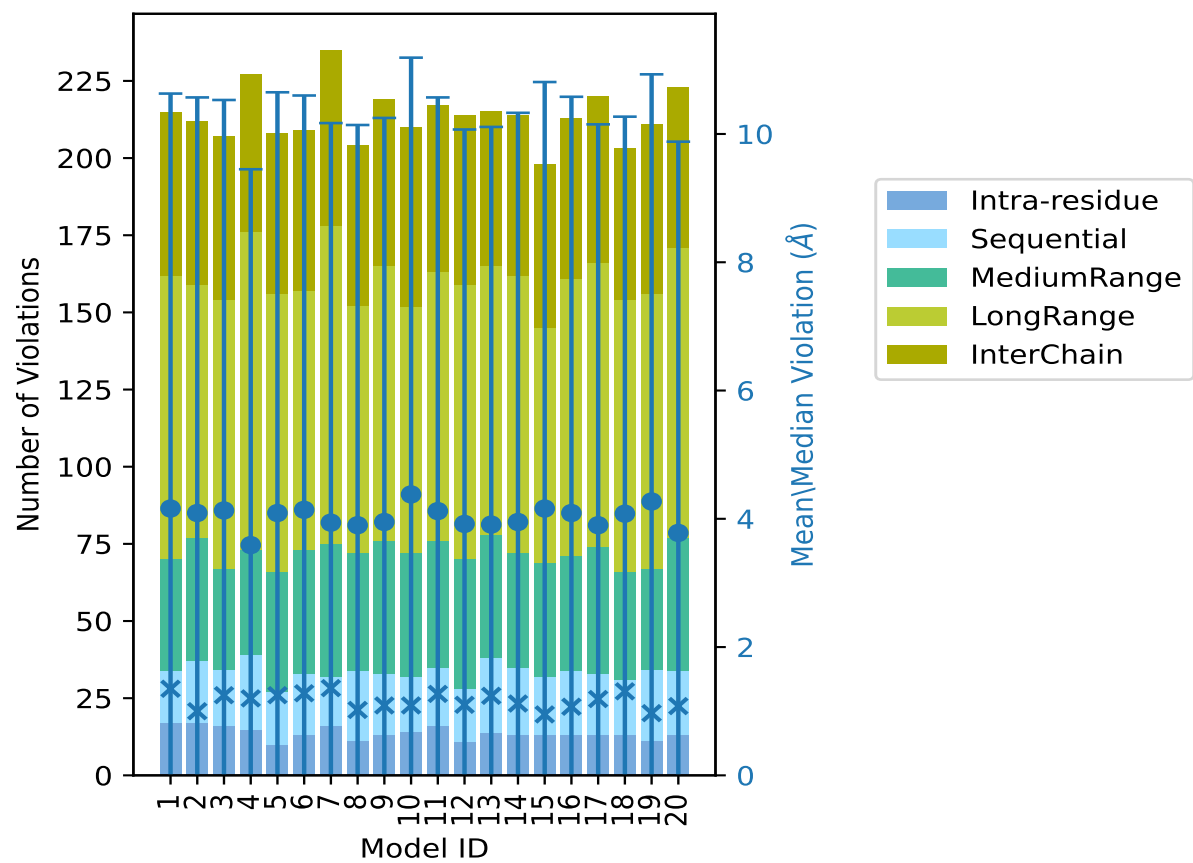
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	16	19	41	87	54	217	4.12	38.69	6.45	1.27
12	11	17	42	89	55	214	3.92	32.01	6.15	1.1
13	14	24	40	87	50	215	3.91	33.78	6.2	1.24
14	13	22	37	90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

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

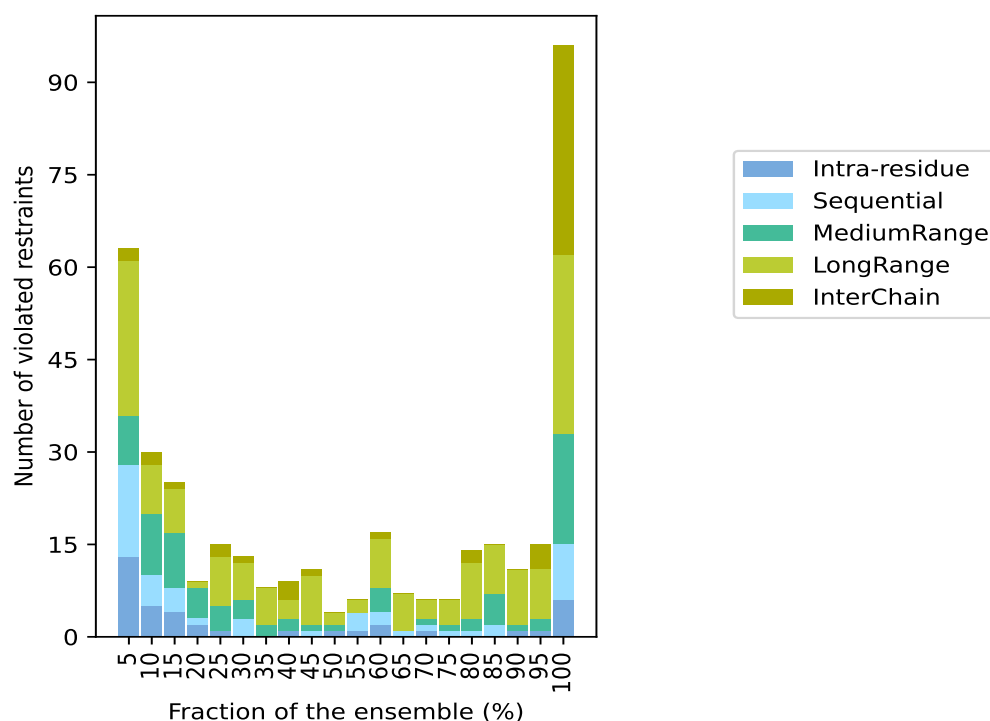
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 795(IR:181, SQ:291, MR:107, LR:145, IC:71) restraints are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

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

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

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

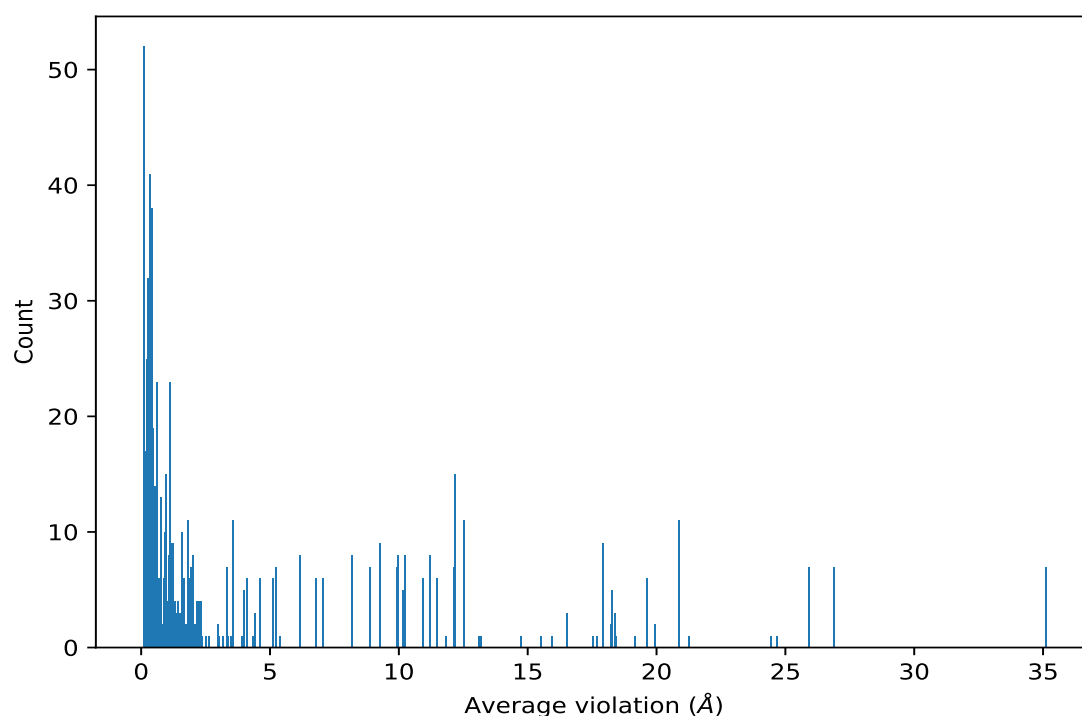
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

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

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,1)	1:5:A:GLY:H	4:349:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:348:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:308:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:317:A:PX4:C35	20	25.93	1.87	25.9
(3,1)	1:5:A:GLY:H	4:330:A:PX4:C35	20	25.93	1.87	25.9
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	20	24.69	0.98	24.88
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	20	24.44	0.49	24.34
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	20	21.26	0.45	21.19
(3,44)	1:34:A:SER:H	4:319:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:321:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:317:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:317:A:PX4:C3	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:310:A:PX4:C4	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:319:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:317:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:321:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:353:A:PX4:C5	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:321:A:PX4:C3	20	20.86	1.82	21.04
(3,44)	1:34:A:SER:H	4:353:A:PX4:C4	20	20.86	1.82	21.04
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	20	19.95	0.65	20.13
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H13	20	19.95	0.65	20.13
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:340:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:352:A:PX4:C35	20	19.65	2.18	19.67
(3,2)	1:21:A:ARG:H	4:324:A:PX4:C35	20	19.65	2.18	19.67
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	20	19.19	0.66	19.25
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	20	18.43	1.22	18.24
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	20	18.39	0.63	18.42
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	20	18.39	0.63	18.42
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	20	18.39	0.63	18.42
(3,3)	1:22:A:PHE:H	4:320:A:PX4:C35	20	18.27	2.14	18.8
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	20	18.27	2.14	18.8
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	20	18.27	2.14	18.8
(3,3)	1:22:A:PHE:H	4:340:A:PX4:C35	20	18.27	2.14	18.8
(3,3)	1:22:A:PHE:H	4:352:A:PX4:C35	20	18.27	2.14	18.8
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	20	18.24	0.64	18.42
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H13	20	18.24	0.64	18.42
(3,6)	1:61:A:ILE:H	4:349:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:353:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:307:A:PX4:C35	20	17.91	2.33	17.85

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,6)	1:61:A:ILE:H	4:348:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:308:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:317:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:325:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:330:A:PX4:C35	20	17.91	2.33	17.85
(3,6)	1:61:A:ILE:H	4:320:A:PX4:C35	20	17.91	2.33	17.85
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	20	17.69	0.65	17.81
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	20	17.53	0.95	17.28
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	20	16.51	0.48	16.46
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	20	16.51	0.48	16.46
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	20	16.51	0.48	16.46
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	20	15.91	0.47	15.87
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	20	15.5	0.56	15.34
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	20	14.73	0.48	14.71
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	20	13.16	0.47	13.33
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	20	13.12	0.31	13.03
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C4	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:310:A:PX4:C4	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C4	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C3	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C3	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:305:A:PX4:C3	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C5	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:308:A:PX4:C3	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C5	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C3	20	12.52	1.16	12.71
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C5	20	12.52	1.16	12.71
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C4	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C3	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:349:A:PX4:C4	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C3	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C5	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C5	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:308:A:PX4:C3	20	12.18	1.3	12.3
(3,39)	1:12:A:TRP:H	4:349:A:PX4:C3	20	12.18	1.3	12.3
(3,31)	1:216:A:TYR:H	4:308:A:PX4:C35	20	12.18	2.64	12.25
(3,31)	1:216:A:TYR:H	4:353:A:PX4:C35	20	12.18	2.64	12.25
(3,31)	1:216:A:TYR:H	4:307:A:PX4:C35	20	12.18	2.64	12.25
(3,31)	1:216:A:TYR:H	4:348:A:PX4:C35	20	12.18	2.64	12.25
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	20	12.18	2.64	12.25
(3,31)	1:216:A:TYR:H	4:317:A:PX4:C35	20	12.18	2.64	12.25
(3,31)	1:216:A:TYR:H	4:320:A:PX4:C35	20	12.18	2.64	12.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,45)	1:51:A:THR:H	4:317:A:PX4:C4	20	12.14	1.55	12.48
(3,45)	1:51:A:THR:H	4:330:A:PX4:C3	20	12.14	1.55	12.48
(3,45)	1:51:A:THR:H	4:317:A:PX4:C3	20	12.14	1.55	12.48
(3,45)	1:51:A:THR:H	4:330:A:PX4:C5	20	12.14	1.55	12.48
(3,45)	1:51:A:THR:H	4:317:A:PX4:C5	20	12.14	1.55	12.48
(3,45)	1:51:A:THR:H	4:307:A:PX4:C4	20	12.14	1.55	12.48
(3,45)	1:51:A:THR:H	4:307:A:PX4:C3	20	12.14	1.55	12.48
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	20	11.84	1.02	11.36
(3,37)	1:7:A:MET:H	4:353:A:PX4:C3	20	11.47	1.28	11.42
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	20	11.47	1.28	11.42
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	20	11.47	1.28	11.42
(3,37)	1:7:A:MET:H	4:317:A:PX4:C4	20	11.47	1.28	11.42
(3,37)	1:7:A:MET:H	4:317:A:PX4:C5	20	11.47	1.28	11.42
(3,37)	1:7:A:MET:H	4:349:A:PX4:C3	20	11.47	1.28	11.42
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C4	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:310:A:PX4:C3	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C3	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:310:A:PX4:C4	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:319:A:PX4:C5	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C5	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:308:A:PX4:C3	20	11.23	0.94	11.04
(3,41)	1:16:A:GLN:H	4:353:A:PX4:C5	20	11.23	0.94	11.04
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C3	20	10.9	1.32	11.38
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	20	10.9	1.32	11.38
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C5	20	10.9	1.32	11.38
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C4	20	10.9	1.32	11.38
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C5	20	10.9	1.32	11.38
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C4	20	10.9	1.32	11.38
(3,38)	1:8:A:SER:H	4:317:A:PX4:C4	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:317:A:PX4:C3	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:349:A:PX4:C4	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:353:A:PX4:C3	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:353:A:PX4:C5	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:317:A:PX4:C5	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:349:A:PX4:C3	20	10.21	1.7	9.84
(3,38)	1:8:A:SER:H	4:349:A:PX4:C5	20	10.21	1.7	9.84
(3,7)	1:69:A:VAL:H	4:320:A:PX4:C35	20	10.19	2.19	10.48
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	20	10.19	2.19	10.48
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	20	10.19	2.19	10.48
(3,7)	1:69:A:VAL:H	4:395:A:PX4:C35	20	10.19	2.19	10.48
(3,7)	1:69:A:VAL:H	4:317:A:PX4:C35	20	10.19	2.19	10.48
(3,23)	1:145:A:ASP:H	4:319:A:PX4:C35	20	9.99	2.22	10.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	20	9.99	2.22	10.86
(3,23)	1:145:A:ASP:H	4:305:A:PX4:C35	20	9.99	2.22	10.86
(3,23)	1:145:A:ASP:H	4:340:A:PX4:C35	20	9.99	2.22	10.86
(3,23)	1:145:A:ASP:H	4:352:A:PX4:C35	20	9.99	2.22	10.86
(3,23)	1:145:A:ASP:H	4:332:A:PX4:C35	20	9.99	2.22	10.86
(3,23)	1:145:A:ASP:H	4:320:A:PX4:C35	20	9.99	2.22	10.86
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	20	9.96	0.36	9.96
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C5	20	9.9	1.0	10.18
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C4	20	9.9	1.0	10.18
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	20	9.9	1.0	10.18
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C5	20	9.9	1.0	10.18
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C4	20	9.9	1.0	10.18
(2,1056)	1:83:A:LYS:H	4:318:A:PX4:C5	20	9.9	1.0	10.18
(2,1056)	1:83:A:LYS:H	4:309:A:PX4:C3	20	9.9	1.0	10.18
(3,22)	1:144:A:GLY:H	4:319:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:341:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:305:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:340:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:352:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:324:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:332:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:310:A:PX4:C35	20	9.25	2.24	9.92
(3,22)	1:144:A:GLY:H	4:320:A:PX4:C35	20	9.25	2.24	9.92
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	20	8.89	1.84	9.4
(3,30)	1:203:A:GLY:H	4:309:A:PX4:C35	20	8.89	1.84	9.4
(3,30)	1:203:A:GLY:H	4:307:A:PX4:C35	20	8.89	1.84	9.4
(3,30)	1:203:A:GLY:H	4:322:A:PX4:C35	20	8.89	1.84	9.4
(3,30)	1:203:A:GLY:H	4:317:A:PX4:C35	20	8.89	1.84	9.4
(3,30)	1:203:A:GLY:H	4:332:A:PX4:C35	20	8.89	1.84	9.4
(3,30)	1:203:A:GLY:H	4:348:A:PX4:C35	20	8.89	1.84	9.4
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C4	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C3	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:317:A:PX4:C3	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C4	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C5	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:341:A:PX4:C3	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:353:A:PX4:C5	20	8.17	2.04	8.66
(3,42)	1:21:A:ARG:H	4:321:A:PX4:C5	20	8.17	2.04	8.66
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C4	20	7.08	1.36	6.98
(3,46)	1:55:A:ASN:H	4:330:A:PX4:C3	20	7.08	1.36	6.98
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	20	7.08	1.36	6.98
(3,46)	1:55:A:ASN:H	4:353:A:PX4:C3	20	7.08	1.36	6.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	20	7.08	1.36	6.98
(3,46)	1:55:A:ASN:H	4:330:A:PX4:C4	20	7.08	1.36	6.98
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C3	20	6.79	1.34	6.94
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	20	6.79	1.34	6.94
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C5	20	6.79	1.34	6.94
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C4	20	6.79	1.34	6.94
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C5	20	6.79	1.34	6.94
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C4	20	6.79	1.34	6.94
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C4	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C4	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:310:A:PX4:C4	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C5	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:317:A:PX4:C5	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C3	20	6.15	1.89	6.72
(3,43)	1:22:A:PHE:H	4:348:A:PX4:C4	20	6.15	1.89	6.72
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	20	5.36	0.72	5.49
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	20	5.24	1.9	5.38
(3,32)	1:233:A:GLY:H	4:307:A:PX4:C35	20	5.24	1.9	5.38
(3,32)	1:233:A:GLY:H	4:322:A:PX4:C35	20	5.24	1.9	5.38
(3,32)	1:233:A:GLY:H	4:309:A:PX4:C35	20	5.24	1.9	5.38
(3,32)	1:233:A:GLY:H	4:332:A:PX4:C35	20	5.24	1.9	5.38
(3,32)	1:233:A:GLY:H	4:345:A:PX4:C35	20	5.24	1.9	5.38
(3,32)	1:233:A:GLY:H	4:429:A:PX4:C35	20	5.24	1.9	5.38
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C3	20	5.11	1.42	5.2
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C3	20	5.11	1.42	5.2
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C5	20	5.11	1.42	5.2
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C4	20	5.11	1.42	5.2
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C5	20	5.11	1.42	5.2
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C4	20	5.11	1.42	5.2
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	20	4.43	0.82	4.48
(2,1064)	1:105:A:VAL:HG21	5:432:A:C3S:H7	20	4.43	0.82	4.48
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	20	4.43	0.82	4.48
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	20	4.31	0.11	4.32
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	20	3.91	0.75	3.97
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	20	3.58	1.02	3.26
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C4	20	3.58	1.02	3.26
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	20	3.58	1.02	3.26
(2,1054)	1:88:A:VAL:H	4:348:A:PX4:C3	20	3.58	1.02	3.26
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	20	3.47	0.81	3.68
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	20	3.4	0.15	3.39
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	20	3.19	0.49	3.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	20	3.01	1.27	3.16
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	20	2.99	1.22	3.44
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	20	2.99	1.2	2.72
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	20	2.6	0.38	2.55
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	20	2.55	1.01	2.68
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	20	2.38	0.19	2.36
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	20	2.32	0.99	2.42
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	20	2.3	0.78	2.24
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	20	2.3	0.78	2.24
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	20	2.2	0.34	2.29
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	20	2.2	0.34	2.29
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	20	2.2	0.23	2.12
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	20	2.2	0.88	2.12
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	20	2.18	0.1	2.2
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	20	2.17	0.95	2.17
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	20	2.16	1.29	1.94
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	20	2.16	0.87	2.32
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	20	1.9	0.9	1.74
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	20	1.9	0.9	1.74
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	20	1.89	0.64	2.03
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	20	1.89	0.64	2.03
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	20	1.85	0.21	1.9
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	20	1.85	0.21	1.9
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	20	1.82	0.75	1.75
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	20	1.82	0.75	1.75
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	20	1.82	0.75	1.75
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	20	1.82	0.87	1.36
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	20	1.74	0.31	1.86
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	20	1.74	0.31	1.86
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	20	1.68	0.78	1.52
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	20	1.68	0.78	1.52
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	20	1.64	0.92	1.48
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	20	1.54	0.18	1.52
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	20	1.35	0.54	1.42
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	20	1.1	0.27	1.1
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	20	1.06	0.41	1.17
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	20	1.03	0.17	1.08
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	20	1.0	0.41	0.98
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	20	0.87	0.47	0.76
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	20	0.78	0.13	0.76
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	20	0.62	0.13	0.64
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	20	0.54	0.13	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	20	0.51	0.12	0.54
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	20	0.44	0.1	0.44
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	20	0.43	0.09	0.44
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	20	0.42	0.14	0.43
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	20	0.42	0.09	0.41
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	20	0.4	0.08	0.38
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	20	0.36	0.08	0.35
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	20	0.35	0.16	0.3
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	20	0.34	0.12	0.32
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	20	0.32	0.1	0.3
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	20	0.31	0.09	0.31
(1,13)	3:304:A:ZN:ZN	1:204:A:HIS:NE2	20	0.31	0.09	0.31
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	20	0.31	0.09	0.31
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	20	0.28	0.06	0.26
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	20	0.28	0.06	0.26
(1,2)	2:301:A:CA:CA	1:133:A:ASP:O	20	0.28	0.06	0.26
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	20	0.27	0.04	0.26
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	20	0.27	0.04	0.26
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	20	0.26	0.04	0.26
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	20	0.26	0.04	0.26
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	20	0.26	0.04	0.26
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	20	0.26	0.04	0.26
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	20	0.25	0.03	0.26
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	20	0.24	0.06	0.24
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	19	4.64	1.72	4.76
(3,24)	1:174:A:GLU:H	4:305:A:PX4:C35	19	4.64	1.72	4.76
(3,24)	1:174:A:GLU:H	4:340:A:PX4:C35	19	4.64	1.72	4.76
(3,24)	1:174:A:GLU:H	4:324:A:PX4:C35	19	4.64	1.72	4.76
(3,24)	1:174:A:GLU:H	4:332:A:PX4:C35	19	4.64	1.72	4.76
(3,24)	1:174:A:GLU:H	4:352:A:PX4:C35	19	4.64	1.72	4.76
(3,29)	1:200:A:LEU:H	4:332:A:PX4:C35	19	3.96	1.53	4.11
(3,29)	1:200:A:LEU:H	4:307:A:PX4:C35	19	3.96	1.53	4.11
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	19	3.96	1.53	4.11
(3,29)	1:200:A:LEU:H	4:338:A:PX4:C35	19	3.96	1.53	4.11
(3,29)	1:200:A:LEU:H	4:309:A:PX4:C35	19	3.96	1.53	4.11
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	19	3.33	1.88	3.62
(3,33)	1:235:A:GLN:H	4:309:A:PX4:C35	19	3.33	1.88	3.62
(3,33)	1:235:A:GLN:H	4:307:A:PX4:C35	19	3.33	1.88	3.62
(3,33)	1:235:A:GLN:H	4:322:A:PX4:C35	19	3.33	1.88	3.62
(3,33)	1:235:A:GLN:H	4:332:A:PX4:C35	19	3.33	1.88	3.62
(3,33)	1:235:A:GLN:H	4:345:A:PX4:C35	19	3.33	1.88	3.62
(3,33)	1:235:A:GLN:H	4:429:A:PX4:C35	19	3.33	1.88	3.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	19	2.27	1.04	2.39
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	19	2.27	1.04	2.39
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	19	2.07	0.95	1.96
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	19	2.07	0.95	1.96
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	19	1.84	1.17	1.54
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	19	1.11	0.72	1.0
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	19	1.11	0.72	1.0
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	19	0.99	0.5	0.88
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	19	0.99	0.5	0.88
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	19	0.88	0.55	0.71
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	19	0.88	0.24	0.9
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	19	0.63	0.29	0.6
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	19	0.61	0.22	0.69
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	19	0.48	0.19	0.48
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	19	0.23	0.08	0.22
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	19	0.23	0.08	0.22
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	18	2.0	0.98	2.52
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	18	2.0	0.98	2.52
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	18	1.83	1.01	1.88
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	18	1.83	1.01	1.88
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	18	1.82	0.92	1.85
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	18	1.82	0.92	1.85
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	18	1.82	0.92	1.85
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	18	1.65	1.12	1.18
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	18	1.55	0.84	1.6
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	18	1.55	0.84	1.6
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	18	1.55	0.84	1.6
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	18	1.31	0.69	1.44
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	18	1.31	0.69	1.44
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	18	1.31	0.69	1.44
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	18	1.31	0.69	1.44
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	18	1.29	0.84	1.23
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	18	1.29	0.84	1.23
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	18	1.06	0.48	0.94
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	18	0.42	0.16	0.4
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	18	0.34	0.12	0.32
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	17	1.47	0.7	1.55
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	17	1.43	0.68	1.72
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	17	1.43	0.68	1.72
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	17	1.43	0.68	1.72
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	17	1.29	0.86	1.28
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	17	1.23	0.73	1.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	17	1.22	0.66	1.2
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	17	1.22	0.66	1.2
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	17	1.2	0.71	1.09
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	17	1.2	0.71	1.09
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	17	1.1	0.86	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	17	1.1	0.86	0.71
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	17	0.99	0.39	1.05
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	17	0.98	0.55	1.04
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	17	0.98	0.55	1.04
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	17	0.59	0.3	0.54
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	17	0.59	0.3	0.54
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	17	0.59	0.3	0.54
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	17	0.49	0.26	0.42
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	17	0.49	0.26	0.42
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	17	0.48	0.25	0.42
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	17	0.4	0.13	0.37
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	17	0.39	0.19	0.35
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	16	4.12	1.26	4.51
(3,28)	1:197:A:GLY:H	4:332:A:PX4:C35	16	4.12	1.26	4.51
(3,28)	1:197:A:GLY:H	4:307:A:PX4:C35	16	4.12	1.26	4.51
(3,28)	1:197:A:GLY:H	4:338:A:PX4:C35	16	4.12	1.26	4.51
(3,28)	1:197:A:GLY:H	4:317:A:PX4:C35	16	4.12	1.26	4.51
(3,28)	1:197:A:GLY:H	4:309:A:PX4:C35	16	4.12	1.26	4.51
(3,27)	1:192:A:ALA:H	4:320:A:PX4:C35	16	3.58	1.51	3.6
(3,27)	1:192:A:ALA:H	4:401:A:PX4:C35	16	3.58	1.51	3.6
(3,27)	1:192:A:ALA:H	4:307:A:PX4:C35	16	3.58	1.51	3.6
(3,27)	1:192:A:ALA:H	4:395:A:PX4:C35	16	3.58	1.51	3.6
(3,27)	1:192:A:ALA:H	4:317:A:PX4:C35	16	3.58	1.51	3.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,27)	1:192:A:ALA:H	4:348:A:PX4:C35	16	3.58	1.51	3.6
(3,27)	1:192:A:ALA:H	4:332:A:PX4:C35	16	3.58	1.51	3.6
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	16	1.84	1.14	1.8
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	16	1.48	0.9	1.53
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	16	1.43	0.97	1.15
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	16	1.23	0.59	1.37
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	16	1.16	0.74	0.97
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	16	1.16	0.74	0.97
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	16	1.16	0.74	0.97
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	16	1.16	0.74	0.97
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	16	1.14	0.75	0.92
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	16	1.14	0.75	0.92
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	16	1.11	0.61	1.25
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	16	0.43	0.26	0.36
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	16	0.42	0.2	0.42
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	16	0.42	0.2	0.42
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	16	0.39	0.13	0.33
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	16	0.33	0.15	0.32
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	15	1.38	1.09	1.11
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	15	0.41	0.22	0.33
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	15	0.4	0.2	0.36
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	15	0.4	0.2	0.36
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	15	0.4	0.2	0.36
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	15	0.34	0.16	0.33
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	15	0.27	0.09	0.25
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	15	0.27	0.11	0.22
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	14	1.5	0.58	1.66
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	14	1.23	0.69	1.14
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	14	1.23	0.69	1.14
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	14	1.23	0.69	1.14
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	14	1.23	0.69	1.14
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	14	0.66	0.28	0.69
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	14	0.61	0.44	0.5
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	14	0.34	0.14	0.32
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	13	1.15	0.7	1.25
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	13	1.15	0.7	1.25
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	13	1.11	0.85	0.94
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	13	1.11	0.85	0.94
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	13	1.09	0.5	0.84
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	13	0.78	0.48	0.69
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	13	0.78	0.48	0.69
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	13	0.68	0.37	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	13	0.68	0.37	0.62
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	13	0.68	0.24	0.72
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	13	0.68	0.24	0.72
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	13	0.3	0.07	0.29
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C3	12	1.94	1.08	1.58
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C4	12	1.94	1.08	1.58
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C5	12	1.94	1.08	1.58
(3,82)	1:147:A:TYR:H	4:340:A:PX4:C3	12	1.94	1.08	1.58
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C4	12	1.94	1.08	1.58
(3,82)	1:147:A:TYR:H	4:340:A:PX4:C4	12	1.94	1.08	1.58
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C3	12	1.94	1.08	1.58
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	12	1.19	0.58	1.29
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	12	1.18	0.73	0.96
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	12	1.15	0.25	1.18
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	12	1.06	0.66	0.86
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	12	0.95	0.34	1.06
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	12	0.92	0.68	0.66
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	12	0.92	0.68	0.66
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	12	0.92	0.68	0.66
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	12	0.87	0.53	0.83
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	12	0.87	0.53	0.83
(2,645)	1:199:A:SER:H	1:202:A:MET:H	12	0.4	0.19	0.36
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	12	0.4	0.2	0.41
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	12	0.4	0.2	0.41
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	12	0.36	0.16	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	12	0.35	0.17	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	12	0.35	0.17	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	12	0.35	0.17	0.36
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	12	0.34	0.22	0.24
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	12	0.27	0.13	0.28
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	12	0.13	0.03	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	12	0.13	0.03	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	12	0.13	0.03	0.12
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	12	0.13	0.03	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	12	0.13	0.03	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	12	0.13	0.03	0.12
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	12	0.13	0.02	0.12
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	12	0.13	0.02	0.12
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	12	0.13	0.02	0.12
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	12	0.13	0.02	0.12
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	12	0.13	0.02	0.12
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	12	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	11	0.63	0.24	0.7
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	11	0.63	0.24	0.7
(2,681)	1:212:A:MET:H	1:227:A:SER:H	11	0.38	0.16	0.39
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	11	0.35	0.14	0.31
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	11	0.35	0.14	0.31
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	11	0.31	0.15	0.3
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	11	0.21	0.09	0.16
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	11	0.21	0.09	0.16
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	10	1.36	0.98	1.02
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	10	0.44	0.2	0.36
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	10	0.44	0.2	0.36
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	10	0.44	0.2	0.36
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	10	0.4	0.23	0.38
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	10	0.4	0.23	0.38
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	10	0.4	0.23	0.38
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	10	0.13	0.02	0.12
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	10	0.13	0.02	0.12
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	10	0.13	0.02	0.12
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	10	0.13	0.02	0.12
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	10	0.13	0.02	0.12
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	10	0.13	0.02	0.12
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	9	1.79	0.8	1.88
(3,84)	1:154:A:ASN:H	4:349:A:PX4:C5	9	1.56	0.66	1.42
(3,84)	1:154:A:ASN:H	4:310:A:PX4:C4	9	1.56	0.66	1.42
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C3	9	1.56	0.66	1.42
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C5	9	1.56	0.66	1.42
(3,84)	1:154:A:ASN:H	4:308:A:PX4:C3	9	1.56	0.66	1.42
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C4	9	1.56	0.66	1.42
(3,84)	1:154:A:ASN:H	4:308:A:PX4:C4	9	1.56	0.66	1.42
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	9	1.19	0.52	1.1
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	9	1.08	0.59	1.03
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	9	1.08	0.59	1.03
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	9	0.91	0.64	0.8
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	9	0.91	0.64	0.8
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	9	0.82	0.69	0.66
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	9	0.82	0.69	0.66
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	9	0.71	0.35	0.65
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	9	0.71	0.35	0.65
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	9	0.61	0.5	0.49
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	9	0.61	0.5	0.49
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	9	0.46	0.18	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	9	0.46	0.18	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	9	0.46	0.18	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	9	0.46	0.18	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	9	0.46	0.18	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	9	0.46	0.18	0.36
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	9	0.36	0.2	0.25
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	9	0.28	0.09	0.31
(3,81)	1:145:A:ASP:H	4:310:A:PX4:C3	8	2.0	0.79	1.9
(3,81)	1:145:A:ASP:H	4:310:A:PX4:C5	8	2.0	0.79	1.9
(3,81)	1:145:A:ASP:H	4:319:A:PX4:C3	8	2.0	0.79	1.9
(3,81)	1:145:A:ASP:H	4:310:A:PX4:C4	8	2.0	0.79	1.9
(3,81)	1:145:A:ASP:H	4:340:A:PX4:C4	8	2.0	0.79	1.9
(3,81)	1:145:A:ASP:H	4:319:A:PX4:C5	8	2.0	0.79	1.9
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C5	8	1.7	0.9	1.74
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C3	8	1.7	0.9	1.74
(3,47)	1:80:A:ASN:H	4:319:A:PX4:C3	8	1.7	0.9	1.74
(3,47)	1:80:A:ASN:H	4:319:A:PX4:C5	8	1.7	0.9	1.74
(3,83)	1:150:A:ASP:H	4:305:A:PX4:C3	8	0.76	0.39	0.62
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C3	8	0.76	0.39	0.62
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C5	8	0.76	0.39	0.62
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C4	8	0.76	0.39	0.62
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	8	0.62	0.4	0.59
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	8	0.62	0.4	0.59
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	8	0.62	0.4	0.59
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	8	0.55	0.37	0.5
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	8	0.55	0.37	0.5
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	8	0.5	0.3	0.45
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	8	0.27	0.05	0.27
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	8	0.27	0.05	0.27
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	8	0.27	0.05	0.27
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	8	0.25	0.13	0.2
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	8	0.23	0.11	0.2
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	7	2.31	0.17	2.39
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	7	2.31	0.17	2.39
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	7	2.31	0.17	2.39
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	7	1.13	0.64	1.26
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	7	0.97	0.76	0.95
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	7	0.62	0.3	0.54
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	7	0.45	0.18	0.5
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	7	0.45	0.18	0.5
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	7	0.45	0.18	0.5
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	7	0.41	0.2	0.36
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	7	0.41	0.2	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	7	0.28	0.12	0.26
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	7	0.28	0.12	0.26
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	7	0.28	0.12	0.26
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	6	1.51	0.94	1.25
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	6	0.86	0.48	0.88
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	6	0.69	0.12	0.65
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	6	0.57	0.1	0.55
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	6	0.55	0.09	0.55
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	6	0.52	0.36	0.36
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	6	0.52	0.36	0.36
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	6	0.5	0.34	0.48
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	6	0.5	0.34	0.48
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	6	0.5	0.16	0.53
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	6	0.5	0.16	0.53
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	6	0.5	0.16	0.53
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	6	0.49	0.22	0.5
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	6	0.32	0.18	0.23
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	6	0.22	0.13	0.18
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	6	0.17	0.05	0.16
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	6	0.15	0.03	0.15
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	6	0.15	0.03	0.15
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	6	0.15	0.03	0.15
(2,1025)	1:58:A:VAL:HG12	1:54:A:LEU:HD21	5	1.22	0.81	1.05
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD22	5	1.11	0.5	1.04
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD23	5	1.11	0.5	1.04
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD22	5	1.06	0.66	0.85
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD23	5	1.06	0.66	0.85
(3,25)	1:180:A:ASP:H	4:320:A:PX4:C35	5	0.92	0.33	0.95
(3,25)	1:180:A:ASP:H	4:414:A:PX4:C35	5	0.92	0.33	0.95
(3,25)	1:180:A:ASP:H	4:324:A:PX4:C35	5	0.92	0.33	0.95
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD22	5	0.78	0.35	0.92
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD23	5	0.78	0.35	0.92
(2,996)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	5	0.74	0.42	0.45
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD22	5	0.63	0.3	0.56
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD23	5	0.63	0.3	0.56
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD22	5	0.51	0.2	0.4
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD23	5	0.51	0.2	0.4
(3,26)	1:181:A:GLY:H	4:414:A:PX4:C35	5	0.35	0.16	0.39
(3,26)	1:181:A:GLY:H	4:308:A:PX4:C35	5	0.35	0.16	0.39
(3,26)	1:181:A:GLY:H	4:320:A:PX4:C35	5	0.35	0.16	0.39
(3,26)	1:181:A:GLY:H	4:324:A:PX4:C35	5	0.35	0.16	0.39
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG13	5	0.26	0.15	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG12	5	0.26	0.15	0.19
(2,815)	1:72:A:VAL:HG11	1:74:A:GLU:H	5	0.22	0.08	0.2
(2,815)	1:72:A:VAL:HG12	1:74:A:GLU:H	5	0.22	0.08	0.2
(2,815)	1:72:A:VAL:HG13	1:74:A:GLU:H	5	0.22	0.08	0.2
(2,279)	1:136:A:ILE:H	1:93:A:ILE:H	5	0.22	0.09	0.19
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG21	5	0.19	0.07	0.21
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG22	5	0.19	0.07	0.21
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG23	5	0.19	0.07	0.21
(2,550)	1:159:A:ALA:H	1:171:A:HIS:H	5	0.15	0.03	0.16
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG13	5	0.13	0.02	0.14
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG13	5	0.13	0.02	0.14
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG13	5	0.13	0.02	0.14
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG12	5	0.13	0.02	0.14
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG12	5	0.13	0.02	0.14
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG12	5	0.13	0.02	0.14
(2,151)	1:55:A:ASN:H	1:58:A:VAL:H	4	0.33	0.17	0.31
(2,171)	1:55:A:ASN:H	1:58:A:VAL:H	4	0.33	0.17	0.31
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD11	4	0.32	0.19	0.24
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD12	4	0.32	0.19	0.24
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD13	4	0.32	0.19	0.24
(2,879)	1:127:A:VAL:HG11	1:91:A:TYR:H	4	0.3	0.12	0.28
(2,879)	1:127:A:VAL:HG12	1:91:A:TYR:H	4	0.3	0.12	0.28
(2,879)	1:127:A:VAL:HG13	1:91:A:TYR:H	4	0.3	0.12	0.28
(2,636)	1:198:A:HIS:H	1:195:A:ALA:H	4	0.22	0.1	0.22
(2,313)	1:105:A:VAL:HG21	1:105:A:VAL:H	4	0.2	0.06	0.21
(2,313)	1:105:A:VAL:HG22	1:105:A:VAL:H	4	0.2	0.06	0.21
(2,313)	1:105:A:VAL:HG23	1:105:A:VAL:H	4	0.2	0.06	0.21
(2,891)	1:105:A:VAL:HG21	1:105:A:VAL:H	4	0.2	0.06	0.21
(2,891)	1:105:A:VAL:HG22	1:105:A:VAL:H	4	0.2	0.06	0.21
(2,891)	1:105:A:VAL:HG23	1:105:A:VAL:H	4	0.2	0.06	0.21
(2,108)	1:43:A:GLN:H	1:46:A:PHE:H	4	0.16	0.05	0.15
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD11	4	0.12	0.02	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD12	4	0.12	0.02	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD13	4	0.12	0.02	0.11
(2,237)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	3	1.0	0.16	0.9
(2,835)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	3	1.0	0.16	0.9
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD22	3	0.96	0.46	0.73
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD23	3	0.96	0.46	0.73
(2,762)	1:19:A:LEU:HD22	1:38:A:LYS:H	3	0.77	0.34	0.62
(2,762)	1:19:A:LEU:HD23	1:38:A:LYS:H	3	0.77	0.34	0.62
(3,8)	1:86:A:SER:H	4:345:A:PX4:C35	3	0.76	0.32	0.71
(3,8)	1:86:A:SER:H	4:332:A:PX4:C35	3	0.76	0.32	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD11	3	0.62	0.28	0.44
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD12	3	0.62	0.28	0.44
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD13	3	0.62	0.28	0.44
(2,70)	1:24:A:LEU:H	1:24:A:LEU:HD21	3	0.54	0.12	0.46
(2,767)	1:24:A:LEU:H	1:24:A:LEU:HD21	3	0.54	0.12	0.46
(2,772)	1:19:A:LEU:HD22	1:22:A:PHE:H	3	0.47	0.22	0.56
(2,772)	1:19:A:LEU:HD23	1:22:A:PHE:H	3	0.47	0.22	0.56
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD11	3	0.45	0.13	0.53
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD12	3	0.45	0.13	0.53
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD13	3	0.45	0.13	0.53
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG21	3	0.43	0.32	0.3
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG22	3	0.43	0.32	0.3
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG23	3	0.43	0.32	0.3
(2,788)	1:58:A:VAL:HG21	1:55:A:ASN:H	3	0.43	0.32	0.3
(2,788)	1:58:A:VAL:HG22	1:55:A:ASN:H	3	0.43	0.32	0.3
(2,788)	1:58:A:VAL:HG23	1:55:A:ASN:H	3	0.43	0.32	0.3
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD11	3	0.42	0.11	0.37
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD12	3	0.42	0.11	0.37
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD13	3	0.42	0.11	0.37
(2,658)	1:200:A:LEU:HD21	1:201:A:GLY:H	3	0.35	0.2	0.32
(2,135)	1:46:A:PHE:H	1:48:A:LEU:H	3	0.3	0.18	0.25
(2,153)	1:55:A:ASN:H	1:55:A:ASN:HD21	3	0.26	0.13	0.25
(2,245)	1:88:A:VAL:H	1:123:A:HIS:H	3	0.26	0.13	0.22
(2,226)	1:75:A:TYR:H	1:73:A:ALA:HA	3	0.24	0.09	0.21
(2,204)	1:66:A:ARG:H	1:67:A:CYS:H	3	0.24	0.02	0.24
(2,542)	1:170:A:ALA:H	1:137:A:GLY:H	3	0.2	0.05	0.23
(2,91)	1:37:A:ALA:H	1:36:A:GLU:H	3	0.17	0.03	0.19
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	3	0.17	0.04	0.14
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	3	0.17	0.04	0.14
(2,103)	1:41:A:GLU:H	1:43:A:GLN:H	3	0.15	0.04	0.13
(2,123)	1:47:A:GLY:H	1:45:A:PHE:H	3	0.14	0.02	0.14
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG13	3	0.13	0.02	0.12
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG13	3	0.13	0.02	0.12
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG13	3	0.13	0.02	0.12
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG12	3	0.13	0.02	0.12
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG12	3	0.13	0.02	0.12
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG12	3	0.13	0.02	0.12
(2,1057)	1:130:A:GLY:H	4:321:A:PX4:C4	2	0.94	0.03	0.94
(3,9)	1:96:A:TYR:H	4:320:A:PX4:C35	2	0.64	0.33	0.64
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD22	2	0.62	0.36	0.62
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD23	2	0.62	0.36	0.62
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD11	2	0.62	0.36	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD12	2	0.62	0.36	0.62
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD13	2	0.62	0.36	0.62
(2,357)	1:113:A:LEU:H	1:196:A:LEU:HD22	2	0.6	0.08	0.6
(2,357)	1:113:A:LEU:H	1:196:A:LEU:HD23	2	0.6	0.08	0.6
(2,913)	1:113:A:LEU:H	1:196:A:LEU:HD22	2	0.6	0.08	0.6
(2,913)	1:113:A:LEU:H	1:196:A:LEU:HD23	2	0.6	0.08	0.6
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG11	2	0.44	0.07	0.44
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG12	2	0.44	0.07	0.44
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG13	2	0.44	0.07	0.44
(2,111)	1:43:A:GLN:H	1:43:A:GLN:HE21	2	0.42	0.21	0.42
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG11	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG12	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG13	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG11	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG12	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG13	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG11	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG12	2	0.34	0.12	0.34
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG13	2	0.34	0.12	0.34
(2,589)	1:179:A:THR:H	1:100:A:LEU:HD22	2	0.32	0.02	0.32
(2,589)	1:179:A:THR:H	1:100:A:LEU:HD23	2	0.32	0.02	0.32
(2,612)	1:108:A:LEU:HD22	1:188:A:PHE:H	2	0.31	0.19	0.31
(2,612)	1:108:A:LEU:HD23	1:188:A:PHE:H	2	0.31	0.19	0.31
(2,133)	1:47:A:GLY:H	1:206:A:SER:HB3	2	0.3	0.12	0.3
(2,133)	1:47:A:GLY:H	1:206:A:SER:HB2	2	0.3	0.12	0.3
(2,639)	1:198:A:HIS:H	1:202:A:MET:H	2	0.21	0.04	0.21
(2,728)	1:236:A:LYS:H	1:237:A:LEU:H	2	0.21	0.06	0.21
(2,728)	1:236:A:LYS:H	1:237:A:LEU:H	2	0.21	0.06	0.21
(2,396)	1:120:A:ILE:H	1:122:A:LEU:H	2	0.21	0.0	0.21
(2,141)	1:50:A:ILE:H	1:50:A:ILE:HG12	2	0.19	0.02	0.19
(2,252)	1:89:A:VAL:H	1:123:A:HIS:H	2	0.18	0.02	0.18
(2,318)	1:104:A:THR:H	1:106:A:ASP:H	2	0.18	0.02	0.18
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD11	2	0.17	0.07	0.17
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD12	2	0.17	0.07	0.17
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD13	2	0.17	0.07	0.17
(2,579)	1:178:A:TRP:HE1	1:175:A:ASP:H	2	0.17	0.01	0.17
(2,117)	1:44:A:LYS:H	1:47:A:GLY:H	2	0.16	0.02	0.16
(2,544)	1:136:A:ILE:H	1:170:A:ALA:H	2	0.16	0.04	0.16
(2,729)	1:237:A:LEU:H	1:239:A:GLY:H	2	0.15	0.02	0.15
(2,740)	1:237:A:LEU:H	1:239:A:GLY:H	2	0.15	0.02	0.15
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG21	2	0.15	0.0	0.15
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG22	2	0.15	0.0	0.15

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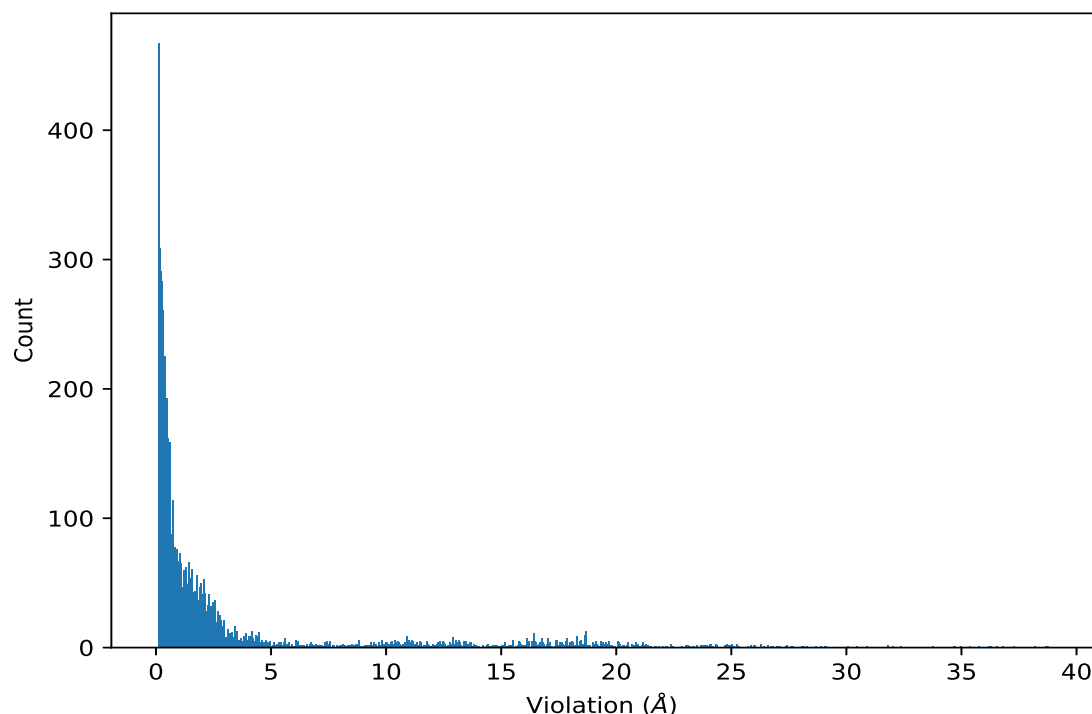
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG23	2	0.15	0.0	0.15
(2,214)	1:72:A:VAL:H	1:71:A:ASP:H	2	0.14	0.03	0.14
(2,706)	1:231:A:ILE:H	1:231:A:ILE:HG13	2	0.13	0.02	0.13
(2,706)	1:231:A:ILE:H	1:231:A:ILE:HG12	2	0.13	0.02	0.13
(2,650)	1:200:A:LEU:HD22	1:199:A:SER:H	2	0.12	0.02	0.12
(2,650)	1:200:A:LEU:HD23	1:199:A:SER:H	2	0.12	0.02	0.12
(2,230)	1:86:A:SER:H	1:85:A:THR:H	2	0.12	0.01	0.12
(2,568)	1:178:A:TRP:HE1	1:176:A:GLU:H	2	0.12	0.0	0.12
(2,580)	1:178:A:TRP:HE1	1:176:A:GLU:H	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	10	38.77
(3,4)	1:33:A:ASN:H	4:309:A:PX4:C35	11	38.69
(3,4)	1:33:A:ASN:H	4:340:A:PX4:C35	5	38.15
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	19	37.25
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	9	36.82
(3,4)	1:33:A:ASN:H	4:352:A:PX4:C35	6	36.54
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	15	36.28
(3,4)	1:33:A:ASN:H	4:320:A:PX4:C35	1	36.22
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	2	36.18
(3,4)	1:33:A:ASN:H	4:352:A:PX4:C35	14	35.76
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	17	35.35
(3,4)	1:33:A:ASN:H	4:320:A:PX4:C35	16	34.96
(3,4)	1:33:A:ASN:H	4:324:A:PX4:C35	7	34.73
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	3	34.66
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	13	33.78
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	18	32.38
(3,4)	1:33:A:ASN:H	4:332:A:PX4:C35	12	32.01
(3,4)	1:33:A:ASN:H	4:320:A:PX4:C35	20	31.81
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	8	31.8
(3,5)	1:51:A:THR:H	4:332:A:PX4:C35	19	30.89
(3,5)	1:51:A:THR:H	4:330:A:PX4:C35	10	30.47
(3,4)	1:33:A:ASN:H	4:348:A:PX4:C35	4	30.06
(3,5)	1:51:A:THR:H	4:322:A:PX4:C35	11	29.14
(3,1)	1:5:A:GLY:H	4:353:A:PX4:C35	19	29.06
(3,5)	1:51:A:THR:H	4:338:A:PX4:C35	1	28.86
(3,1)	1:5:A:GLY:H	4:330:A:PX4:C35	7	28.67
(3,5)	1:51:A:THR:H	4:322:A:PX4:C35	2	28.27
(3,5)	1:51:A:THR:H	4:322:A:PX4:C35	14	28.18
(3,1)	1:5:A:GLY:H	4:308:A:PX4:C35	5	28.06
(3,1)	1:5:A:GLY:H	4:330:A:PX4:C35	15	27.66
(3,1)	1:5:A:GLY:H	4:317:A:PX4:C35	6	27.58
(3,1)	1:5:A:GLY:H	4:317:A:PX4:C35	14	27.42
(3,1)	1:5:A:GLY:H	4:330:A:PX4:C35	16	27.42
(3,5)	1:51:A:THR:H	4:348:A:PX4:C35	17	27.35
(3,5)	1:51:A:THR:H	4:330:A:PX4:C35	5	27.14
(3,5)	1:51:A:THR:H	4:317:A:PX4:C35	7	27.02
(3,5)	1:51:A:THR:H	4:317:A:PX4:C35	20	26.95
(3,5)	1:51:A:THR:H	4:322:A:PX4:C35	6	26.8
(3,5)	1:51:A:THR:H	4:307:A:PX4:C35	16	26.74
(3,1)	1:5:A:GLY:H	4:349:A:PX4:C35	9	26.59
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	18	26.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	1:5:A:GLY:H	4:353:A:PX4:C35	10	26.44
(3,5)	1:51:A:THR:H	4:330:A:PX4:C35	15	26.29
(3,5)	1:51:A:THR:H	4:322:A:PX4:C35	9	26.26
(3,5)	1:51:A:THR:H	4:348:A:PX4:C35	13	26.26
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	5	26.03
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	4	26.01
(3,5)	1:51:A:THR:H	4:332:A:PX4:C35	12	25.98
(3,1)	1:5:A:GLY:H	4:349:A:PX4:C35	3	25.95
(3,1)	1:5:A:GLY:H	4:325:A:PX4:C35	1	25.86
(3,1)	1:5:A:GLY:H	4:349:A:PX4:C35	20	25.86
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	16	25.7
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	6	25.33
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	12	25.28
(3,1)	1:5:A:GLY:H	4:349:A:PX4:C35	13	25.24
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	17	25.24
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	1	25.23
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	6	25.11
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	16	25.03
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	8	25.02
(3,1)	1:5:A:GLY:H	4:353:A:PX4:C35	11	25.0
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	4	24.97
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	2	24.96
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	15	24.94
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	20	24.9
(3,5)	1:51:A:THR:H	4:307:A:PX4:C35	3	24.87
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	8	24.87
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	15	24.84
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	5	24.83
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	3	24.81
(3,1)	1:5:A:GLY:H	4:353:A:PX4:C35	17	24.71
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	13	24.7
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	18	24.38
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	12	24.35
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	13	24.32
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	11	24.31
(3,1)	1:5:A:GLY:H	4:353:A:PX4:C35	2	24.3
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	10	24.21
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	9	24.13
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	2	24.12
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	20	24.11
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	10	24.08
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	14	24.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	7	24.05
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	17	24.03
(3,1)	1:5:A:GLY:H	4:330:A:PX4:C35	12	23.91
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	14	23.9
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	7	23.88
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	3	23.85
(3,5)	1:51:A:THR:H	4:348:A:PX4:C35	8	23.78
(3,5)	1:51:A:THR:H	4:348:A:PX4:C35	18	23.76
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	11	23.68
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	1	23.68
(3,44)	1:34:A:SER:H	4:321:A:PX4:C5	10	23.52
(2,53)	1:22:A:PHE:H	1:183:A:SER:H	19	23.51
(3,1)	1:5:A:GLY:H	4:348:A:PX4:C35	8	23.37
(3,44)	1:34:A:SER:H	4:321:A:PX4:C3	15	23.34
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	10	23.2
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	19	23.13
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	11	23.11
(3,1)	1:5:A:GLY:H	4:348:A:PX4:C35	18	23.08
(2,62)	1:23:A:TYR:H	1:219:A:GLY:H	9	23.04
(3,5)	1:51:A:THR:H	4:348:A:PX4:C35	4	23.03
(3,44)	1:34:A:SER:H	4:321:A:PX4:C4	2	22.89
(3,44)	1:34:A:SER:H	4:317:A:PX4:C3	19	22.47
(3,6)	1:61:A:ILE:H	4:320:A:PX4:C35	19	22.43
(3,1)	1:5:A:GLY:H	4:348:A:PX4:C35	4	22.37
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	16	22.37
(3,44)	1:34:A:SER:H	4:353:A:PX4:C5	11	22.36
(3,44)	1:34:A:SER:H	4:319:A:PX4:C4	1	22.2
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	11	22.16
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	13	22.03
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	5	21.86
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	20	21.7
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	6	21.69
(3,44)	1:34:A:SER:H	4:353:A:PX4:C4	17	21.51
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	15	21.47
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	19	21.41
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	10	21.39
(3,44)	1:34:A:SER:H	4:317:A:PX4:C3	16	21.36
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	8	21.29
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	17	21.28
(3,44)	1:34:A:SER:H	4:321:A:PX4:C5	12	21.27
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	2	21.22
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	3	21.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	11	21.19
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	14	21.19
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	17	21.17
(3,2)	1:21:A:ARG:H	4:340:A:PX4:C35	5	21.16
(3,44)	1:34:A:SER:H	4:310:A:PX4:C4	5	21.13
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	2	21.1
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	19	21.08
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	1	20.95
(3,44)	1:34:A:SER:H	4:321:A:PX4:C5	20	20.94
(3,44)	1:34:A:SER:H	4:317:A:PX4:C4	3	20.93
(3,2)	1:21:A:ARG:H	4:324:A:PX4:C35	7	20.9
(3,44)	1:34:A:SER:H	4:317:A:PX4:C5	9	20.89
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	4	20.89
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	18	20.89
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	10	20.85
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	9	20.79
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	13	20.75
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	12	20.74
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	8	20.67
(2,52)	1:21:A:ARG:H	1:185:A:GLY:H	7	20.67
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	9	20.66
(3,44)	1:34:A:SER:H	4:319:A:PX4:C5	13	20.53
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	1	20.53
(3,6)	1:61:A:ILE:H	4:330:A:PX4:C35	15	20.51
(3,6)	1:61:A:ILE:H	4:317:A:PX4:C35	7	20.5
(3,6)	1:61:A:ILE:H	4:353:A:PX4:C35	10	20.49
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	18	20.48
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	7	20.41
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	16	20.31
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	17	20.3
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	5	20.27
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	7	20.25
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	4	20.2
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	10	20.19
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	15	20.17
(3,6)	1:61:A:ILE:H	4:308:A:PX4:C35	5	20.15
(3,3)	1:22:A:PHE:H	4:340:A:PX4:C35	5	20.14
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	4	20.14
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	14	20.12
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	6	20.1
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	3	20.08
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	8	20.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	4	20.07
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	6	20.07
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	17	20.07
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	12	19.94
(3,44)	1:34:A:SER:H	4:319:A:PX4:C4	7	19.85
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	1	19.83
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	16	19.8
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	16	19.79
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	19	19.76
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	13	19.74
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	3	19.72
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	20	19.67
(3,44)	1:34:A:SER:H	4:317:A:PX4:C3	8	19.66
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	6	19.66
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	3	19.66
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	9	19.65
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	5	19.64
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	15	19.6
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	18	19.6
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	19	19.57
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	16	19.56
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	16	19.56
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	16	19.56
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	2	19.52
(3,2)	1:21:A:ARG:H	4:352:A:PX4:C35	6	19.52
(3,44)	1:34:A:SER:H	4:317:A:PX4:C5	18	19.51
(3,6)	1:61:A:ILE:H	4:307:A:PX4:C35	3	19.46
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	1	19.43
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	1	19.43
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	1	19.43
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	7	19.4
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	9	19.39
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	17	19.38
(3,44)	1:34:A:SER:H	4:317:A:PX4:C3	4	19.37
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	3	19.34
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	20	19.34
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	20	19.34
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	20	19.34
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	15	19.31
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	9	19.26
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	8	19.22
(3,3)	1:22:A:PHE:H	4:352:A:PX4:C35	6	19.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	20	19.19
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	16	19.17
(3,2)	1:21:A:ARG:H	4:352:A:PX4:C35	14	19.16
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	18	19.13
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	12	19.11
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	3	19.1
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	3	19.1
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	3	19.1
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	4	19.08
(3,3)	1:22:A:PHE:H	4:320:A:PX4:C35	1	19.02
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	8	19.01
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	1	19.0
(3,6)	1:61:A:ILE:H	4:349:A:PX4:C35	1	18.99
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	7	18.98
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	9	18.96
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	6	18.95
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	20	18.87
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	14	18.85
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	13	18.78
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	1	18.77
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	18	18.71
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H7	2	18.68
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	13	18.67
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	13	18.66
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	14	18.66
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	14	18.66
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	14	18.66
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	16	18.65
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	5	18.65
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	5	18.65
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	5	18.65
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	8	18.65
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	8	18.65
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	8	18.65
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	14	18.64
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	13	18.63
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	4	18.63
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	4	18.63
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	4	18.63
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	7	18.63
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	14	18.61
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	12	18.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	12	18.6
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	12	18.6
(3,3)	1:22:A:PHE:H	4:352:A:PX4:C35	14	18.57
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	17	18.57
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	1	18.55
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	15	18.53
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	2	18.51
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	8	18.51
(3,6)	1:61:A:ILE:H	4:320:A:PX4:C35	16	18.49
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	5	18.47
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	10	18.45
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	17	18.45
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	17	18.45
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	17	18.45
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	3	18.44
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	12	18.41
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	7	18.4
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	7	18.4
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	7	18.4
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	1	18.38
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	4	18.34
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	16	18.31
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	7	18.28
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	7	18.26
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	8	18.26
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	18	18.26
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	18	18.26
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	18	18.26
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	11	18.25
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	11	18.25
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	11	18.25
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	19	18.22
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	16	18.21
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	19	18.17
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	14	18.15
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	10	18.14
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	19	18.13
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	15	18.13
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	13	18.11
(2,1067)	1:90:A:THR:H	5:432:A:C3S:H13	11	18.08
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	2	18.08
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	2	18.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	2	18.08
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	18	18.06
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	14	18.01
(2,60)	1:22:A:PHE:H	1:217:A:GLY:H	11	18.01
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	15	17.98
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	15	17.98
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	15	17.98
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	17	17.98
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	20	17.94
(3,6)	1:61:A:ILE:H	4:317:A:PX4:C35	6	17.91
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	12	17.88
(3,6)	1:61:A:ILE:H	4:353:A:PX4:C35	11	17.87
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	3	17.85
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	6	17.85
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	6	17.85
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	6	17.85
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	6	17.85
(3,6)	1:61:A:ILE:H	4:325:A:PX4:C35	9	17.83
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	10	17.82
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	4	17.81
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	17	17.8
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	11	17.8
(3,3)	1:22:A:PHE:H	4:320:A:PX4:C35	16	17.77
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	19	17.76
(3,6)	1:61:A:ILE:H	4:317:A:PX4:C35	14	17.74
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	3	17.72
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	19	17.66
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	19	17.66
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	19	17.66
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	3	17.63
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	8	17.63
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	5	17.61
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	6	17.61
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	13	17.58
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	13	17.58
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	13	17.58
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	19	17.58
(3,6)	1:61:A:ILE:H	4:330:A:PX4:C35	12	17.52
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	18	17.51
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	17	17.49
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	5	17.49
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	14	17.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	14	17.44
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	14	17.44
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	9	17.4
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	9	17.4
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	9	17.4
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	9	17.39
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	9	17.39
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	18	17.38
(2,297)	1:105:A:VAL:HG21	1:237:A:LEU:H	10	17.36
(2,297)	1:105:A:VAL:HG22	1:237:A:LEU:H	10	17.36
(2,297)	1:105:A:VAL:HG23	1:237:A:LEU:H	10	17.36
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	12	17.34
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	10	17.22
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	18	17.18
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	15	17.1
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	2	17.1
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	2	17.1
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	2	17.1
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	5	17.07
(3,6)	1:61:A:ILE:H	4:320:A:PX4:C35	20	17.06
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	11	17.05
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	6	17.04
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	6	17.04
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	6	17.04
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H7	2	17.02
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	10	17.01
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	10	17.01
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	10	17.01
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	9	16.99
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	9	16.99
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	9	16.99
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	20	16.94
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	9	16.89
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	8	16.88
(3,6)	1:61:A:ILE:H	4:353:A:PX4:C35	2	16.85
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	3	16.83
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	3	16.83
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	3	16.83
(3,44)	1:34:A:SER:H	4:319:A:PX4:C5	14	16.82
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	2	16.78
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	18	16.76
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	18	16.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	18	16.76
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	7	16.75
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	7	16.75
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	7	16.75
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	1	16.73
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	17	16.73
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	2	16.7
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	20	16.69
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	6	16.68
(3,6)	1:61:A:ILE:H	4:317:A:PX4:C35	13	16.66
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	18	16.65
(3,6)	1:61:A:ILE:H	4:348:A:PX4:C35	17	16.64
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	10	16.63
(3,44)	1:34:A:SER:H	4:319:A:PX4:C5	6	16.6
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	12	16.58
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	19	16.55
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	15	16.53
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	15	16.53
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	15	16.53
(2,1068)	1:133:A:ASP:H	5:432:A:C3S:H13	11	16.52
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	10	16.49
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	20	16.49
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	20	16.49
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	20	16.49
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	8	16.45
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	1	16.43
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	1	16.43
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	1	16.43
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	4	16.43
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	4	16.43
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	4	16.43
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	2	16.42
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	13	16.4
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	13	16.4
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	13	16.4
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	3	16.4
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	13	16.33
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	12	16.32
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	12	16.32
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	12	16.32
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	11	16.3
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	13	16.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	16	16.21
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	16	16.21
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	16	16.21
(2,1069)	1:134:A:ILE:H	5:432:A:C3S:H7	11	16.2
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	4	16.18
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	16	16.16
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	19	16.14
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	19	16.14
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	19	16.14
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	17	16.13
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	17	16.13
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	17	16.13
(2,75)	1:25:A:TYR:H	1:11:A:GLN:HE21	15	16.11
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	14	16.09
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	5	16.08
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	12	16.03
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	6	15.99
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	2	15.97
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	1	15.92
(2,750)	1:10:A:LEU:H	1:25:A:TYR:H	15	15.91
(3,2)	1:21:A:ARG:H	4:348:A:PX4:C35	4	15.89
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	12	15.88
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	9	15.85
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	11	15.83
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	11	15.83
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	11	15.83
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	19	15.82
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	20	15.79
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	8	15.77
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	8	15.77
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	8	15.77
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	13	15.76
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	10	15.74
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	14	15.73
(3,2)	1:21:A:ARG:H	4:332:A:PX4:C35	12	15.66
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	7	15.6
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD11	5	15.53
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD12	5	15.53
(2,296)	1:100:A:LEU:H	1:120:A:ILE:HD13	5	15.53
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	16	15.52
(3,2)	1:21:A:ARG:H	4:320:A:PX4:C35	20	15.51
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	4	15.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	14	15.46
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	17	15.45
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	15	15.43
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	6	15.41
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	20	15.38
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	7	15.36
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	10	15.33
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	13	15.31
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	19	15.29
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	16	15.2
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	18	15.18
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	1	15.16
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	8	15.16
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	3	15.15
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	4	15.13
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C3	2	15.12
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	15	15.08
(3,3)	1:22:A:PHE:H	4:348:A:PX4:C35	4	15.02
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	11	15.01
(2,73)	1:11:A:GLN:H	1:24:A:LEU:H	9	14.99
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	5	14.91
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	11	14.87
(3,31)	1:216:A:TYR:H	4:308:A:PX4:C35	1	14.84
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	17	14.8
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	7	14.79
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	3	14.76
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	1	14.72
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	20	14.7
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	5	14.67
(3,45)	1:51:A:THR:H	4:307:A:PX4:C4	10	14.65
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	8	14.63
(3,40)	1:13:A:GLU:H	4:310:A:PX4:C4	2	14.6
(2,65)	1:23:A:TYR:H	1:205:A:SER:H	2	14.55
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	10	14.51
(3,45)	1:51:A:THR:H	4:317:A:PX4:C4	15	14.46
(3,31)	1:216:A:TYR:H	4:353:A:PX4:C35	11	14.44
(3,45)	1:51:A:THR:H	4:330:A:PX4:C5	5	14.43
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	19	14.41
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	2	14.38
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	9	14.36
(3,22)	1:144:A:GLY:H	4:332:A:PX4:C35	10	14.3
(3,3)	1:22:A:PHE:H	4:320:A:PX4:C35	20	14.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:61:A:ILE:H	4:348:A:PX4:C35	18	14.21
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	15	14.03
(3,3)	1:22:A:PHE:H	4:332:A:PX4:C35	12	13.98
(3,6)	1:61:A:ILE:H	4:348:A:PX4:C35	8	13.92
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C4	12	13.9
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C5	20	13.88
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	12	13.88
(2,77)	1:11:A:GLN:H	1:26:A:ASP:H	18	13.84
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	8	13.83
(3,7)	1:69:A:VAL:H	4:320:A:PX4:C35	11	13.82
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	16	13.79
(3,37)	1:7:A:MET:H	4:353:A:PX4:C3	10	13.69
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	12	13.69
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	4	13.68
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C4	12	13.67
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	19	13.63
(3,39)	1:12:A:TRP:H	4:308:A:PX4:C3	10	13.62
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	4	13.62
(3,37)	1:7:A:MET:H	4:317:A:PX4:C5	20	13.6
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	3	13.56
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	4	13.55
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	14	13.55
(3,45)	1:51:A:THR:H	4:317:A:PX4:C5	17	13.53
(3,23)	1:145:A:ASP:H	4:332:A:PX4:C35	10	13.48
(3,40)	1:13:A:GLU:H	4:308:A:PX4:C3	10	13.47
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C5	20	13.47
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	5	13.47
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	13	13.45
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	9	13.44
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	17	13.43
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	6	13.43
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	6	13.41
(3,31)	1:216:A:TYR:H	4:320:A:PX4:C35	20	13.4
(3,41)	1:16:A:GLN:H	4:310:A:PX4:C3	2	13.39
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	20	13.39
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	7	13.37
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	18	13.36
(3,45)	1:51:A:THR:H	4:317:A:PX4:C4	11	13.35
(3,45)	1:51:A:THR:H	4:330:A:PX4:C3	2	13.31
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	10	13.29
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C4	1	13.26
(3,31)	1:216:A:TYR:H	4:353:A:PX4:C35	2	13.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C3	10	13.23
(3,40)	1:13:A:GLU:H	4:305:A:PX4:C3	6	13.22
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	8	13.22
(3,37)	1:7:A:MET:H	4:317:A:PX4:C4	7	13.19
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	10	13.19
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	2	13.19
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	15	13.19
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	6	13.18
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	11	13.17
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C5	16	13.12
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	10	13.12
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C4	1	13.09
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	13	13.07
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	8	13.05
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	18	13.05
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	7	13.04
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	1	13.04
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C4	7	13.03
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	14	13.02
(3,45)	1:51:A:THR:H	4:307:A:PX4:C3	16	13.01
(3,45)	1:51:A:THR:H	4:317:A:PX4:C5	14	13.0
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	14	12.99
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C4	3	12.97
(3,6)	1:61:A:ILE:H	4:348:A:PX4:C35	4	12.95
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	15	12.93
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	12	12.93
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C4	7	12.92
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	5	12.92
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	7	12.92
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	13	12.91
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	19	12.91
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	20	12.91
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C5	9	12.89
(3,23)	1:145:A:ASP:H	4:305:A:PX4:C35	18	12.86
(3,45)	1:51:A:THR:H	4:317:A:PX4:C3	19	12.83
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	3	12.82
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	7	12.82
(3,38)	1:8:A:SER:H	4:317:A:PX4:C5	20	12.78
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	2	12.78
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	9	12.77
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	1	12.77
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	12	12.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,751)	1:11:A:GLN:H	1:22:A:PHE:H	16	12.7
(3,45)	1:51:A:THR:H	4:317:A:PX4:C3	6	12.69
(3,39)	1:12:A:TRP:H	4:349:A:PX4:C4	3	12.68
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C3	20	12.6
(3,41)	1:16:A:GLN:H	4:310:A:PX4:C4	15	12.58
(3,41)	1:16:A:GLN:H	4:308:A:PX4:C3	10	12.55
(3,31)	1:216:A:TYR:H	4:307:A:PX4:C35	3	12.55
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	16	12.54
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C3	13	12.53
(3,38)	1:8:A:SER:H	4:317:A:PX4:C3	2	12.5
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	15	12.5
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C3	19	12.46
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C5	9	12.45
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	8	12.45
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	19	12.45
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	11	12.45
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	5	12.44
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C5	19	12.41
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	2	12.4
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C3	16	12.39
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C3	13	12.37
(3,38)	1:8:A:SER:H	4:317:A:PX4:C3	12	12.36
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C3	4	12.33
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	3	12.32
(3,38)	1:8:A:SER:H	4:317:A:PX4:C4	7	12.31
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	7	12.31
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	2	12.31
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C3	1	12.29
(3,45)	1:51:A:THR:H	4:317:A:PX4:C4	1	12.28
(3,23)	1:145:A:ASP:H	4:319:A:PX4:C35	11	12.28
(2,67)	1:24:A:LEU:H	1:204:A:HIS:HE1	17	12.25
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	9	12.24
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C5	6	12.23
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C5	15	12.22
(3,7)	1:69:A:VAL:H	4:395:A:PX4:C35	5	12.18
(3,37)	1:7:A:MET:H	4:353:A:PX4:C3	1	12.15
(3,38)	1:8:A:SER:H	4:317:A:PX4:C4	1	12.06
(3,37)	1:7:A:MET:H	4:317:A:PX4:C5	9	12.05
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C4	7	12.03
(3,30)	1:203:A:GLY:H	4:332:A:PX4:C35	19	12.02
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	16	12.0
(3,31)	1:216:A:TYR:H	4:317:A:PX4:C35	9	11.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C3	8	11.93
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	12	11.88
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C5	20	11.85
(3,38)	1:8:A:SER:H	4:317:A:PX4:C5	9	11.82
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C4	12	11.81
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C5	18	11.81
(3,40)	1:13:A:GLU:H	4:317:A:PX4:C5	18	11.79
(3,37)	1:7:A:MET:H	4:349:A:PX4:C3	14	11.78
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	2	11.76
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C4	1	11.75
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C5	15	11.75
(3,23)	1:145:A:ASP:H	4:305:A:PX4:C35	4	11.71
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C5	19	11.67
(3,31)	1:216:A:TYR:H	4:317:A:PX4:C35	6	11.67
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C5	14	11.63
(2,1056)	1:83:A:LYS:H	4:318:A:PX4:C5	14	11.63
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	16	11.59
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	15	11.54
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	17	11.54
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C5	15	11.51
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	2	11.5
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C3	8	11.49
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C5	9	11.48
(3,22)	1:144:A:GLY:H	4:305:A:PX4:C35	8	11.48
(3,40)	1:13:A:GLU:H	4:349:A:PX4:C3	14	11.47
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	19	11.45
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C5	11	11.42
(3,23)	1:145:A:ASP:H	4:332:A:PX4:C35	19	11.42
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	9	11.35
(3,23)	1:145:A:ASP:H	4:319:A:PX4:C35	3	11.34
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C3	16	11.33
(3,39)	1:12:A:TRP:H	4:317:A:PX4:C3	4	11.3
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	16	11.3
(3,39)	1:12:A:TRP:H	4:349:A:PX4:C3	14	11.29
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	19	11.29
(3,45)	1:51:A:THR:H	4:317:A:PX4:C4	3	11.28
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C5	11	11.17
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	11	11.17
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	11	11.16
(3,7)	1:69:A:VAL:H	4:317:A:PX4:C35	6	11.15
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	18	11.15
(3,41)	1:16:A:GLN:H	4:353:A:PX4:C5	11	11.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,23)	1:145:A:ASP:H	4:352:A:PX4:C35	17	11.13
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	9	11.12
(3,45)	1:51:A:THR:H	4:317:A:PX4:C4	7	11.11
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C3	13	11.11
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	3	11.11
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	10	11.09
(3,42)	1:21:A:ARG:H	4:321:A:PX4:C5	19	11.06
(3,45)	1:51:A:THR:H	4:317:A:PX4:C5	18	11.04
(3,31)	1:216:A:TYR:H	4:317:A:PX4:C35	14	11.04
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	5	11.04
(3,38)	1:8:A:SER:H	4:353:A:PX4:C3	10	11.02
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C4	3	10.98
(3,22)	1:144:A:GLY:H	4:319:A:PX4:C35	3	10.98
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	19	10.98
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	15	10.96
(3,22)	1:144:A:GLY:H	4:319:A:PX4:C35	11	10.96
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	1	10.95
(3,22)	1:144:A:GLY:H	4:305:A:PX4:C35	4	10.94
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	1	10.94
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	20	10.94
(3,42)	1:21:A:ARG:H	4:353:A:PX4:C5	11	10.93
(3,31)	1:216:A:TYR:H	4:348:A:PX4:C35	17	10.93
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	5	10.92
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	14	10.91
(3,38)	1:8:A:SER:H	4:349:A:PX4:C5	16	10.9
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	3	10.9
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C5	11	10.87
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	2	10.83
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C5	9	10.82
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	13	10.82
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C4	7	10.81
(3,22)	1:144:A:GLY:H	4:352:A:PX4:C35	17	10.77
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	6	10.76
(3,23)	1:145:A:ASP:H	4:319:A:PX4:C35	7	10.76
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	12	10.74
(3,22)	1:144:A:GLY:H	4:305:A:PX4:C35	18	10.7
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	15	10.7
(3,30)	1:203:A:GLY:H	4:307:A:PX4:C35	14	10.69
(3,45)	1:51:A:THR:H	4:317:A:PX4:C3	13	10.67
(3,38)	1:8:A:SER:H	4:349:A:PX4:C4	3	10.64
(3,7)	1:69:A:VAL:H	4:320:A:PX4:C35	1	10.64
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C3	5	10.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	1:51:A:THR:H	4:307:A:PX4:C4	12	10.59
(3,31)	1:216:A:TYR:H	4:330:A:PX4:C35	12	10.58
(3,30)	1:203:A:GLY:H	4:322:A:PX4:C35	9	10.57
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	16	10.55
(3,22)	1:144:A:GLY:H	4:332:A:PX4:C35	19	10.53
(3,45)	1:51:A:THR:H	4:317:A:PX4:C5	9	10.52
(3,30)	1:203:A:GLY:H	4:322:A:PX4:C35	6	10.52
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C4	2	10.52
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	12	10.52
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C5	18	10.46
(3,30)	1:203:A:GLY:H	4:307:A:PX4:C35	10	10.45
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C5	7	10.44
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	9	10.41
(3,41)	1:16:A:GLN:H	4:319:A:PX4:C5	6	10.4
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C5	12	10.4
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	1	10.39
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	8	10.37
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	7	10.37
(3,45)	1:51:A:THR:H	4:317:A:PX4:C3	8	10.36
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	13	10.36
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	14	10.35
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	17	10.33
(3,37)	1:7:A:MET:H	4:317:A:PX4:C5	18	10.32
(3,41)	1:16:A:GLN:H	4:310:A:PX4:C4	5	10.31
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C4	6	10.29
(2,78)	1:14:A:GLN:H	1:25:A:TYR:H	15	10.29
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C3	4	10.28
(3,41)	1:16:A:GLN:H	4:353:A:PX4:C5	17	10.26
(3,22)	1:144:A:GLY:H	4:341:A:PX4:C35	2	10.26
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C4	17	10.23
(3,30)	1:203:A:GLY:H	4:309:A:PX4:C35	2	10.23
(3,37)	1:7:A:MET:H	4:353:A:PX4:C3	5	10.22
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	6	10.21
(3,41)	1:16:A:GLN:H	4:319:A:PX4:C5	14	10.17
(3,41)	1:16:A:GLN:H	4:317:A:PX4:C3	8	10.12
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C3	5	10.11
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C3	5	10.1
(3,30)	1:203:A:GLY:H	4:317:A:PX4:C35	7	10.08
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C4	17	10.06
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	8	10.04
(3,46)	1:55:A:ASN:H	4:330:A:PX4:C4	10	10.03
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C5	3	10.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C5	6	10.01
(3,22)	1:144:A:GLY:H	4:324:A:PX4:C35	7	9.99
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	11	9.99
(3,45)	1:51:A:THR:H	4:317:A:PX4:C3	4	9.98
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	17	9.98
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	4	9.94
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	13	9.93
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	20	9.92
(3,38)	1:8:A:SER:H	4:353:A:PX4:C5	6	9.86
(3,22)	1:144:A:GLY:H	4:310:A:PX4:C35	15	9.85
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	16	9.84
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C4	16	9.83
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C4	15	9.82
(3,38)	1:8:A:SER:H	4:349:A:PX4:C3	13	9.82
(3,30)	1:203:A:GLY:H	4:309:A:PX4:C35	11	9.81
(3,31)	1:216:A:TYR:H	4:317:A:PX4:C35	13	9.8
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	15	9.79
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	5	9.72
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	2	9.7
(3,38)	1:8:A:SER:H	4:317:A:PX4:C5	18	9.67
(3,45)	1:51:A:THR:H	4:307:A:PX4:C3	20	9.65
(3,38)	1:8:A:SER:H	4:349:A:PX4:C3	14	9.65
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C5	1	9.65
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	15	9.61
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	3	9.59
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	10	9.55
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	18	9.55
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C5	20	9.54
(3,40)	1:13:A:GLU:H	4:353:A:PX4:C5	17	9.48
(3,7)	1:69:A:VAL:H	4:320:A:PX4:C35	16	9.48
(2,1056)	1:83:A:LYS:H	4:321:A:PX4:C3	13	9.47
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	16	9.46
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	3	9.42
(2,1056)	1:83:A:LYS:H	4:309:A:PX4:C3	18	9.42
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C4	10	9.34
(3,38)	1:8:A:SER:H	4:317:A:PX4:C3	8	9.33
(3,30)	1:203:A:GLY:H	4:348:A:PX4:C35	20	9.33
(3,23)	1:145:A:ASP:H	4:332:A:PX4:C35	12	9.33
(3,38)	1:8:A:SER:H	4:317:A:PX4:C3	4	9.29
(3,39)	1:12:A:TRP:H	4:353:A:PX4:C5	17	9.28
(3,37)	1:7:A:MET:H	4:317:A:PX4:C3	4	9.21
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C5	18	9.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	19	9.18
(2,551)	1:159:A:ALA:H	1:92:A:ARG:H	19	9.18
(3,36)	1:5:A:GLY:H	4:353:A:PX4:C4	17	9.12
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C3	10	9.12
(3,37)	1:7:A:MET:H	4:353:A:PX4:C5	17	9.09
(3,42)	1:21:A:ARG:H	4:317:A:PX4:C3	8	9.08
(3,43)	1:22:A:PHE:H	4:348:A:PX4:C4	17	9.01
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C4	1	8.96
(3,42)	1:21:A:ARG:H	4:317:A:PX4:C3	4	8.93
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C5	4	8.84
(3,23)	1:145:A:ASP:H	4:320:A:PX4:C35	16	8.83
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C3	2	8.82
(3,23)	1:145:A:ASP:H	4:319:A:PX4:C35	1	8.82
(3,38)	1:8:A:SER:H	4:353:A:PX4:C5	19	8.81
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C4	18	8.8
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	8	8.79
(3,22)	1:144:A:GLY:H	4:320:A:PX4:C35	16	8.79
(3,22)	1:144:A:GLY:H	4:332:A:PX4:C35	12	8.76
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C5	20	8.72
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	18	8.71
(3,38)	1:8:A:SER:H	4:353:A:PX4:C5	15	8.69
(3,23)	1:145:A:ASP:H	4:340:A:PX4:C35	5	8.67
(3,38)	1:8:A:SER:H	4:353:A:PX4:C5	11	8.66
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C5	10	8.64
(3,31)	1:216:A:TYR:H	4:348:A:PX4:C35	8	8.61
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C4	15	8.53
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C5	11	8.52
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C4	8	8.51
(3,36)	1:5:A:GLY:H	4:317:A:PX4:C3	4	8.43
(3,42)	1:21:A:ARG:H	4:321:A:PX4:C5	20	8.41
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C4	3	8.36
(3,46)	1:55:A:ASN:H	4:353:A:PX4:C3	5	8.34
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C3	1	8.3
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C3	11	8.27
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	12	8.24
(3,42)	1:21:A:ARG:H	4:341:A:PX4:C3	9	8.24
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	5	8.17
(3,22)	1:144:A:GLY:H	4:319:A:PX4:C35	1	8.14
(3,32)	1:233:A:GLY:H	4:332:A:PX4:C35	12	8.11
(3,22)	1:144:A:GLY:H	4:340:A:PX4:C35	5	8.11
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	19	8.09
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	15	8.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	6	8.04
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	2	7.99
(3,30)	1:203:A:GLY:H	4:348:A:PX4:C35	13	7.96
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C4	7	7.94
(2,1056)	1:83:A:LYS:H	4:349:A:PX4:C4	19	7.88
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	13	7.86
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	14	7.72
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	11	7.7
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C4	7	7.67
(3,24)	1:174:A:GLU:H	4:324:A:PX4:C35	10	7.65
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	17	7.59
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	16	7.58
(3,31)	1:216:A:TYR:H	4:348:A:PX4:C35	18	7.57
(3,7)	1:69:A:VAL:H	4:332:A:PX4:C35	12	7.57
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C5	15	7.55
(3,38)	1:8:A:SER:H	4:353:A:PX4:C3	5	7.54
(3,42)	1:21:A:ARG:H	4:321:A:PX4:C5	12	7.53
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C4	16	7.5
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	12	7.44
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	10	7.43
(3,31)	1:216:A:TYR:H	4:348:A:PX4:C35	4	7.42
(3,30)	1:203:A:GLY:H	4:332:A:PX4:C35	12	7.41
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	11	7.4
(3,23)	1:145:A:ASP:H	4:352:A:PX4:C35	6	7.34
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	8	7.34
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C5	14	7.33
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	13	7.32
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C4	2	7.25
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C3	20	7.24
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	16	7.23
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C3	10	7.19
(3,32)	1:233:A:GLY:H	4:309:A:PX4:C35	11	7.15
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	1	7.14
(3,46)	1:55:A:ASN:H	4:330:A:PX4:C3	2	7.11
(3,24)	1:174:A:GLU:H	4:324:A:PX4:C35	17	7.05
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C5	9	7.04
(3,30)	1:203:A:GLY:H	4:307:A:PX4:C35	3	7.04
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	20	6.99
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	17	6.98
(3,43)	1:22:A:PHE:H	4:317:A:PX4:C5	18	6.95
(3,7)	1:69:A:VAL:H	4:320:A:PX4:C35	20	6.93
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C4	8	6.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	19	6.88
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C5	11	6.84
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	19	6.84
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C3	15	6.78
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	9	6.78
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	1	6.75
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C4	7	6.74
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C5	7	6.74
(3,42)	1:21:A:ARG:H	4:310:A:PX4:C4	5	6.72
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	4	6.7
(3,23)	1:145:A:ASP:H	4:341:A:PX4:C35	14	6.68
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	6	6.67
(3,43)	1:22:A:PHE:H	4:317:A:PX4:C5	9	6.66
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C5	3	6.61
(3,32)	1:233:A:GLY:H	4:307:A:PX4:C35	7	6.57
(3,38)	1:8:A:SER:H	4:353:A:PX4:C5	17	6.56
(3,32)	1:233:A:GLY:H	4:307:A:PX4:C35	10	6.55
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	19	6.51
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	8	6.45
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C5	6	6.41
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	1	6.4
(3,22)	1:144:A:GLY:H	4:341:A:PX4:C35	13	6.37
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C4	1	6.3
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C5	13	6.3
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C4	3	6.27
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	12	6.27
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C4	3	6.22
(3,27)	1:192:A:ALA:H	4:348:A:PX4:C35	10	6.19
(3,22)	1:144:A:GLY:H	4:352:A:PX4:C35	6	6.19
(3,32)	1:233:A:GLY:H	4:345:A:PX4:C35	14	6.17
(3,23)	1:145:A:ASP:H	4:320:A:PX4:C35	20	6.16
(3,30)	1:203:A:GLY:H	4:348:A:PX4:C35	18	6.15
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C3	12	6.14
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	1	6.14
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	9	6.13
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	13	6.11
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	7	6.11
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C3	1	6.09
(3,32)	1:233:A:GLY:H	4:429:A:PX4:C35	20	6.09
(3,22)	1:144:A:GLY:H	4:341:A:PX4:C35	14	6.09
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C5	14	6.08
(3,43)	1:22:A:PHE:H	4:310:A:PX4:C4	5	6.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C3	2	6.07
(3,22)	1:144:A:GLY:H	4:341:A:PX4:C35	9	6.01
(3,7)	1:69:A:VAL:H	4:348:A:PX4:C35	4	5.98
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	2	5.92
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C3	5	5.91
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	6	5.9
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	13	5.86
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	3	5.8
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	19	5.79
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	14	5.78
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	8	5.76
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	4	5.75
(3,22)	1:144:A:GLY:H	4:320:A:PX4:C35	20	5.74
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	9	5.73
(3,29)	1:200:A:LEU:H	4:307:A:PX4:C35	14	5.66
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C5	9	5.65
(3,32)	1:233:A:GLY:H	4:322:A:PX4:C35	6	5.65
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	13	5.64
(2,1054)	1:88:A:VAL:H	4:348:A:PX4:C3	14	5.64
(3,27)	1:192:A:ALA:H	4:320:A:PX4:C35	19	5.63
(3,28)	1:197:A:GLY:H	4:307:A:PX4:C35	10	5.62
(3,28)	1:197:A:GLY:H	4:309:A:PX4:C35	11	5.61
(3,29)	1:200:A:LEU:H	4:332:A:PX4:C35	1	5.6
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	19	5.6
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	9	5.59
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	2	5.59
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	10	5.59
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	13	5.55
(3,30)	1:203:A:GLY:H	4:338:A:PX4:C35	4	5.54
(2,1064)	1:105:A:VAL:HG21	5:432:A:C3S:H7	7	5.51
(3,28)	1:197:A:GLY:H	4:317:A:PX4:C35	14	5.49
(3,33)	1:235:A:GLN:H	4:332:A:PX4:C35	12	5.46
(3,29)	1:200:A:LEU:H	4:307:A:PX4:C35	10	5.44
(3,27)	1:192:A:ALA:H	4:320:A:PX4:C35	11	5.43
(2,1054)	1:88:A:VAL:H	4:348:A:PX4:C3	6	5.43
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	6	5.42
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	18	5.39
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	14	5.38
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C5	15	5.34
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C5	19	5.33
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	20	5.32
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	4	5.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	18	5.29
(3,24)	1:174:A:GLU:H	4:332:A:PX4:C35	12	5.28
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	16	5.27
(3,29)	1:200:A:LEU:H	4:332:A:PX4:C35	7	5.24
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	10	5.22
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	19	5.15
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	9	5.14
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	9	5.12
(3,32)	1:233:A:GLY:H	4:322:A:PX4:C35	9	5.11
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C5	18	5.1
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C5	11	5.07
(3,28)	1:197:A:GLY:H	4:332:A:PX4:C35	19	5.07
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C4	16	5.03
(3,32)	1:233:A:GLY:H	4:307:A:PX4:C35	13	4.99
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	18	4.99
(3,33)	1:235:A:GLN:H	4:307:A:PX4:C35	7	4.98
(3,28)	1:197:A:GLY:H	4:338:A:PX4:C35	5	4.98
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	3	4.97
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	2	4.93
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	9	4.93
(3,35)	1:4:A:ALA:H	4:353:A:PX4:C4	17	4.9
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	15	4.9
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	16	4.89
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C3	8	4.88
(3,33)	1:235:A:GLN:H	4:322:A:PX4:C35	6	4.88
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	19	4.86
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	10	4.83
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C5	7	4.79
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	6	4.79
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	20	4.78
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	17	4.77
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	15	4.76
(3,28)	1:197:A:GLY:H	4:317:A:PX4:C35	6	4.75
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	9	4.72
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	8	4.71
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	17	4.71
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	5	4.7
(3,27)	1:192:A:ALA:H	4:307:A:PX4:C35	3	4.69
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	9	4.69
(3,43)	1:22:A:PHE:H	4:321:A:PX4:C5	12	4.68
(3,33)	1:235:A:GLN:H	4:307:A:PX4:C35	10	4.67
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	16	4.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	8	4.64
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C5	3	4.63
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	12	4.63
(3,46)	1:55:A:ASN:H	4:317:A:PX4:C5	18	4.61
(2,1064)	1:105:A:VAL:HG21	5:432:A:C3S:H7	13	4.61
(3,24)	1:174:A:GLU:H	4:305:A:PX4:C35	18	4.58
(2,1064)	1:105:A:VAL:HG21	5:432:A:C3S:H7	16	4.57
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	16	4.56
(3,27)	1:192:A:ALA:H	4:401:A:PX4:C35	2	4.56
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	19	4.52
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	13	4.52
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	20	4.51
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	15	4.48
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	14	4.48
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	18	4.48
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C4	17	4.48
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	18	4.48
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	18	4.48
(3,27)	1:192:A:ALA:H	4:317:A:PX4:C35	7	4.47
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	7	4.47
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	1	4.46
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	13	4.46
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	20	4.46
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	9	4.45
(3,29)	1:200:A:LEU:H	4:338:A:PX4:C35	16	4.44
(3,28)	1:197:A:GLY:H	4:332:A:PX4:C35	2	4.43
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	6	4.43
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C3	13	4.41
(3,24)	1:174:A:GLU:H	4:340:A:PX4:C35	5	4.4
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	10	4.4
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	4	4.4
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	8	4.4
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	10	4.4
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	1	4.39
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	19	4.39
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	7	4.38
(3,29)	1:200:A:LEU:H	4:309:A:PX4:C35	11	4.37
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	3	4.37
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	2	4.35
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	9	4.34
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	14	4.34
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	1	4.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	1	4.33
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	2	4.32
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	1	4.32
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	11	4.31
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	3	4.31
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	18	4.31
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	2	4.31
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	13	4.29
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	16	4.28
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	18	4.28
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	16	4.27
(3,29)	1:200:A:LEU:H	4:332:A:PX4:C35	19	4.26
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C5	13	4.24
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	3	4.24
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	11	4.23
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	17	4.22
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	12	4.21
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	17	4.21
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	13	4.2
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	11	4.19
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	14	4.19
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	19	4.19
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	12	4.18
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	17	4.18
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	12	4.18
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	5	4.17
(3,82)	1:147:A:TYR:H	4:340:A:PX4:C4	11	4.16
(3,28)	1:197:A:GLY:H	4:317:A:PX4:C35	7	4.16
(2,1064)	1:105:A:VAL:HG22	5:432:A:C3S:H7	8	4.16
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	6	4.15
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	6	4.15
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	7	4.15
(2,1064)	1:105:A:VAL:HG21	5:432:A:C3S:H7	3	4.13
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	19	4.13
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	15	4.12
(3,29)	1:200:A:LEU:H	4:338:A:PX4:C35	15	4.11
(2,1064)	1:105:A:VAL:HG21	5:432:A:C3S:H7	5	4.11
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	10	4.11
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	11	4.11
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	8	4.1
(2,268)	1:136:A:ILE:H	1:171:A:HIS:H	15	4.1
(3,35)	1:4:A:ALA:H	4:317:A:PX4:C3	4	4.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:235:A:GLN:H	4:322:A:PX4:C35	9	4.09
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	20	4.08
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	17	4.08
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C5	6	4.05
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	18	4.05
(3,33)	1:235:A:GLN:H	4:309:A:PX4:C35	2	4.04
(3,33)	1:235:A:GLN:H	4:429:A:PX4:C35	20	4.03
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C3	5	4.01
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	10	4.01
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	10	4.01
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	3	4.0
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	13	4.0
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	3	4.0
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	13	4.0
(3,24)	1:174:A:GLU:H	4:305:A:PX4:C35	8	3.99
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	15	3.99
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	5	3.98
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	15	3.96
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	19	3.96
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	11	3.95
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	4	3.94
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	16	3.94
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	16	3.94
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	17	3.94
(3,29)	1:200:A:LEU:H	4:338:A:PX4:C35	5	3.93
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	20	3.93
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	20	3.93
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	20	3.93
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	9	3.91
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	11	3.9
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	11	3.9
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	12	3.89
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	17	3.89
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	11	3.88
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	11	3.88
(3,27)	1:192:A:ALA:H	4:320:A:PX4:C35	16	3.87
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	8	3.87
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	14	3.87
(2,1065)	1:96:A:TYR:H	5:432:A:C3S:H7	2	3.86
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	14	3.84
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	4	3.84
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	5	3.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	1	3.83
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	18	3.82
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	18	3.82
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	2	3.82
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	5	3.81
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	18	3.81
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C4	8	3.78
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	5	3.78
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	3	3.77
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	13	3.77
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	10	3.75
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	12	3.72
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	17	3.72
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	17	3.72
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	13	3.71
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	5	3.71
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	4	3.69
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	11	3.67
(3,27)	1:192:A:ALA:H	4:317:A:PX4:C35	9	3.66
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	5	3.66
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	12	3.66
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	7	3.65
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	2	3.65
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	20	3.64
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	15	3.63
(3,33)	1:235:A:GLN:H	4:309:A:PX4:C35	11	3.62
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	18	3.6
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	18	3.6
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	19	3.6
(3,29)	1:200:A:LEU:H	4:332:A:PX4:C35	2	3.58
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	11	3.58
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	5	3.57
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	6	3.56
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	10	3.55
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	20	3.55
(3,27)	1:192:A:ALA:H	4:332:A:PX4:C35	15	3.54
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	11	3.54
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	19	3.53
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	9	3.52
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	9	3.52
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	9	3.51
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	9	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	16	3.51
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	4	3.51
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	4	3.51
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	4	3.51
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	14	3.5
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	17	3.5
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	5	3.48
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	19	3.48
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	11	3.48
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	17	3.47
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	6	3.47
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	7	3.45
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	18	3.44
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	6	3.44
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C5	14	3.43
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	17	3.43
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	9	3.43
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	9	3.43
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	1	3.42
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	18	3.42
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	16	3.41
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	5	3.41
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	5	3.41
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	5	3.41
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C5	18	3.4
(3,24)	1:174:A:GLU:H	4:324:A:PX4:C35	7	3.4
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	12	3.4
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	1	3.4
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	12	3.4
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	2	3.39
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	3	3.39
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	14	3.39
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	1	3.38
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	9	3.38
(3,32)	1:233:A:GLY:H	4:322:A:PX4:C35	18	3.37
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	20	3.37
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	13	3.35
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	2	3.34
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	4	3.34
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	8	3.33
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	16	3.33
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	1	3.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	1	3.32
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	18	3.32
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	6	3.32
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	19	3.31
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	19	3.31
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	7	3.3
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	4	3.3
(3,29)	1:200:A:LEU:H	4:338:A:PX4:C35	17	3.29
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	10	3.28
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C3	8	3.27
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	14	3.27
(3,28)	1:197:A:GLY:H	4:332:A:PX4:C35	15	3.26
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	17	3.26
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	4	3.26
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	4	3.26
(3,82)	1:147:A:TYR:H	4:340:A:PX4:C3	8	3.25
(3,29)	1:200:A:LEU:H	4:307:A:PX4:C35	3	3.25
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	7	3.25
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	10	3.24
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	10	3.24
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	4	3.24
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	12	3.23
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	15	3.23
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	12	3.21
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	11	3.21
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	11	3.2
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	12	3.19
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	3	3.18
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	19	3.18
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	19	3.18
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	20	3.18
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	2	3.17
(3,42)	1:21:A:ARG:H	4:319:A:PX4:C5	6	3.16
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C4	7	3.15
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	4	3.15
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	7	3.15
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	2	3.15
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	4	3.14
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	13	3.14
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	13	3.14
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	8	3.14
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	20	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	13	3.12
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	12	3.12
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	20	3.12
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	1	3.11
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	1	3.11
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	1	3.11
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	14	3.11
(3,34)	1:3:A:GLU:H	4:353:A:PX4:C4	17	3.1
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	2	3.1
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C3	20	3.07
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	19	3.07
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	19	3.07
(2,271)	1:135:A:MET:H	1:171:A:HIS:H	5	3.06
(3,81)	1:145:A:ASP:H	4:310:A:PX4:C5	4	3.05
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	6	3.04
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	6	3.04
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	3	3.04
(3,28)	1:197:A:GLY:H	4:307:A:PX4:C35	3	3.03
(3,27)	1:192:A:ALA:H	4:395:A:PX4:C35	5	3.03
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	1	3.03
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	18	3.02
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	10	3.01
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	15	2.99
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	15	2.99
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	15	2.99
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	8	2.99
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C5	12	2.98
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	1	2.98
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	1	2.98
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	7	2.98
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	13	2.97
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	13	2.97
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	13	2.97
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	13	2.97
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	4	2.97
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	20	2.97
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	20	2.97
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	20	2.97
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	15	2.96
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	9	2.96
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	9	2.96
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	3	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	15	2.95
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	14	2.94
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	14	2.94
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	7	2.94
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C3	19	2.93
(3,33)	1:235:A:GLN:H	4:345:A:PX4:C35	14	2.93
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	20	2.92
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	9	2.92
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C3	3	2.91
(3,24)	1:174:A:GLU:H	4:305:A:PX4:C35	4	2.91
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	10	2.91
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	10	2.91
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	11	2.9
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	11	2.9
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	19	2.9
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	19	2.9
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	14	2.89
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	17	2.89
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	11	2.89
(3,81)	1:145:A:ASP:H	4:340:A:PX4:C4	11	2.88
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	1	2.88
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	13	2.88
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	13	2.88
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	4	2.87
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	3	2.87
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	13	2.87
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	13	2.87
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	5	2.87
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	5	2.87
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	1	2.86
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	16	2.86
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	11	2.85
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	4	2.85
(3,32)	1:233:A:GLY:H	4:307:A:PX4:C35	3	2.84
(3,24)	1:174:A:GLU:H	4:352:A:PX4:C35	14	2.84
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	1	2.84
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	18	2.84
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	18	2.84
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	16	2.84
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	6	2.83
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	5	2.83
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	5	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	18	2.81
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	18	2.81
(3,27)	1:192:A:ALA:H	4:320:A:PX4:C35	1	2.8
(3,27)	1:192:A:ALA:H	4:348:A:PX4:C35	13	2.8
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	4	2.8
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	4	2.8
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	17	2.8
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	17	2.8
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	17	2.8
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	15	2.8
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	15	2.8
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	1	2.8
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	10	2.79
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	17	2.79
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	18	2.79
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	18	2.79
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	14	2.79
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	19	2.78
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	4	2.78
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	4	2.78
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	12	2.78
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	12	2.78
(3,81)	1:145:A:ASP:H	4:319:A:PX4:C5	17	2.77
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	11	2.77
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	11	2.77
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	4	2.77
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	3	2.76
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	3	2.76
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	3	2.76
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	3	2.76
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	3	2.76
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	3	2.76
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	3	2.76
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	3	2.76
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	3	2.76
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	10	2.75
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	10	2.75
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	2	2.74
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	2	2.74
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	1	2.73
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	11	2.72
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	11	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	5	2.72
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	18	2.72
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	18	2.72
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	6	2.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	6	2.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	6	2.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	6	2.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	6	2.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	6	2.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	6	2.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	6	2.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	6	2.71
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	16	2.71
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	13	2.71
(3,27)	1:192:A:ALA:H	4:317:A:PX4:C35	14	2.7
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	3	2.7
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	3	2.7
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	17	2.7
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	17	2.7
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	11	2.68
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	16	2.68
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	8	2.68
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	18	2.68
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	18	2.68
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	18	2.68
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	10	2.67
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	7	2.67
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	3	2.67
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	3	2.67
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	15	2.67
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	2	2.67
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	2	2.67
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	5	2.67
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	5	2.67
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	6	2.67
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	13	2.67
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	13	2.67
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	7	2.66
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	2	2.66
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	6	2.66
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	6	2.66
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	16	2.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	6	2.66
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	6	2.66
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	16	2.66
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	7	2.66
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	12	2.65
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	10	2.64
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	19	2.64
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	6	2.64
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	6	2.64
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	15	2.64
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	3	2.63
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	3	2.63
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	3	2.63
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	3	2.63
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	19	2.63
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	19	2.63
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	6	2.63
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	9	2.61
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	9	2.61
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	8	2.61
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	8	2.61
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	2	2.61
(2,1025)	1:58:A:VAL:HG12	1:54:A:LEU:HD21	7	2.6
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	20	2.6
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	20	2.6
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	17	2.59
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	17	2.59
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	2	2.59
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	8	2.59
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	16	2.59
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	16	2.59
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	16	2.59
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	18	2.58
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C4	2	2.58
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	7	2.58
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	7	2.58
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	16	2.58
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	20	2.58
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	14	2.58
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	12	2.58
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	13	2.58
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	13	2.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C4	17	2.57
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	9	2.57
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	4	2.57
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	7	2.57
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	15	2.57
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	18	2.56
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	18	2.56
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	17	2.56
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	1	2.56
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	10	2.56
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	20	2.56
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	20	2.56
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	7	2.56
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	7	2.56
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	7	2.56
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	5	2.55
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	8	2.55
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	17	2.55
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	17	2.55
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	17	2.55
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	16	2.54
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	7	2.54
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	13	2.54
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	8	2.54
(3,33)	1:235:A:GLN:H	4:307:A:PX4:C35	13	2.53
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	6	2.53
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	19	2.53
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	1	2.53
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	6	2.53
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	6	2.53
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	6	2.53
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	6	2.53
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	7	2.53
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	7	2.53
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	14	2.53
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	13	2.52
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	11	2.52
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	11	2.52
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	10	2.52
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	10	2.52
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	16	2.52
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	5	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	7	2.51
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	11	2.51
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	11	2.51
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	5	2.51
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	5	2.51
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	20	2.51
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C3	12	2.5
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	6	2.5
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	6	2.5
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	17	2.5
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	2	2.5
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	16	2.5
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	16	2.5
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	5	2.49
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	6	2.49
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	8	2.48
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	13	2.48
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	9	2.48
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	6	2.48
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	10	2.48
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	10	2.48
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	12	2.47
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	12	2.47
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	12	2.47
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	3	2.47
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	3	2.47
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	3	2.47
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	14	2.47
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	14	2.47
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	14	2.47
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	3	2.47
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	3	2.47
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	8	2.46
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	17	2.46
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	17	2.46
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	17	2.46
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	5	2.46
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	5	2.46
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	6	2.45
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	13	2.45
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	13	2.45
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	13	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	13	2.45
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	8	2.45
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	8	2.45
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	9	2.45
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	9	2.45
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	17	2.45
(3,32)	1:233:A:GLY:H	4:338:A:PX4:C35	4	2.44
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	13	2.44
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	13	2.44
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	13	2.44
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	10	2.44
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	1	2.44
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	1	2.44
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	1	2.44
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	5	2.43
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	20	2.42
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	7	2.42
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	7	2.42
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	18	2.42
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	18	2.42
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	18	2.42
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	20	2.42
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	13	2.41
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	13	2.41
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	13	2.41
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	13	2.41
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	13	2.41
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	13	2.41
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	13	2.41
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	13	2.41
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	13	2.41
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	7	2.41
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	19	2.41
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	19	2.4
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	7	2.4
(3,34)	1:3:A:GLU:H	4:317:A:PX4:C3	4	2.39
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	3	2.39
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	5	2.39
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	5	2.39
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	18	2.39
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	6	2.39
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	6	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	6	2.39
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	13	2.39
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	10	2.39
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	18	2.38
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	1	2.38
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	1	2.38
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	5	2.38
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	15	2.38
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C5	1	2.37
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	9	2.37
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	17	2.37
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	17	2.37
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	5	2.37
(3,81)	1:145:A:ASP:H	4:319:A:PX4:C3	8	2.36
(2,1054)	1:88:A:VAL:H	4:321:A:PX4:C3	18	2.36
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	4	2.36
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	3	2.36
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	3	2.36
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	3	2.36
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	19	2.36
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	3	2.35
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	12	2.35
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	12	2.35
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	20	2.35
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	3	2.35
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	17	2.34
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	12	2.34
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	12	2.34
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	12	2.34
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	2	2.34
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	13	2.33
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	3	2.33
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	6	2.33
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	3	2.33
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	6	2.33
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	6	2.33
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	6	2.33
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	8	2.33
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	2	2.33
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	2	2.33
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	20	2.32
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	17	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	1	2.32
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	3	2.32
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	9	2.32
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	7	2.32
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	7	2.32
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	5	2.31
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	7	2.31
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	12	2.31
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	4	2.31
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	4	2.31
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	1	2.31
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	9	2.31
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	12	2.31
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	9	2.31
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	18	2.31
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	4	2.3
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	16	2.3
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	16	2.3
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	10	2.3
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	10	2.3
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	20	2.3
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	2	2.3
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	6	2.3
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	6	2.3
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	3	2.29
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	19	2.29
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	8	2.29
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	8	2.29
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	8	2.29
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	10	2.29
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	16	2.29
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	1	2.28
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	9	2.28
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	9	2.28
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	18	2.28
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	18	2.28
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	20	2.28
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	13	2.27
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	12	2.27
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	8	2.27
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	8	2.27
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	8	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	1	2.27
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	1	2.27
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	1	2.27
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	7	2.26
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	13	2.26
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	20	2.26
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	20	2.26
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	2	2.26
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	9	2.26
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	14	2.25
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	14	2.25
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	11	2.25
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	11	2.25
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	20	2.25
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	20	2.25
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	20	2.24
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	1	2.24
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	1	2.24
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	9	2.24
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	3	2.24
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	16	2.23
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	16	2.23
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	16	2.23
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	11	2.23
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	4	2.22
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	4	2.22
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	17	2.22
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	17	2.22
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	5	2.22
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	14	2.22
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	7	2.22
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	1	2.21
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	7	2.21
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	7	2.21
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	3	2.21
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	1	2.21
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	9	2.2
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	16	2.2
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	16	2.2
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	11	2.2
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	12	2.2
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	13	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	13	2.19
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	7	2.19
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	6	2.18
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	19	2.18
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	19	2.18
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	16	2.18
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	4	2.18
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	9	2.18
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	9	2.18
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	9	2.18
(2,125)	1:45:A:PHE:H	1:48:A:LEU:HD21	3	2.18
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	9	2.17
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	9	2.17
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	9	2.17
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	9	2.17
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	8	2.17
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	8	2.17
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	8	2.17
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	10	2.17
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	11	2.17
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	14	2.17
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	15	2.16
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	19	2.16
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	12	2.15
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	20	2.15
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	20	2.15
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	16	2.15
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	18	2.15
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	7	2.14
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	7	2.14
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	7	2.14
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	7	2.14
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	7	2.14
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	7	2.14
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	7	2.14
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	10	2.14
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	4	2.14
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	16	2.13
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	16	2.13
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	7	2.13
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	7	2.13
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	7	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	18	2.13
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	16	2.13
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	15	2.13
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	15	2.13
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	14	2.12
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	17	2.12
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD22	20	2.12
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD23	20	2.12
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	7	2.12
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	7	2.12
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	11	2.12
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	7	2.12
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	7	2.12
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	11	2.12
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	9	2.12
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	1	2.12
(3,27)	1:192:A:ALA:H	4:317:A:PX4:C35	6	2.11
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	14	2.11
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	10	2.11
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	3	2.11
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	3	2.11
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	8	2.11
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	2	2.11
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	3	2.11
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	16	2.1
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	16	2.1
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	11	2.1
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	11	2.1
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	11	2.09
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	6	2.09
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	6	2.09
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	10	2.09
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	10	2.09
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	18	2.09
(3,47)	1:80:A:ASN:H	4:319:A:PX4:C3	9	2.08
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	13	2.08
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	13	2.08
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	13	2.08
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	4	2.08
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	4	2.08
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	15	2.07
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	2	2.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	14	2.07
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	2	2.07
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	14	2.07
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	12	2.07
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	12	2.07
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	1	2.07
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	1	2.07
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	1	2.06
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	6	2.06
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	12	2.06
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	12	2.06
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	7	2.06
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	7	2.06
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	5	2.06
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	14	2.05
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	2	2.05
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	2	2.05
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	6	2.05
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	6	2.05
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	11	2.05
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	11	2.05
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	18	2.05
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	18	2.05
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	6	2.05
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	6	2.05
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	11	2.05
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	11	2.05
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	18	2.05
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	18	2.05
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	17	2.05
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	17	2.05
(2,501)	1:158:A:HIS:H	1:156:A:LEU:H	4	2.05
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	5	2.05
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	20	2.05
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	20	2.05
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	8	2.05
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	7	2.05
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	6	2.05
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	8	2.05
(3,84)	1:154:A:ASN:H	4:349:A:PX4:C5	1	2.04
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	10	2.04
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	5	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	3	2.04
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	3	2.04
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	3	2.04
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	1	2.04
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	1	2.04
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	1	2.04
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	9	2.04
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	5	2.03
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	5	2.03
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	13	2.03
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	8	2.03
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	2	2.03
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	17	2.02
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	17	2.02
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	19	2.02
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	5	2.02
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	5	2.02
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	16	2.02
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	2	2.02
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	16	2.01
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	11	2.01
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	15	2.01
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	15	2.01
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	3	2.01
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	3	2.01
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	3	2.01
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	4	2.01
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	17	2.0
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	15	2.0
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	7	2.0
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	11	2.0
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	7	2.0
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	5	2.0
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	5	2.0
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	15	2.0
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	15	2.0
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	13	2.0
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	13	2.0
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	9	1.99
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	17	1.99
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	19	1.99
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	19	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	14	1.99
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	14	1.99
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	15	1.99
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	17	1.98
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	19	1.98
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	19	1.98
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	4	1.98
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	4	1.98
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	4	1.98
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	4	1.98
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	14	1.98
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	14	1.98
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	14	1.98
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	14	1.98
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	14	1.98
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	14	1.98
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	14	1.98
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	14	1.98
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	14	1.98
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	13	1.98
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	13	1.98
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	13	1.98
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	15	1.98
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	15	1.98
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	15	1.98
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	16	1.98
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	16	1.98
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	16	1.98
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	19	1.98
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	2	1.97
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	8	1.97
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	8	1.97
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	8	1.97
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	8	1.97
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD11	8	1.97
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD12	8	1.97
(2,603)	1:186:A:ILE:H	1:156:A:LEU:HD13	8	1.97
(1,5)	2:302:A:CA:CA	1:176:A:GLU:OE2	17	1.97
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	5	1.96
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	5	1.96
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	16	1.96
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	16	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	17	1.96
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	5	1.96
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	14	1.95
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	20	1.95
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	11	1.94
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	11	1.94
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	11	1.94
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	11	1.94
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	1	1.94
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	1	1.94
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	2	1.94
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	2	1.94
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	18	1.94
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	18	1.94
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	17	1.94
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	3	1.94
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	3	1.94
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	7	1.93
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	6	1.93
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	6	1.93
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	8	1.93
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	8	1.93
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	15	1.93
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	15	1.93
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C5	14	1.92
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	4	1.92
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	4	1.92
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	9	1.92
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	9	1.92
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	9	1.92
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	9	1.92
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	9	1.92
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	9	1.92
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	9	1.92
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	9	1.92
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	9	1.92
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	2	1.92
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	2	1.92
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	2	1.92
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	14	1.92
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	14	1.92
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	14	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	7	1.92
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	14	1.92
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	11	1.91
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	18	1.91
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	18	1.91
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	2	1.91
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	14	1.9
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	14	1.9
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	19	1.9
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	20	1.89
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	10	1.89
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	10	1.89
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	1	1.89
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	1	1.89
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	20	1.89
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	20	1.89
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	18	1.89
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	18	1.89
(3,33)	1:235:A:GLN:H	4:322:A:PX4:C35	18	1.88
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	4	1.88
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	9	1.88
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	9	1.88
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	7	1.88
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	3	1.87
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	16	1.87
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	16	1.87
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	10	1.87
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	10	1.87
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	10	1.87
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	8	1.87
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	8	1.87
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	8	1.87
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	19	1.87
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	19	1.87
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	19	1.87
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	7	1.86
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	20	1.86
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	14	1.86
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	14	1.86
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	9	1.86
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	5	1.85
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	8	1.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	11	1.83
(2,807)	1:61:A:ILE:HD12	1:48:A:LEU:HD21	4	1.83
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	7	1.83
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	7	1.83
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	15	1.83
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	15	1.83
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	15	1.83
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	13	1.82
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	1	1.82
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	19	1.82
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	19	1.82
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	8	1.82
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	8	1.82
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD22	17	1.81
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD23	17	1.81
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	17	1.81
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	17	1.81
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	17	1.81
(2,769)	1:19:A:LEU:HD21	1:17:A:ASP:H	6	1.81
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	14	1.81
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	18	1.81
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	14	1.81
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	14	1.81
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	14	1.81
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C3	16	1.8
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	3	1.8
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	13	1.8
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	13	1.8
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	17	1.8
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	14	1.8
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	14	1.8
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	13	1.8
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	13	1.8
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	17	1.8
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	14	1.8
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	14	1.8
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	10	1.79
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	10	1.79
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	10	1.79
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	10	1.79
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	10	1.79
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	10	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	10	1.79
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	10	1.79
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	10	1.79
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	5	1.79
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	14	1.79
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	12	1.79
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	19	1.79
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	19	1.79
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	19	1.79
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	12	1.79
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	1	1.79
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	17	1.79
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	17	1.79
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	5	1.79
(2,64)	1:205:A:SER:H	1:204:A:HIS:HE1	8	1.79
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	4	1.78
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	4	1.78
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	3	1.78
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	9	1.78
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	9	1.78
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	14	1.78
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	14	1.78
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	19	1.78
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	18	1.78
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	16	1.77
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	18	1.77
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	18	1.77
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	18	1.77
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	6	1.77
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	6	1.77
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	13	1.77
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	13	1.77
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	13	1.77
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	20	1.76
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	20	1.76
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	12	1.76
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	12	1.76
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	12	1.76
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	16	1.76
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	19	1.76
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	19	1.76
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C5	4	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	7	1.75
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	7	1.75
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	2	1.75
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	2	1.75
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	14	1.75
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	20	1.75
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	12	1.75
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	15	1.75
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	1	1.74
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	11	1.74
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	11	1.74
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	1	1.74
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	11	1.74
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	11	1.74
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	11	1.74
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	10	1.73
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	10	1.73
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	12	1.73
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	20	1.73
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	5	1.73
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	5	1.73
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	5	1.73
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	15	1.73
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	15	1.73
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	6	1.73
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	17	1.73
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	5	1.72
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	9	1.72
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	9	1.72
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	9	1.72
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	15	1.72
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	2	1.71
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	2	1.71
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	2	1.71
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	2	1.71
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	2	1.71
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	2	1.71
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	2	1.71
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	2	1.71
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	2	1.71
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	2	1.71
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	14	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	14	1.71
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	12	1.7
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	3	1.7
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	7	1.7
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	7	1.7
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	17	1.7
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	17	1.7
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	20	1.7
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C5	20	1.69
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	4	1.69
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	16	1.69
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	1	1.69
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	9	1.69
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	9	1.69
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	9	1.69
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	13	1.69
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	13	1.69
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	13	1.69
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	1	1.69
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	1	1.69
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	1	1.68
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	13	1.68
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	13	1.68
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	1	1.68
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	13	1.68
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	13	1.68
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	7	1.68
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	10	1.68
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	16	1.67
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	16	1.67
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	16	1.67
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	16	1.67
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	1	1.67
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	1	1.67
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	16	1.67
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	16	1.67
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	16	1.67
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	9	1.67
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	2	1.67
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	2	1.67
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	10	1.67
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	11	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	6	1.66
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	7	1.66
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	6	1.66
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	13	1.65
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	13	1.65
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	11	1.65
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	11	1.65
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	7	1.65
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	7	1.65
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	14	1.65
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	20	1.64
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	20	1.64
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	3	1.64
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	3	1.64
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	19	1.64
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	4	1.64
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	10	1.64
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	5	1.63
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	10	1.63
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	12	1.63
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	11	1.63
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	2	1.63
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	2	1.63
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	2	1.63
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	4	1.63
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	12	1.62
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	12	1.62
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	8	1.62
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	11	1.62
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	4	1.62
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	4	1.62
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	4	1.62
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	16	1.61
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	7	1.61
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	9	1.61
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	9	1.61
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	13	1.61
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	13	1.61
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	19	1.61
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	19	1.61
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	19	1.61
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	3	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	10	1.61
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	16	1.61
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	16	1.61
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	16	1.61
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	6	1.6
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD22	10	1.6
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD23	10	1.6
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	11	1.6
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	11	1.6
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	11	1.6
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	11	1.6
(3,84)	1:154:A:ASN:H	4:310:A:PX4:C4	2	1.59
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	3	1.59
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	1	1.59
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	19	1.58
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	19	1.58
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	19	1.58
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	19	1.58
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	19	1.58
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	19	1.58
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	19	1.58
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	19	1.58
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	19	1.58
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	18	1.58
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	5	1.58
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	16	1.58
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	16	1.58
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	16	1.58
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	16	1.58
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	8	1.58
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	9	1.58
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	9	1.58
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	9	1.58
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	13	1.57
(2,1025)	1:58:A:VAL:HG12	1:54:A:LEU:HD21	17	1.57
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	1	1.57
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	1	1.57
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	4	1.57
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	4	1.57
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	17	1.57
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	6	1.57
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	6	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	6	1.57
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	5	1.56
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	7	1.56
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	7	1.56
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	12	1.56
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	12	1.56
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	9	1.56
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	13	1.56
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	7	1.56
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	19	1.56
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	19	1.55
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	1	1.55
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	1	1.55
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	19	1.55
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	1	1.55
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	1	1.55
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	5	1.55
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	4	1.55
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	4	1.55
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	4	1.55
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	15	1.55
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	15	1.55
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	15	1.55
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	13	1.55
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	8	1.55
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	8	1.55
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	20	1.55
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	20	1.55
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	20	1.55
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	20	1.55
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	20	1.54
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	3	1.54
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	20	1.54
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	9	1.54
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	8	1.54
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	12	1.54
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	17	1.54
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	9	1.54
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	6	1.54
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	6	1.54
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	18	1.54
(3,28)	1:197:A:GLY:H	4:348:A:PX4:C35	13	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD22	7	1.53
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD23	7	1.53
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	17	1.53
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	17	1.53
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	17	1.53
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	17	1.53
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	17	1.53
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	17	1.53
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	17	1.53
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	17	1.53
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	17	1.53
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	10	1.53
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	14	1.53
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	14	1.53
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	20	1.53
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	7	1.52
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	16	1.52
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	1	1.52
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	6	1.52
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	4	1.52
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	4	1.52
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	2	1.51
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	11	1.51
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	5	1.51
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	5	1.51
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	5	1.51
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	5	1.51
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	12	1.51
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	12	1.51
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	14	1.51
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	14	1.51
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	14	1.51
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	11	1.51
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	11	1.51
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C5	7	1.5
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	17	1.5
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	3	1.5
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	3	1.5
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	1	1.5
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	2	1.5
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	10	1.5
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	17	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	9	1.49
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	9	1.49
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	9	1.49
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	9	1.49
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	3	1.49
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	3	1.49
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	20	1.49
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	20	1.49
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	20	1.49
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	2	1.49
(3,43)	1:22:A:PHE:H	4:319:A:PX4:C5	6	1.48
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	7	1.48
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	1	1.48
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	4	1.48
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	7	1.48
(2,1064)	1:105:A:VAL:HG23	5:432:A:C3S:H7	20	1.47
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	18	1.47
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	2	1.47
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	2	1.47
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	6	1.47
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	19	1.47
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	3	1.47
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	18	1.47
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	18	1.47
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	18	1.47
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	13	1.47
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	18	1.46
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	18	1.46
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	18	1.46
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	18	1.46
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	13	1.46
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	8	1.46
(3,81)	1:145:A:ASP:H	4:310:A:PX4:C4	10	1.45
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	19	1.45
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	5	1.45
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	18	1.45
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	4	1.45
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	4	1.45
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C5	19	1.44
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	1	1.44
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	1	1.44
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	1	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	1	1.44
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	1	1.44
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	1	1.44
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	1	1.44
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	1	1.44
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	1	1.44
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	16	1.44
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	20	1.44
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	4	1.44
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	13	1.44
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	16	1.44
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	4	1.44
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C3	12	1.43
(2,1055)	1:123:A:HIS:H	4:348:A:PX4:C3	18	1.43
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	5	1.43
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	5	1.43
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	5	1.43
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	5	1.43
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	5	1.43
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	5	1.43
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	5	1.43
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	5	1.43
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	5	1.43
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	20	1.43
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	7	1.43
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	13	1.43
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	13	1.43
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	4	1.43
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	14	1.43
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	13	1.43
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	2	1.43
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	18	1.43
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	18	1.43
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	4	1.43
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	4	1.43
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C3	4	1.42
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C4	3	1.42
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	4	1.42
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	12	1.42
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	4	1.41
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	4	1.41
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD22	7	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD23	7	1.41
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	12	1.41
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C3	8	1.4
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	17	1.4
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	5	1.4
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	11	1.4
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	9	1.4
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	9	1.4
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	3	1.4
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	3	1.4
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	14	1.4
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	8	1.4
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	16	1.4
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	2	1.4
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	2	1.4
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	2	1.4
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	20	1.4
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	20	1.4
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	20	1.4
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	20	1.4
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	7	1.39
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	7	1.39
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	15	1.39
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	9	1.39
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	7	1.39
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	7	1.39
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	7	1.39
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	2	1.39
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	5	1.39
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	4	1.39
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	12	1.39
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	12	1.39
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	20	1.38
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	18	1.38
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	7	1.38
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	7	1.38
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	15	1.38
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	5	1.37
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	6	1.37
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	17	1.37
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	15	1.37
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	14	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C4	16	1.36
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	4	1.36
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	6	1.36
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	6	1.36
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	4	1.36
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	7	1.36
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	1	1.36
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	17	1.36
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	19	1.36
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	20	1.36
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	20	1.36
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	20	1.36
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	9	1.36
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	13	1.36
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	15	1.36
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	15	1.36
(3,81)	1:145:A:ASP:H	4:319:A:PX4:C3	12	1.35
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	4	1.35
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	10	1.35
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	19	1.35
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	20	1.35
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	8	1.35
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	8	1.35
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	14	1.35
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	1	1.35
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	1	1.35
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	1	1.35
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	4	1.34
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	4	1.34
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	4	1.34
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	4	1.34
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	10	1.34
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	5	1.34
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	17	1.34
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	4	1.34
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C4	11	1.33
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	10	1.33
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	20	1.33
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	20	1.33
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	20	1.33
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	20	1.33
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	20	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	20	1.33
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	20	1.33
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	20	1.33
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	20	1.33
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	1	1.33
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	14	1.33
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	3	1.33
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	3	1.33
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	14	1.33
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	3	1.33
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	3	1.33
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	4	1.33
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	4	1.33
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	6	1.33
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD22	8	1.33
(2,126)	1:45:A:PHE:H	1:48:A:LEU:HD23	8	1.33
(3,25)	1:180:A:ASP:H	4:320:A:PX4:C35	7	1.32
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	3	1.32
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	3	1.32
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	6	1.32
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	6	1.32
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	12	1.32
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	12	1.32
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	8	1.32
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	6	1.32
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	6	1.32
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	4	1.32
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	17	1.32
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	15	1.31
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	18	1.31
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	18	1.31
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	17	1.31
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	17	1.31
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	11	1.31
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	10	1.3
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	11	1.3
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	13	1.3
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	13	1.3
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	6	1.3
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	6	1.3
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	12	1.3
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	12	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	11	1.3
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	16	1.3
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	16	1.3
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	3	1.3
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	18	1.3
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	9	1.29
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	11	1.29
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	14	1.29
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	7	1.29
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD22	17	1.28
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD23	17	1.28
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	6	1.28
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	6	1.28
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	6	1.28
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	6	1.28
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	7	1.28
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	11	1.28
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	11	1.28
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	16	1.28
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	14	1.28
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	19	1.28
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	2	1.28
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	1	1.28
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	2	1.28
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	11	1.27
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	11	1.27
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	5	1.27
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	20	1.27
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	20	1.27
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	14	1.27
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	19	1.27
(3,84)	1:154:A:ASN:H	4:317:A:PX4:C4	12	1.26
(3,84)	1:154:A:ASN:H	4:308:A:PX4:C4	19	1.26
(2,996)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	7	1.26
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	12	1.26
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	12	1.26
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	14	1.26
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	11	1.26
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	15	1.26
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	7	1.25
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	6	1.25
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	1	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	1	1.25
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	2	1.25
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	5	1.25
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	4	1.25
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	4	1.25
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	3	1.25
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	14	1.25
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	6	1.25
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	5	1.25
(2,996)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	20	1.24
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	3	1.24
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	13	1.24
(2,762)	1:19:A:LEU:HD22	1:38:A:LYS:H	6	1.24
(2,762)	1:19:A:LEU:HD23	1:38:A:LYS:H	6	1.24
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	20	1.24
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	20	1.24
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	20	1.24
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	18	1.24
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	17	1.24
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	15	1.24
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	4	1.24
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	4	1.24
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	4	1.24
(3,25)	1:180:A:ASP:H	4:414:A:PX4:C35	10	1.23
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	3	1.23
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	3	1.23
(2,835)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	18	1.23
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	3	1.23
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	3	1.23
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	18	1.23
(2,237)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	18	1.23
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	4	1.23
(2,1063)	1:126:A:LYS:H	4:332:A:PX4:C24	17	1.22
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	9	1.22
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	9	1.22
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	11	1.22
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	11	1.22
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	4	1.22
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	4	1.22
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	3	1.22
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	18	1.22
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	9	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	9	1.22
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	2	1.22
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	2	1.22
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	8	1.22
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	12	1.22
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	12	1.22
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	12	1.22
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	5	1.21
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	14	1.21
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	8	1.21
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	16	1.21
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	18	1.21
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	18	1.21
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	5	1.21
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	12	1.21
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	17	1.21
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	3	1.2
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	3	1.2
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	2	1.2
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	2	1.2
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	10	1.2
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	12	1.2
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	12	1.2
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	11	1.2
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	11	1.2
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	13	1.2
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	4	1.2
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	20	1.19
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	20	1.19
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	12	1.19
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	12	1.19
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	13	1.18
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	13	1.18
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	8	1.18
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	6	1.18
(3,8)	1:86:A:SER:H	4:345:A:PX4:C35	9	1.17
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	9	1.17
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	17	1.17
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	17	1.17
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	10	1.17
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	10	1.17
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	10	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	10	1.17
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	7	1.17
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	7	1.17
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	7	1.17
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	9	1.17
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	9	1.17
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	19	1.17
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	12	1.17
(3,81)	1:145:A:ASP:H	4:319:A:PX4:C3	19	1.16
(2,1029)	1:54:A:LEU:HD21	1:39:A:LEU:HD11	16	1.16
(2,1029)	1:54:A:LEU:HD21	1:39:A:LEU:HD12	16	1.16
(2,1029)	1:54:A:LEU:HD21	1:39:A:LEU:HD13	16	1.16
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	19	1.16
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	10	1.16
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	10	1.16
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	14	1.16
(3,33)	1:235:A:GLN:H	4:307:A:PX4:C35	3	1.15
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	11	1.15
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	4	1.15
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	8	1.15
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	8	1.14
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	20	1.14
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	8	1.14
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	5	1.14
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	16	1.14
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	16	1.14
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	9	1.14
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	4	1.14
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	15	1.14
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	17	1.14
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD22	13	1.14
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD23	13	1.14
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	17	1.13
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	6	1.13
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	16	1.13
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	14	1.13
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	14	1.13
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	17	1.12
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	17	1.12
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	17	1.12
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	17	1.12
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	17	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	6	1.12
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	1	1.12
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	7	1.11
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	2	1.11
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	6	1.11
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	6	1.11
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	10	1.11
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	6	1.11
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	6	1.11
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	10	1.11
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	13	1.11
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	2	1.11
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	13	1.11
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	2	1.11
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	20	1.1
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	20	1.1
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	12	1.1
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	12	1.1
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	12	1.1
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	12	1.1
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	12	1.1
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	12	1.1
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	14	1.1
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	17	1.1
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	10	1.1
(3,24)	1:174:A:GLU:H	4:320:A:PX4:C35	16	1.09
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	6	1.09
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	6	1.09
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	6	1.09
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	9	1.09
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	6	1.09
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	7	1.09
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	7	1.09
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	7	1.09
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	12	1.09
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	3	1.09
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	8	1.09
(2,1066)	1:100:A:LEU:H	5:432:A:C3S:H7	20	1.08
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	4	1.08
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	4	1.08
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	4	1.08
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	4	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	4	1.08
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	4	1.08
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	4	1.08
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	4	1.08
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	4	1.08
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	1	1.08
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	1	1.08
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	10	1.08
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	1	1.08
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	1	1.08
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	10	1.08
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	3	1.08
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	11	1.08
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	10	1.08
(2,464)	1:137:A:GLY:H	1:135:A:MET:H	8	1.08
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	7	1.08
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	20	1.08
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	12	1.08
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	3	1.07
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	16	1.07
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	7	1.07
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	7	1.07
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	2	1.07
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	2	1.07
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	17	1.07
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	18	1.07
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	16	1.07
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	11	1.07
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	12	1.07
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	12	1.07
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	18	1.07
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	8	1.06
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	6	1.06
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	8	1.06
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	8	1.06
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	13	1.06
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	10	1.06
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	1	1.06
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	15	1.06
(2,1025)	1:58:A:VAL:HG12	1:54:A:LEU:HD21	10	1.05
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	20	1.05
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	20	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	5	1.05
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	15	1.05
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	9	1.05
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	18	1.05
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	18	1.05
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	18	1.05
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD22	10	1.04
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD23	10	1.04
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	15	1.04
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	15	1.04
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	15	1.04
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	15	1.04
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	15	1.04
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	15	1.04
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	15	1.04
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	15	1.04
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	15	1.04
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	14	1.04
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	14	1.04
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	14	1.04
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	14	1.04
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	18	1.04
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	8	1.04
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	9	1.04
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C4	10	1.03
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	3	1.03
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	3	1.03
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	18	1.03
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	16	1.03
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	16	1.03
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	15	1.03
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	9	1.03
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	9	1.03
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	17	1.03
(3,81)	1:145:A:ASP:H	4:310:A:PX4:C3	2	1.02
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	15	1.02
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	17	1.02
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	15	1.02
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	15	1.02
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	5	1.02
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	15	1.02
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	5	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	7	1.02
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	4	1.02
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	3	1.02
(3,27)	1:192:A:ALA:H	4:348:A:PX4:C35	17	1.01
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	11	1.01
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	10	1.01
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	11	1.01
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	15	1.01
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	15	1.01
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	10	1.01
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	10	1.01
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	7	1.01
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	7	1.01
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	6	1.01
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	6	1.01
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	10	1.01
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	11	1.01
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD11	5	1.01
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD12	5	1.01
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD13	5	1.01
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	7	1.0
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	7	1.0
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	7	1.0
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	7	1.0
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	7	1.0
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	7	1.0
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	7	1.0
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	7	1.0
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	7	1.0
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	4	1.0
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	4	1.0
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	14	1.0
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	16	1.0
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	15	1.0
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	15	1.0
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	11	1.0
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	14	1.0
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	10	0.99
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	1	0.99
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	1	0.99
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	4	0.99
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	4	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	12	0.99
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	12	0.99
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	20	0.99
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	20	0.99
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	12	0.99
(2,341)	1:189:A:LEU:HD21	1:111:A:LYS:H	9	0.99
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	18	0.99
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	6	0.99
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	8	0.99
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C3	2	0.98
(2,1057)	1:130:A:GLY:H	4:321:A:PX4:C4	1	0.98
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	8	0.98
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	11	0.98
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	11	0.98
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	4	0.98
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	4	0.98
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	13	0.98
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	13	0.98
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	13	0.98
(3,9)	1:96:A:TYR:H	4:320:A:PX4:C35	10	0.97
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	2	0.97
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	5	0.97
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	20	0.97
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	19	0.97
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	15	0.97
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD22	12	0.97
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD23	12	0.97
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD11	12	0.97
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD12	12	0.97
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD13	12	0.97
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	19	0.96
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	12	0.96
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	12	0.96
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	12	0.96
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	12	0.96
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	12	0.96
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	12	0.96
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	12	0.96
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	12	0.96
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	12	0.96
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	4	0.96
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	19	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	9	0.96
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	6	0.96
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	6	0.96
(3,25)	1:180:A:ASP:H	4:320:A:PX4:C35	15	0.95
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	4	0.95
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD22	7	0.95
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD23	7	0.95
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	7	0.95
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	14	0.95
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	14	0.95
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	15	0.95
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	15	0.95
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	11	0.95
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	11	0.95
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	11	0.95
(2,604)	1:186:A:ILE:H	1:156:A:LEU:HD21	16	0.95
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	16	0.95
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	16	0.95
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	16	0.95
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	1	0.95
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	17	0.94
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	15	0.94
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	15	0.94
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	4	0.94
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	9	0.94
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	9	0.94
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	8	0.94
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	8	0.94
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	10	0.94
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	10	0.94
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	10	0.94
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	10	0.94
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	1	0.94
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	3	0.94
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	16	0.94
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	7	0.94
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	16	0.94
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	19	0.94
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	2	0.93
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	18	0.93
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	18	0.93
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	18	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	18	0.93
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	18	0.93
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	18	0.93
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	18	0.93
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	18	0.93
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	18	0.93
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	13	0.93
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	7	0.93
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	9	0.93
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	9	0.93
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	9	0.93
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	7	0.93
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	6	0.93
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	11	0.93
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	9	0.93
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	9	0.93
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	7	0.93
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD22	8	0.92
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD23	8	0.92
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	7	0.92
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	4	0.92
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	1	0.92
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	17	0.92
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	4	0.92
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	11	0.92
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	7	0.92
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	12	0.92
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C5	7	0.91
(2,1057)	1:130:A:GLY:H	4:321:A:PX4:C4	18	0.91
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	13	0.91
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	13	0.91
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	16	0.91
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	16	0.91
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	20	0.91
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	10	0.91
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	6	0.91
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	11	0.91
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	20	0.91
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	4	0.9
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	1	0.9
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	8	0.9
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	8	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,835)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	19	0.9
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	8	0.9
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	8	0.9
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD22	16	0.9
(2,808)	1:61:A:ILE:HD12	1:48:A:LEU:HD23	16	0.9
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	14	0.9
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	14	0.9
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	2	0.9
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	13	0.9
(2,237)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	19	0.9
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	10	0.9
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	8	0.9
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	19	0.89
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	1	0.89
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	7	0.89
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	7	0.89
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	7	0.89
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	19	0.89
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	19	0.89
(2,770)	1:19:A:LEU:HD22	1:17:A:ASP:H	6	0.89
(2,770)	1:19:A:LEU:HD23	1:17:A:ASP:H	6	0.89
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	3	0.89
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	3	0.89
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	16	0.89
(2,540)	1:169:A:ASP:H	1:166:A:LEU:HD21	14	0.89
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	3	0.89
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD22	12	0.88
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD23	12	0.88
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	19	0.88
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	19	0.88
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	19	0.88
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	19	0.88
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	19	0.88
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	19	0.88
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	12	0.88
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	12	0.88
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	12	0.88
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	15	0.88
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	15	0.88
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	17	0.88
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	17	0.88
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	8	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	8	0.88
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	8	0.88
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	14	0.87
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	14	0.87
(2,835)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	20	0.87
(2,788)	1:58:A:VAL:HG21	1:55:A:ASN:H	1	0.87
(2,788)	1:58:A:VAL:HG22	1:55:A:ASN:H	1	0.87
(2,788)	1:58:A:VAL:HG23	1:55:A:ASN:H	1	0.87
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	5	0.87
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	5	0.87
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	5	0.87
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	10	0.87
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	14	0.87
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	6	0.87
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	6	0.87
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	6	0.87
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	12	0.87
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	11	0.87
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	17	0.87
(2,237)	1:84:A:TRP:HE1	1:200:A:LEU:HD21	20	0.87
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG21	1	0.87
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG22	1	0.87
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG23	1	0.87
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	1	0.86
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	7	0.86
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	12	0.86
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	13	0.86
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	16	0.86
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	7	0.86
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	13	0.86
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	4	0.85
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	19	0.85
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD22	4	0.85
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD23	4	0.85
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	20	0.85
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	20	0.85
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	6	0.85
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	10	0.85
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	11	0.85
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	11	0.85
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	10	0.85
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	2	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	3	0.85
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	4	0.84
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	19	0.84
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	15	0.84
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	11	0.84
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	5	0.84
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	14	0.84
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	16	0.84
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	16	0.84
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	15	0.83
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	10	0.83
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	4	0.83
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	8	0.83
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	8	0.83
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	10	0.83
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	10	0.83
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	10	0.83
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	10	0.83
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	10	0.83
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	10	0.83
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	7	0.83
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	2	0.83
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	20	0.83
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	9	0.83
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	3	0.83
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	3	0.83
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	11	0.83
(3,47)	1:80:A:ASN:H	4:319:A:PX4:C5	14	0.82
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	10	0.82
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	17	0.82
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	12	0.82
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	12	0.82
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	12	0.82
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	12	0.82
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	15	0.82
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	15	0.82
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	16	0.82
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	16	0.82
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	20	0.82
(3,82)	1:147:A:TYR:H	4:319:A:PX4:C4	20	0.81
(3,29)	1:200:A:LEU:H	4:348:A:PX4:C35	4	0.81
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	5	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	5	0.81
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	10	0.81
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	19	0.81
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	7	0.81
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	20	0.81
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	6	0.81
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	19	0.81
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	12	0.81
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	12	0.81
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	18	0.81
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	18	0.81
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	18	0.81
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	1	0.81
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	6	0.81
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	9	0.81
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	1	0.81
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	1	0.81
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	1	0.81
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	13	0.81
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	13	0.81
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	7	0.8
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	19	0.8
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	19	0.8
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	14	0.8
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	14	0.8
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	17	0.8
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	17	0.8
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	15	0.8
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	15	0.8
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	17	0.8
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	17	0.8
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	17	0.8
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	17	0.8
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	1	0.8
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	20	0.8
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	20	0.8
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	20	0.8
(3,83)	1:150:A:ASP:H	4:305:A:PX4:C3	20	0.79
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	20	0.79
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	20	0.79
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	19	0.79
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	19	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	19	0.79
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	19	0.79
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	8	0.79
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	11	0.79
(2,645)	1:199:A:SER:H	1:202:A:MET:H	14	0.79
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	12	0.79
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	7	0.79
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	7	0.79
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	6	0.79
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	9	0.79
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	13	0.79
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	14	0.79
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	8	0.79
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	14	0.79
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	14	0.79
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	10	0.78
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	11	0.78
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	11	0.78
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	17	0.78
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	17	0.78
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	17	0.78
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	17	0.78
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	17	0.78
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	17	0.78
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	17	0.78
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	17	0.78
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	17	0.78
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	4	0.78
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	5	0.78
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	14	0.78
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	6	0.78
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	17	0.78
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	17	0.78
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	9	0.77
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	6	0.77
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	7	0.77
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	7	0.77
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	7	0.77
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	7	0.77
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	17	0.77
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	2	0.77
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	12	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	4	0.77
(3,27)	1:192:A:ALA:H	4:332:A:PX4:C35	12	0.76
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	15	0.76
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	15	0.76
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	15	0.76
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	2	0.76
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	14	0.76
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	11	0.76
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	5	0.76
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	5	0.76
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	20	0.76
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	5	0.76
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	8	0.75
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	8	0.75
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	3	0.75
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD22	5	0.75
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD23	5	0.75
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	17	0.75
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	2	0.75
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	2	0.75
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	2	0.75
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	2	0.75
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	12	0.75
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	12	0.75
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	3	0.75
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	3	0.75
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	3	0.75
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	16	0.75
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD22	5	0.74
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD23	5	0.74
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	1	0.74
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	5	0.74
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	4	0.74
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	4	0.74
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	9	0.74
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	16	0.74
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	2	0.74
(2,847)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	7	0.74
(2,828)	1:89:A:VAL:HG13	1:200:A:LEU:HD21	7	0.74
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	13	0.74
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	13	0.74
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	13	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	13	0.74
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	11	0.74
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD22	17	0.73
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD23	17	0.73
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	20	0.73
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	20	0.73
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	8	0.73
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	20	0.73
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	20	0.73
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	8	0.73
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	20	0.73
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	8	0.73
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	8	0.73
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	8	0.73
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	2	0.73
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	16	0.73
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	16	0.73
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	18	0.73
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	15	0.72
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	15	0.72
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	13	0.72
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	13	0.72
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	12	0.72
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	12	0.72
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	3	0.72
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	5	0.72
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	5	0.72
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	1	0.72
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	11	0.72
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	10	0.72
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	19	0.72
(2,262)	1:134:A:ILE:HD11	1:90:A:THR:H	16	0.72
(2,262)	1:134:A:ILE:HD12	1:90:A:THR:H	16	0.72
(2,262)	1:134:A:ILE:HD13	1:90:A:THR:H	16	0.72
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	7	0.72
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	7	0.72
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	9	0.72
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	9	0.72
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	20	0.72
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	9	0.72
(3,8)	1:86:A:SER:H	4:332:A:PX4:C35	7	0.71
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	15	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	16	0.71
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	16	0.71
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	16	0.71
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	2	0.71
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	11	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	2	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	2	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	2	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	2	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	2	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	2	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	2	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	2	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	2	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	4	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	4	0.71
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	4	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	4	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	4	0.71
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	4	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	4	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	4	0.71
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	4	0.71
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	4	0.71
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	4	0.71
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	4	0.71
(2,767)	1:24:A:LEU:H	1:24:A:LEU:HD21	4	0.71
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	6	0.71
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	6	0.71
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	19	0.71
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	4	0.71
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	5	0.71
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	5	0.71
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	3	0.71
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	3	0.71
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	3	0.71
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	1	0.71
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	13	0.71
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	20	0.71
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD22	16	0.71
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD23	16	0.71
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	3	0.71
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	3	0.71
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	1	0.71
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	12	0.71
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	16	0.71
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	18	0.71
(2,70)	1:24:A:LEU:H	1:24:A:LEU:HD21	4	0.71
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	15	0.7
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	2	0.7
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	12	0.7
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	7	0.7
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	15	0.7
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	10	0.7
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	17	0.7
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	6	0.7
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	6	0.7
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	4	0.69
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	4	0.69
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	19	0.69
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	19	0.69
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	14	0.69
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	14	0.69
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	14	0.69
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	8	0.69
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	10	0.69
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	10	0.69
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	15	0.69
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	15	0.69
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	8	0.69
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	15	0.69
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	15	0.69
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	12	0.69
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	12	0.69
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	2	0.69
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	1	0.69
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	19	0.69
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	1	0.68
(2,913)	1:113:A:LEU:H	1:196:A:LEU:HD22	5	0.68
(2,913)	1:113:A:LEU:H	1:196:A:LEU:HD23	5	0.68
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	7	0.68
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	11	0.68
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	11	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	11	0.68
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	11	0.68
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	20	0.68
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	20	0.68
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	20	0.68
(2,772)	1:19:A:LEU:HD22	1:22:A:PHE:H	20	0.68
(2,772)	1:19:A:LEU:HD23	1:22:A:PHE:H	20	0.68
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	19	0.68
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	20	0.68
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	5	0.68
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	19	0.68
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	1	0.68
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	19	0.68
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	5	0.68
(2,357)	1:113:A:LEU:H	1:196:A:LEU:HD22	5	0.68
(2,357)	1:113:A:LEU:H	1:196:A:LEU:HD23	5	0.68
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C3	7	0.67
(2,870)	1:89:A:VAL:HG11	1:122:A:LEU:HD21	20	0.67
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	12	0.67
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	12	0.67
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	12	0.67
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	12	0.67
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	14	0.67
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	17	0.67
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	8	0.67
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	8	0.67
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	14	0.67
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	1	0.67
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	11	0.66
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	5	0.66
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	5	0.66
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	17	0.66
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	17	0.66
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	17	0.66
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	17	0.66
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD22	1	0.66
(2,806)	1:61:A:ILE:HD11	1:48:A:LEU:HD23	1	0.66
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	1	0.66
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	1	0.66
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	7	0.66
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	7	0.66
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	10	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	5	0.66
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	5	0.66
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	11	0.66
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	11	0.66
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	11	0.66
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	7	0.66
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	7	0.66
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	16	0.66
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	7	0.65
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	4	0.65
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	4	0.65
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	1	0.65
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	1	0.65
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	1	0.65
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	16	0.65
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	13	0.65
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	19	0.65
(2,59)	1:217:A:GLY:H	1:219:A:GLY:H	12	0.65
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	16	0.65
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	16	0.65
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	8	0.64
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	8	0.64
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	11	0.64
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	11	0.64
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	11	0.64
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	11	0.64
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	11	0.64
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	11	0.64
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	11	0.64
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	11	0.64
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	11	0.64
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	2	0.64
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	2	0.64
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	11	0.64
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	11	0.64
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	7	0.64
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	7	0.64
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	7	0.64
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	7	0.64
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	7	0.64
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	7	0.64
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	7	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	7	0.64
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	7	0.64
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	2	0.64
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	2	0.64
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	2	0.64
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	2	0.64
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	2	0.64
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	2	0.64
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	5	0.64
(2,645)	1:199:A:SER:H	1:202:A:MET:H	12	0.64
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	16	0.64
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	16	0.64
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	19	0.64
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	2	0.64
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	15	0.64
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	3	0.64
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	7	0.64
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	11	0.64
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	13	0.64
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	17	0.64
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	15	0.63
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	12	0.63
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	17	0.63
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	17	0.63
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	18	0.63
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD11	19	0.63
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD12	19	0.63
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD13	19	0.63
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	12	0.63
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	18	0.63
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	12	0.63
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	20	0.63
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	5	0.63
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	5	0.63
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	5	0.63
(2,111)	1:43:A:GLN:H	1:43:A:GLN:HE21	2	0.63
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	12	0.63
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	12	0.62
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	12	0.62
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	12	0.62
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	12	0.62
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	12	0.62
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	12	0.62
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	12	0.62
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	12	0.62
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	18	0.62
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	18	0.62
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	18	0.62
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	18	0.62
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	18	0.62
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	18	0.62
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	18	0.62
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	18	0.62
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	18	0.62
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	18	0.62
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	6	0.62
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	6	0.62
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	13	0.62
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	13	0.62
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	8	0.62
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	8	0.62
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	8	0.62
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	8	0.62
(2,762)	1:19:A:LEU:HD22	1:38:A:LYS:H	11	0.62
(2,762)	1:19:A:LEU:HD23	1:38:A:LYS:H	11	0.62
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	17	0.62
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	4	0.62
(2,681)	1:212:A:MET:H	1:227:A:SER:H	5	0.62
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	19	0.62
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	9	0.62
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	1	0.62
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	11	0.62
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	11	0.62
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	10	0.62
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	3	0.62
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	8	0.62
(3,25)	1:180:A:ASP:H	4:324:A:PX4:C35	19	0.61
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	20	0.61
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	9	0.61
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	9	0.61
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	9	0.61
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	1	0.61
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	16	0.61
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	16	0.61
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	9	0.61
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	9	0.61
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	9	0.61
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	9	0.61
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	7	0.61
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	7	0.61
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	7	0.61
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	9	0.61
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	9	0.61
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	9	0.61
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	9	0.61
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	9	0.61
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	6	0.61
(2,658)	1:200:A:LEU:HD21	1:201:A:GLY:H	14	0.61
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	20	0.61
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	20	0.61
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	6	0.61
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	16	0.61
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	3	0.61
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	19	0.61
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	1	0.61
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	1	0.61
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	16	0.61
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	13	0.61
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	6	0.61
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	6	0.61
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	6	0.61
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	3	0.61
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	5	0.61
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	15	0.6
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	15	0.6
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	7	0.6
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	7	0.6
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	19	0.6
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	19	0.6
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	13	0.6
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	9	0.6
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD22	2	0.6
(2,810)	1:61:A:ILE:HD13	1:48:A:LEU:HD23	2	0.6
(2,752)	1:22:A:PHE:H	1:25:A:TYR:H	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,645)	1:199:A:SER:H	1:202:A:MET:H	16	0.6
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	20	0.6
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	3	0.6
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	18	0.6
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	14	0.6
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	13	0.6
(2,316)	1:106:A:ASP:H	1:109:A:VAL:H	14	0.6
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	10	0.6
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	8	0.6
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	8	0.6
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	13	0.6
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	18	0.59
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	18	0.59
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	18	0.59
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	18	0.59
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	11	0.59
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	11	0.59
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	11	0.59
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	11	0.59
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	11	0.59
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	11	0.59
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	11	0.59
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	11	0.59
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	11	0.59
(2,681)	1:212:A:MET:H	1:227:A:SER:H	3	0.59
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	16	0.59
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	16	0.59
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	16	0.59
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	5	0.59
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	7	0.59
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	20	0.59
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	6	0.59
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	14	0.59
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	2	0.59
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	9	0.59
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	20	0.59
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	16	0.59
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C5	8	0.58
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	18	0.58
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	5	0.58
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD22	7	0.58
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD23	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	17	0.58
(2,863)	1:89:A:VAL:HG21	1:200:A:LEU:HD21	14	0.58
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	16	0.58
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	16	0.58
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	16	0.58
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	19	0.58
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	19	0.58
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	19	0.58
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	19	0.58
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	19	0.58
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	19	0.58
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	2	0.58
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	2	0.58
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	2	0.58
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	7	0.58
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	7	0.58
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	6	0.58
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	6	0.58
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	6	0.58
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	6	0.58
(2,512)	1:160:A:PHE:H	1:167:A:GLY:HA3	7	0.58
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	4	0.58
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	18	0.58
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	16	0.58
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	17	0.58
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	3	0.58
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	3	0.58
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	3	0.58
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	8	0.58
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	6	0.58
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	12	0.58
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	8	0.58
(3,33)	1:235:A:GLN:H	4:338:A:PX4:C35	4	0.57
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	13	0.57
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD11	19	0.57
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD12	19	0.57
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD13	19	0.57
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	10	0.57
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	1	0.57
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	2	0.57
(2,336)	1:111:A:LYS:H	1:108:A:LEU:H	3	0.57
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	17	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	2	0.57
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	10	0.57
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	5	0.57
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	11	0.57
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	17	0.57
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	14	0.57
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	18	0.57
(3,26)	1:181:A:GLY:H	4:320:A:PX4:C35	12	0.56
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD22	7	0.56
(2,1028)	1:58:A:VAL:HG13	1:54:A:LEU:HD23	7	0.56
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	18	0.56
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD11	9	0.56
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD12	9	0.56
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD13	9	0.56
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	13	0.56
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	11	0.56
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	11	0.56
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	19	0.56
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	19	0.56
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	9	0.56
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	9	0.56
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	20	0.56
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	20	0.56
(2,772)	1:19:A:LEU:HD22	1:22:A:PHE:H	16	0.56
(2,772)	1:19:A:LEU:HD23	1:22:A:PHE:H	16	0.56
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	4	0.56
(2,681)	1:212:A:MET:H	1:227:A:SER:H	1	0.56
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	9	0.56
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	10	0.56
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	20	0.56
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	16	0.56
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	17	0.56
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	9	0.56
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	17	0.56
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD22	9	0.56
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD23	9	0.56
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	8	0.56
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	11	0.56
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	14	0.56
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	14	0.56
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	14	0.56
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	20	0.55
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	16	0.55
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	18	0.55
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	15	0.55
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	7	0.55
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	15	0.55
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	11	0.55
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	8	0.55
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	16	0.55
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	2	0.55
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	2	0.55
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	20	0.55
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	14	0.55
(2,248)	1:88:A:VAL:H	1:122:A:LEU:HD21	8	0.55
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	2	0.55
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	2	0.55
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	2	0.55
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	3	0.55
(2,171)	1:55:A:ASN:H	1:58:A:VAL:H	9	0.55
(2,151)	1:55:A:ASN:H	1:58:A:VAL:H	9	0.55
(2,135)	1:46:A:PHE:H	1:48:A:LEU:H	17	0.55
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	18	0.55
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C3	9	0.54
(2,1025)	1:58:A:VAL:HG12	1:54:A:LEU:HD21	5	0.54
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	20	0.54
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	18	0.54
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	18	0.54
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	18	0.54
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	18	0.54
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	4	0.54
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	4	0.54
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	4	0.54
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	16	0.54
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	17	0.54
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	17	0.54
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	3	0.54
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	18	0.54
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	18	0.54
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	18	0.54
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	12	0.54
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	12	0.54
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	2	0.54
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	16	0.54
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	15	0.54
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	8	0.54
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	8	0.54
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	1	0.54
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	7	0.54
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	7	0.54
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	7	0.54
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	19	0.54
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	14	0.54
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	15	0.54
(3,83)	1:150:A:ASP:H	4:340:A:PX4:C4	13	0.53
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	10	0.53
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	20	0.53
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	20	0.53
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	20	0.53
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD11	18	0.53
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD12	18	0.53
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD13	18	0.53
(2,913)	1:113:A:LEU:H	1:196:A:LEU:HD22	1	0.53
(2,913)	1:113:A:LEU:H	1:196:A:LEU:HD23	1	0.53
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	15	0.53
(2,872)	1:89:A:VAL:HG12	1:122:A:LEU:HD21	14	0.53
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	15	0.53
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	14	0.53
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	14	0.53
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	12	0.53
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	3	0.53
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	3	0.53
(2,547)	1:170:A:ALA:H	1:171:A:HIS:HD2	20	0.53
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	18	0.53
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	18	0.53
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	18	0.53
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	4	0.53
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	15	0.53
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	4	0.53
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	11	0.53
(2,357)	1:113:A:LEU:H	1:196:A:LEU:HD22	1	0.53
(2,357)	1:113:A:LEU:H	1:196:A:LEU:HD23	1	0.53
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	1	0.53
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	9	0.53
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	16	0.53
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	9	0.53
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	9	0.53
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	9	0.53
(2,149)	1:43:A:GLN:HE22	1:52:A:GLY:H	6	0.53
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	5	0.53
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	2	0.53
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	19	0.53
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	3	0.53
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	7	0.52
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	2	0.52
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	2	0.52
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	2	0.52
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	1	0.52
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	1	0.52
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	15	0.52
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	15	0.52
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	15	0.52
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	10	0.52
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	10	0.52
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	10	0.52
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	13	0.52
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	13	0.52
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	17	0.52
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG13	5	0.52
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG12	5	0.52
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	13	0.52
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	7	0.52
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	19	0.52
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	3	0.52
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	13	0.52
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	2	0.51
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	6	0.51
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	6	0.51
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG11	20	0.51
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG12	20	0.51
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG13	20	0.51
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	14	0.51
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	4	0.51
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	15	0.51
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	2	0.51
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	2	0.51
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	6	0.51
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	18	0.51
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	4	0.51
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	4	0.51
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	4	0.51
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	7	0.51
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	2	0.51
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	6	0.51
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	12	0.51
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	15	0.51
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	2	0.51
(3,25)	1:180:A:ASP:H	4:320:A:PX4:C35	12	0.5
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	12	0.5
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	12	0.5
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	12	0.5
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	7	0.5
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	7	0.5
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	8	0.5
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	8	0.5
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	20	0.5
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	20	0.5
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	20	0.5
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	20	0.5
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	19	0.5
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	19	0.5
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	19	0.5
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	17	0.5
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	17	0.5
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	17	0.5
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	17	0.5
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	17	0.5
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	17	0.5
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	3	0.5
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	11	0.5
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	11	0.5
(2,612)	1:108:A:LEU:HD22	1:188:A:PHE:H	8	0.5
(2,612)	1:108:A:LEU:HD23	1:188:A:PHE:H	8	0.5
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	13	0.5
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	20	0.5
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	16	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	17	0.5
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	17	0.5
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	6	0.5
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	3	0.5
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD22	18	0.5
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD23	18	0.5
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	6	0.5
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	6	0.5
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	6	0.5
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	9	0.5
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	10	0.5
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	10	0.5
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	2	0.5
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	3	0.5
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	12	0.5
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	5	0.5
(3,82)	1:147:A:TYR:H	4:310:A:PX4:C4	15	0.49
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	2	0.49
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	17	0.49
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	17	0.49
(2,924)	1:113:A:LEU:HD22	1:196:A:LEU:HD21	1	0.49
(2,879)	1:127:A:VAL:HG11	1:91:A:TYR:H	4	0.49
(2,879)	1:127:A:VAL:HG12	1:91:A:TYR:H	4	0.49
(2,879)	1:127:A:VAL:HG13	1:91:A:TYR:H	4	0.49
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	10	0.49
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	10	0.49
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	11	0.49
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	11	0.49
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	17	0.49
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	17	0.49
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	10	0.49
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	10	0.49
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	10	0.49
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	10	0.49
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	10	0.49
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	10	0.49
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	10	0.49
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	10	0.49
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	10	0.49
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	13	0.49
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	13	0.49
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	18	0.49
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	20	0.49
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	15	0.49
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	6	0.49
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	8	0.49
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	10	0.49
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	15	0.49
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	13	0.49
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	13	0.49
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	13	0.49
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	3	0.49
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	9	0.49
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	3	0.49
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	9	0.49
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	10	0.49
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	15	0.49
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	1	0.48
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	5	0.48
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	5	0.48
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	18	0.48
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	17	0.48
(2,645)	1:199:A:SER:H	1:202:A:MET:H	10	0.48
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	15	0.48
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	8	0.48
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	16	0.48
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	19	0.48
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	13	0.48
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	6	0.48
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	11	0.48
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	13	0.48
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	17	0.48
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	4	0.48
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	15	0.48
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	14	0.48
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	16	0.48
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	17	0.48
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	18	0.48
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	18	0.48
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	18	0.48
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	18	0.48
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	4	0.48
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	16	0.48
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	7	0.48
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	13	0.48
(3,84)	1:154:A:ASN:H	4:308:A:PX4:C3	10	0.47
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD22	10	0.47
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD23	10	0.47
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	4	0.47
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	16	0.47
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	16	0.47
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	13	0.47
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	2	0.47
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	2	0.47
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	2	0.47
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	2	0.47
(2,809)	1:61:A:ILE:HD13	1:48:A:LEU:HD21	4	0.47
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	2	0.47
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	2	0.47
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	2	0.47
(2,783)	1:58:A:VAL:HG11	1:54:A:LEU:HD11	5	0.47
(2,783)	1:58:A:VAL:HG11	1:54:A:LEU:HD12	5	0.47
(2,783)	1:58:A:VAL:HG11	1:54:A:LEU:HD13	5	0.47
(2,783)	1:58:A:VAL:HG12	1:54:A:LEU:HD11	5	0.47
(2,783)	1:58:A:VAL:HG12	1:54:A:LEU:HD12	5	0.47
(2,783)	1:58:A:VAL:HG12	1:54:A:LEU:HD13	5	0.47
(2,783)	1:58:A:VAL:HG13	1:54:A:LEU:HD11	5	0.47
(2,783)	1:58:A:VAL:HG13	1:54:A:LEU:HD12	5	0.47
(2,783)	1:58:A:VAL:HG13	1:54:A:LEU:HD13	5	0.47
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	2	0.47
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	15	0.47
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	5	0.47
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	13	0.47
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	1	0.47
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	3	0.47
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	14	0.47
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	13	0.47
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	19	0.47
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	5	0.47
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	17	0.47
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	18	0.47
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	18	0.47
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	18	0.47
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	3	0.47
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	4	0.47
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	10	0.47
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	13	0.47
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	18	0.47
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	10	0.47
(3,26)	1:181:A:GLY:H	4:414:A:PX4:C35	10	0.46
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	3	0.46
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	3	0.46
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	3	0.46
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG11	1	0.46
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG12	1	0.46
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG13	1	0.46
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG11	1	0.46
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG12	1	0.46
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG13	1	0.46
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG11	1	0.46
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG12	1	0.46
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG13	1	0.46
(2,789)	1:58:A:VAL:HG21	1:55:A:ASN:HD22	12	0.46
(2,789)	1:58:A:VAL:HG22	1:55:A:ASN:HD22	12	0.46
(2,789)	1:58:A:VAL:HG23	1:55:A:ASN:HD22	12	0.46
(2,767)	1:24:A:LEU:H	1:24:A:LEU:HD21	11	0.46
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	3	0.46
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	20	0.46
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	20	0.46
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	11	0.46
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	2	0.46
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	13	0.46
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	14	0.46
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	3	0.46
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	10	0.46
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	15	0.46
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	2	0.46
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	16	0.46
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	16	0.46
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	12	0.46
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	8	0.46
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	12	0.46
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	20	0.46
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	20	0.46
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	20	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:24:A:LEU:H	1:24:A:LEU:HD21	11	0.46
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	16	0.46
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	20	0.46
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	8	0.45
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	8	0.45
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	8	0.45
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	8	0.45
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	8	0.45
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	8	0.45
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	8	0.45
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	8	0.45
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	8	0.45
(2,996)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	19	0.45
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	14	0.45
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	14	0.45
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	10	0.45
(2,767)	1:24:A:LEU:H	1:24:A:LEU:HD21	15	0.45
(2,762)	1:19:A:LEU:HD22	1:38:A:LYS:H	3	0.45
(2,762)	1:19:A:LEU:HD23	1:38:A:LYS:H	3	0.45
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	10	0.45
(2,681)	1:212:A:MET:H	1:227:A:SER:H	13	0.45
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	1	0.45
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	15	0.45
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	16	0.45
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	19	0.45
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	14	0.45
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	2	0.45
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	13	0.45
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	6	0.45
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	13	0.45
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	4	0.45
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	1	0.45
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	18	0.45
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	4	0.45
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	4	0.45
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	14	0.45
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	12	0.45
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	14	0.45
(2,70)	1:24:A:LEU:H	1:24:A:LEU:HD21	15	0.45
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	19	0.45
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	1	0.45
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD22	12	0.44
(2,1024)	1:58:A:VAL:HG11	1:54:A:LEU:HD23	12	0.44
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	17	0.44
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	10	0.44
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	10	0.44
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	16	0.44
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	10	0.44
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	18	0.44
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	3	0.44
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	3	0.44
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	19	0.44
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	19	0.44
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	19	0.44
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	1	0.44
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	11	0.44
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	9	0.44
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	7	0.44
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	3	0.44
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	15	0.44
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	15	0.44
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	2	0.44
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	9	0.44
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	9	0.44
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	19	0.44
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	19	0.44
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	6	0.44
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	6	0.44
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	6	0.44
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	18	0.44
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	18	0.44
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	18	0.44
(2,171)	1:55:A:ASN:H	1:58:A:VAL:H	6	0.44
(2,151)	1:55:A:ASN:H	1:58:A:VAL:H	6	0.44
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	13	0.44
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	13	0.44
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD11	7	0.44
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD12	7	0.44
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD13	7	0.44
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	20	0.44
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	9	0.44
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	14	0.44
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,998)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	20	0.43
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	5	0.43
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	8	0.43
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	8	0.43
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	8	0.43
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	8	0.43
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	8	0.43
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	8	0.43
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	8	0.43
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	8	0.43
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	8	0.43
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	15	0.43
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	18	0.43
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	16	0.43
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	19	0.43
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	14	0.43
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	4	0.43
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	7	0.43
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	9	0.43
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	5	0.43
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	5	0.43
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	1	0.43
(2,245)	1:88:A:VAL:H	1:123:A:HIS:H	13	0.43
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	19	0.43
(2,163)	1:55:A:ASN:HD21	1:48:A:LEU:HD21	19	0.43
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	5	0.43
(2,133)	1:47:A:GLY:H	1:206:A:SER:HB3	4	0.43
(2,133)	1:47:A:GLY:H	1:206:A:SER:HB2	4	0.43
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	9	0.43
(1,13)	3:304:A:ZN:ZN	1:204:A:HIS:NE2	2	0.43
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	16	0.43
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	7	0.42
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	7	0.42
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	7	0.42
(2,899)	1:108:A:LEU:HD21	1:109:A:VAL:H	18	0.42
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	16	0.42
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	3	0.42
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	10	0.42
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	2	0.42
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	2	0.42
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	19	0.42
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	12	0.42
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	6	0.42
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	1	0.42
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	20	0.42
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	20	0.42
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	16	0.42
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	2	0.42
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	2	0.42
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	5	0.42
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	19	0.42
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	15	0.42
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	13	0.42
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	13	0.42
(2,153)	1:55:A:ASN:H	1:55:A:ASN:HD21	20	0.42
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	9	0.42
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	6	0.42
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	6	0.42
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	20	0.42
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	5	0.41
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	3	0.41
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	3	0.41
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	15	0.41
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	15	0.41
(2,790)	1:43:A:GLN:HE22	1:58:A:VAL:HG21	1	0.41
(2,790)	1:43:A:GLN:HE22	1:58:A:VAL:HG22	1	0.41
(2,790)	1:43:A:GLN:HE22	1:58:A:VAL:HG23	1	0.41
(2,645)	1:199:A:SER:H	1:202:A:MET:H	18	0.41
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	15	0.41
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	15	0.41
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	9	0.41
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	5	0.41
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	4	0.41
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	12	0.41
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	11	0.41
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	13	0.41
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	6	0.41
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	16	0.41
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	20	0.41
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	1	0.41
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	3	0.41
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	11	0.41
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	20	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	1:86:A:SER:H	4:345:A:PX4:C35	6	0.4
(2,996)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	17	0.4
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD22	20	0.4
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD23	20	0.4
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	12	0.4
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	1	0.4
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	1	0.4
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	1	0.4
(2,681)	1:212:A:MET:H	1:227:A:SER:H	7	0.4
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	4	0.4
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	16	0.4
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	9	0.4
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	8	0.4
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	8	0.4
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD11	15	0.4
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD12	15	0.4
(2,124)	1:45:A:PHE:H	1:48:A:LEU:HD13	15	0.4
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	17	0.4
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	10	0.4
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	6	0.4
(3,26)	1:181:A:GLY:H	4:324:A:PX4:C35	19	0.39
(2,1023)	1:58:A:VAL:HG11	1:54:A:LEU:HD21	12	0.39
(2,865)	1:89:A:VAL:HG22	1:200:A:LEU:HD21	8	0.39
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	4	0.39
(2,846)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	4	0.39
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD22	4	0.39
(2,827)	1:89:A:VAL:HG12	1:200:A:LEU:HD23	4	0.39
(2,805)	1:61:A:ILE:HD11	1:48:A:LEU:HD21	4	0.39
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	19	0.39
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	19	0.39
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	19	0.39
(2,681)	1:212:A:MET:H	1:227:A:SER:H	16	0.39
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	14	0.39
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	14	0.39
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	19	0.39
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	6	0.39
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	12	0.39
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	20	0.39
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	12	0.39
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	4	0.39
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	4	0.39
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	18	0.39
(2,154)	1:55:A:ASN:H	1:59:A:ILE:H	13	0.39
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	6	0.39
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	12	0.39
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	8	0.39
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	8	0.39
(2,76)	1:11:A:GLN:H	1:14:A:GLN:H	15	0.39
(1,13)	3:304:A:ZN:ZN	1:204:A:HIS:NE2	5	0.39
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	2	0.39
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	15	0.39
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	6	0.39
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	9	0.39
(1,2)	2:301:A:CA:CA	1:133:A:ASP:O	18	0.39
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	6	0.39
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	18	0.38
(2,938)	1:196:A:LEU:HD21	1:200:A:LEU:HD21	14	0.38
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	17	0.38
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	13	0.38
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	13	0.38
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	19	0.38
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	8	0.38
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	8	0.38
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	9	0.38
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	10	0.38
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	10	0.38
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	10	0.38
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	8	0.38
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	8	0.38
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	8	0.38
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	3	0.38
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	11	0.38
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	5	0.38
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	9	0.38
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	17	0.38
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	3	0.38
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	5	0.38
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	18	0.38
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	15	0.38
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	5	0.38
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	5	0.38
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	5	0.38
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	19	0.38
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	7	0.38
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	9	0.38
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	11	0.38
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	13	0.38
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	17	0.38
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	11	0.38
(3,47)	1:80:A:ASN:H	4:321:A:PX4:C5	1	0.37
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	6	0.37
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	14	0.37
(2,815)	1:72:A:VAL:HG11	1:74:A:GLU:H	5	0.37
(2,815)	1:72:A:VAL:HG12	1:74:A:GLU:H	5	0.37
(2,815)	1:72:A:VAL:HG13	1:74:A:GLU:H	5	0.37
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG11	18	0.37
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG12	18	0.37
(2,814)	1:71:A:ASP:H	1:72:A:VAL:HG13	18	0.37
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	19	0.37
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	19	0.37
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	19	0.37
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	13	0.37
(2,645)	1:199:A:SER:H	1:202:A:MET:H	11	0.37
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD11	20	0.37
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD12	20	0.37
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD13	20	0.37
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	11	0.37
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	11	0.37
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	11	0.37
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	6	0.37
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	6	0.37
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	6	0.37
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	5	0.37
(2,489)	1:154:A:ASN:H	1:64:A:LYS:H	15	0.37
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	9	0.37
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	19	0.37
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	19	0.37
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	9	0.37
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	7	0.37
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	1	0.37
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	1	0.37
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	1	0.37
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	1	0.37
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	6	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	16	0.37
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	11	0.37
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	10	0.37
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	18	0.37
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	2	0.37
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	2	0.37
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	17	0.37
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	17	0.36
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	17	0.36
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	18	0.36
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	18	0.36
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	18	0.36
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	19	0.36
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	19	0.36
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	19	0.36
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	17	0.36
(2,845)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	2	0.36
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	15	0.36
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	15	0.36
(2,826)	1:89:A:VAL:HG12	1:200:A:LEU:HD21	2	0.36
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	15	0.36
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	15	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	1	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	1	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	1	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	1	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	1	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	1	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	5	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	5	0.36
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	5	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	5	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	5	0.36
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	5	0.36
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	14	0.36
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	14	0.36
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	14	0.36
(2,653)	1:200:A:LEU:H	1:202:A:MET:H	16	0.36
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	11	0.36
(2,645)	1:199:A:SER:H	1:202:A:MET:H	5	0.36
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	8	0.36
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	17	0.36
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	3	0.36
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	11	0.36
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	2	0.36
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	2	0.36
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	4	0.36
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	3	0.36
(2,226)	1:75:A:TYR:H	1:73:A:ALA:HA	2	0.36
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	19	0.36
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	19	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	8	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	8	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	8	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	10	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	10	0.36
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	10	0.36
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	13	0.36
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	20	0.36
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	9	0.36
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	19	0.36
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	2	0.36
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	1	0.36
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	1	0.36
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	16	0.36
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	1	0.36
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	11	0.36
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	16	0.36
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	17	0.36
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	19	0.36
(2,996)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	4	0.35
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD22	4	0.35
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD23	4	0.35
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	5	0.35
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	5	0.35
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	14	0.35
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	10	0.35
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	10	0.35
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	10	0.35
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	12	0.35
(2,681)	1:212:A:MET:H	1:227:A:SER:H	8	0.35
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	4	0.35
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,645)	1:199:A:SER:H	1:202:A:MET:H	1	0.35
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	17	0.35
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	3	0.35
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	13	0.35
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	13	0.35
(2,589)	1:179:A:THR:H	1:100:A:LEU:HD22	6	0.35
(2,589)	1:179:A:THR:H	1:100:A:LEU:HD23	6	0.35
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	20	0.35
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	10	0.35
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	9	0.35
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	12	0.35
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	9	0.35
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	15	0.35
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	4	0.35
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	14	0.35
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	14	0.35
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	17	0.35
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	14	0.35
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	20	0.35
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	17	0.35
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	17	0.35
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	17	0.35
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	16	0.35
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	16	0.35
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	10	0.35
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	10	0.35
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	10	0.35
(1,13)	3:304:A:ZN:ZN	1:204:A:HIS:NE2	12	0.35
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	9	0.35
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	4	0.35
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	7	0.35
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	8	0.35
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	1	0.35
(1,2)	2:301:A:CA:CA	1:133:A:ASP:O	3	0.35
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	19	0.35
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	13	0.34
(2,1025)	1:58:A:VAL:HG12	1:54:A:LEU:HD21	8	0.34
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD22	19	0.34
(2,991)	1:186:A:ILE:HD12	1:156:A:LEU:HD23	19	0.34
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	11	0.34
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	6	0.34
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,636)	1:198:A:HIS:H	1:195:A:ALA:H	4	0.34
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	4	0.34
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	4	0.34
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	4	0.34
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	2	0.34
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	11	0.34
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	11	0.34
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	12	0.34
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	16	0.34
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	7	0.34
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	11	0.34
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	11	0.34
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	3	0.34
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	10	0.34
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	4	0.34
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	14	0.34
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	1	0.34
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	3	0.34
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	15	0.34
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	19	0.34
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	20	0.34
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	20	0.34
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	9	0.34
(2,325)	1:108:A:LEU:H	1:108:A:LEU:HD21	7	0.34
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	16	0.34
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD11	15	0.34
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD12	15	0.34
(2,162)	1:55:A:ASN:HD21	1:48:A:LEU:HD13	15	0.34
(2,72)	1:11:A:GLN:H	1:11:A:GLN:HE21	6	0.34
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	7	0.34
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	4	0.34
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	8	0.34
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	11	0.34
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	15	0.34
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	16	0.34
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	12	0.34
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	1	0.33
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	20	0.33
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	20	0.33
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	20	0.33
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	20	0.33
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	20	0.33
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	20	0.33
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	20	0.33
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	20	0.33
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	1	0.33
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	7	0.33
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	16	0.33
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	7	0.33
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	1	0.33
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	12	0.33
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	12	0.33
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	13	0.33
(2,279)	1:136:A:ILE:H	1:93:A:ILE:H	12	0.33
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	12	0.33
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	12	0.33
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	12	0.33
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	16	0.33
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	12	0.33
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	12	0.33
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	17	0.33
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	17	0.33
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	17	0.33
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	13	0.33
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	18	0.33
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	6	0.33
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	18	0.33
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	9	0.33
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	12	0.33
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	4	0.33
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	20	0.32
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	12	0.32
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	12	0.32
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	5	0.32
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	1	0.32
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	1	0.32
(2,940)	1:196:A:LEU:HD22	1:200:A:LEU:HD21	15	0.32
(2,912)	1:113:A:LEU:H	1:196:A:LEU:HD21	9	0.32
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	5	0.32
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	5	0.32
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	5	0.32
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	5	0.32
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	8	0.32
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	8	0.32
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	8	0.32
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	8	0.32
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	8	0.32
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	19	0.32
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	19	0.32
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	3	0.32
(2,658)	1:200:A:LEU:HD21	1:201:A:GLY:H	6	0.32
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	1	0.32
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD11	1	0.32
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD12	1	0.32
(2,548)	1:170:A:ALA:H	1:136:A:ILE:HD13	1	0.32
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	16	0.32
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	16	0.32
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	5	0.32
(2,389)	1:120:A:ILE:HD11	1:119:A:GLU:H	3	0.32
(2,389)	1:120:A:ILE:HD12	1:119:A:GLU:H	3	0.32
(2,389)	1:120:A:ILE:HD13	1:119:A:GLU:H	3	0.32
(2,356)	1:113:A:LEU:H	1:196:A:LEU:HD21	9	0.32
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	2	0.32
(2,138)	1:48:A:LEU:HD21	1:47:A:GLY:H	2	0.32
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	18	0.32
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	2	0.32
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	2	0.32
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	7	0.32
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	10	0.32
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	15	0.32
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	4	0.32
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	7	0.32
(3,9)	1:96:A:TYR:H	4:320:A:PX4:C35	11	0.31
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	15	0.31
(2,862)	1:123:A:HIS:H	1:122:A:LEU:HD11	19	0.31
(2,862)	1:123:A:HIS:H	1:122:A:LEU:HD12	19	0.31
(2,862)	1:123:A:HIS:H	1:122:A:LEU:HD13	19	0.31
(2,760)	1:15:A:ALA:H	1:59:A:ILE:HD11	18	0.31
(2,760)	1:15:A:ALA:H	1:59:A:ILE:HD12	18	0.31
(2,760)	1:15:A:ALA:H	1:59:A:ILE:HD13	18	0.31
(2,753)	1:15:A:ALA:H	1:59:A:ILE:HD11	18	0.31
(2,753)	1:15:A:ALA:H	1:59:A:ILE:HD12	18	0.31
(2,753)	1:15:A:ALA:H	1:59:A:ILE:HD13	18	0.31
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	3	0.31
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	2	0.31
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	3	0.31
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	2	0.31
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	3	0.31
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	11	0.31
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD22	2	0.31
(2,591)	1:178:A:TRP:H	1:100:A:LEU:HD23	2	0.31
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	12	0.31
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	10	0.31
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	19	0.31
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	3	0.31
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	2	0.31
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	10	0.31
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	19	0.31
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	11	0.31
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	16	0.31
(2,279)	1:136:A:ILE:H	1:93:A:ILE:H	1	0.31
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	4	0.31
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	11	0.31
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	8	0.31
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	11	0.31
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	19	0.31
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	14	0.31
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	14	0.31
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	8	0.31
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	11	0.31
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	19	0.31
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	19	0.31
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	19	0.31
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	19	0.31
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	11	0.31
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	4	0.31
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	10	0.31
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	3	0.31
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	4	0.31
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	12	0.3
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD22	11	0.3
(2,1026)	1:58:A:VAL:HG12	1:54:A:LEU:HD23	11	0.3
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	5	0.3
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	5	0.3
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	13	0.3
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	9	0.3
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	9	0.3
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	20	0.3
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	20	0.3
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	20	0.3
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	14	0.3
(2,788)	1:58:A:VAL:HG21	1:55:A:ASN:H	20	0.3
(2,788)	1:58:A:VAL:HG22	1:55:A:ASN:H	20	0.3
(2,788)	1:58:A:VAL:HG23	1:55:A:ASN:H	20	0.3
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	4	0.3
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	4	0.3
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	4	0.3
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	4	0.3
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	4	0.3
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	4	0.3
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	9	0.3
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	9	0.3
(2,763)	1:19:A:LEU:HD21	1:40:A:LYS:H	18	0.3
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	20	0.3
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	8	0.3
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	12	0.3
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	12	0.3
(2,636)	1:198:A:HIS:H	1:195:A:ALA:H	1	0.3
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	8	0.3
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	15	0.3
(2,589)	1:179:A:THR:H	1:100:A:LEU:HD22	20	0.3
(2,589)	1:179:A:THR:H	1:100:A:LEU:HD23	20	0.3
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	2	0.3
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	4	0.3
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	12	0.3
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG13	4	0.3
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG12	4	0.3
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	5	0.3
(2,543)	1:170:A:ALA:H	1:169:A:ASP:H	9	0.3
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	13	0.3
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	6	0.3
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	17	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	2	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	2	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	3	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	6	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	6	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	12	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	12	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	20	0.3
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	20	0.3
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	7	0.3
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD11	1	0.3
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD12	1	0.3
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD13	1	0.3
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	12	0.3
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	7	0.3
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	11	0.3
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	8	0.3
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	11	0.3
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	18	0.3
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	12	0.3
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	11	0.3
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	11	0.3
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	11	0.3
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	8	0.3
(2,202)	1:64:A:LYS:H	1:64:A:LYS:HG3	18	0.3
(2,202)	1:64:A:LYS:H	1:64:A:LYS:HG2	18	0.3
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	11	0.3
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	9	0.3
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	14	0.3
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD22	16	0.3
(2,164)	1:55:A:ASN:HD21	1:48:A:LEU:HD23	16	0.3
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	9	0.3
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	14	0.3
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG21	20	0.3
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG22	20	0.3
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG23	20	0.3
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	4	0.3
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	1	0.3
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	20	0.3
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	4	0.3
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	19	0.3
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	4	0.3
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	6	0.3
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	20	0.3
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	17	0.3
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	6	0.3
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	10	0.29
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	10	0.29
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	10	0.29
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD22	20	0.29
(2,941)	1:196:A:LEU:HD22	1:200:A:LEU:HD23	20	0.29
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	13	0.29
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	13	0.29
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	13	0.29
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	14	0.29
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	14	0.29
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	14	0.29
(2,879)	1:127:A:VAL:HG11	1:91:A:TYR:H	6	0.29
(2,879)	1:127:A:VAL:HG12	1:91:A:TYR:H	6	0.29
(2,879)	1:127:A:VAL:HG13	1:91:A:TYR:H	6	0.29
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	19	0.29
(2,645)	1:199:A:SER:H	1:202:A:MET:H	9	0.29
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG21	14	0.29
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG22	14	0.29
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG23	14	0.29
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	13	0.29
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	19	0.29
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	20	0.29
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	13	0.29
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	6	0.29
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	6	0.29
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	6	0.29
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	13	0.29
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	14	0.29
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	14	0.29
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	14	0.29
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	9	0.29
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	2	0.29
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	10	0.29
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	3	0.29
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	13	0.29
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	15	0.29
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	18	0.29
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	9	0.29
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	6	0.29
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	2	0.28
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	3	0.28
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	3	0.28
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	3	0.28
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	4	0.28
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	4	0.28
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	19	0.28
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	19	0.28
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	19	0.28
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	19	0.28
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	19	0.28
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	19	0.28
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	19	0.28
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	19	0.28
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	19	0.28
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	10	0.28
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	13	0.28
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	10	0.28
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	13	0.28
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	14	0.28
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	13	0.28
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	13	0.28
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	13	0.28
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	8	0.28
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	8	0.28
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	16	0.28
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	1	0.28
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	8	0.28
(2,398)	1:122:A:LEU:H	1:120:A:ILE:HG13	20	0.28
(2,398)	1:122:A:LEU:H	1:120:A:ILE:HG12	20	0.28
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	14	0.28
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	19	0.28
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	11	0.28
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	7	0.28
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	5	0.28
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	9	0.28
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	1	0.28
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	6	0.28
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	15	0.28
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	1	0.28
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	6	0.28
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	15	0.28
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	9	0.28
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	11	0.28
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	12	0.28
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	11	0.28
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	17	0.28
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	17	0.28
(1,13)	3:304:A:ZN:ZN	1:204:A:HIS:NE2	8	0.28
(1,13)	3:304:A:ZN:ZN	1:204:A:HIS:NE2	16	0.28
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	14	0.28
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	13	0.28
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	17	0.28
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	14	0.28
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	3	0.27
(2,995)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	11	0.27
(2,995)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	11	0.27
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD11	13	0.27
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD12	13	0.27
(2,963)	1:200:A:LEU:HD21	1:122:A:LEU:HD13	13	0.27
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	6	0.27
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	6	0.27
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	6	0.27
(2,891)	1:105:A:VAL:HG21	1:105:A:VAL:H	1	0.27
(2,891)	1:105:A:VAL:HG22	1:105:A:VAL:H	1	0.27
(2,891)	1:105:A:VAL:HG23	1:105:A:VAL:H	1	0.27
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	16	0.27
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	16	0.27
(2,843)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	14	0.27
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	16	0.27
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	16	0.27
(2,824)	1:89:A:VAL:HG11	1:200:A:LEU:HD21	14	0.27
(2,728)	1:236:A:LYS:H	1:237:A:LEU:H	14	0.27
(2,728)	1:236:A:LYS:H	1:237:A:LEU:H	14	0.27
(2,681)	1:212:A:MET:H	1:227:A:SER:H	17	0.27
(2,675)	1:210:A:ALA:H	1:209:A:ASN:HD22	12	0.27
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	1	0.27
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	7	0.27
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	19	0.27
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	1	0.27
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	7	0.27
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	19	0.27
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	9	0.27
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	9	0.27
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	14	0.27
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	14	0.27
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	8	0.27
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	20	0.27
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	5	0.27
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	6	0.27
(2,313)	1:105:A:VAL:HG21	1:105:A:VAL:H	1	0.27
(2,313)	1:105:A:VAL:HG22	1:105:A:VAL:H	1	0.27
(2,313)	1:105:A:VAL:HG23	1:105:A:VAL:H	1	0.27
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	14	0.27
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	14	0.27
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	14	0.27
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	15	0.27
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	15	0.27
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	3	0.27
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	3	0.27
(2,157)	1:55:A:ASN:H	1:59:A:ILE:HG13	5	0.27
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	2	0.27
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	5	0.27
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	6	0.27
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	19	0.27
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	10	0.27
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	7	0.27
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	4	0.27
(1,4)	2:302:A:CA:CA	1:155:A:THR:O	5	0.27
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	12	0.27
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	9	0.27
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	15	0.27
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	5	0.27
(1,1)	2:301:A:CA:CA	1:167:A:GLY:O	14	0.27
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	4	0.26
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	4	0.26
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	4	0.26
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	4	0.26
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	4	0.26
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	9	0.26
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	9	0.26
(2,879)	1:127:A:VAL:HG11	1:91:A:TYR:H	1	0.26
(2,879)	1:127:A:VAL:HG12	1:91:A:TYR:H	1	0.26
(2,879)	1:127:A:VAL:HG13	1:91:A:TYR:H	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,874)	1:89:A:VAL:HG13	1:122:A:LEU:HD21	6	0.26
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	1	0.26
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	1	0.26
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	1	0.26
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	10	0.26
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	5	0.26
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	8	0.26
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	14	0.26
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	20	0.26
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	5	0.26
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	8	0.26
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	14	0.26
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	20	0.26
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	12	0.26
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	8	0.26
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	4	0.26
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	11	0.26
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	5	0.26
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	5	0.26
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	6	0.26
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	12	0.26
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	16	0.26
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	4	0.26
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD22	19	0.26
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD23	19	0.26
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD11	19	0.26
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD12	19	0.26
(2,217)	1:74:A:GLU:H	1:24:A:LEU:HD13	19	0.26
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	3	0.26
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	3	0.26
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	3	0.26
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	8	0.26
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	8	0.26
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	8	0.26
(2,204)	1:66:A:ARG:H	1:67:A:CYS:H	14	0.26
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	13	0.26
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	13	0.26
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	18	0.26
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	13	0.26
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	18	0.26
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	8	0.26
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	12	0.26
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	13	0.26
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	16	0.26
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	16	0.26
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	15	0.26
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	18	0.26
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	8	0.26
(1,13)	3:304:A:ZN:ZN	1:194:A:HIS:NE2	20	0.26
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	18	0.26
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	3	0.26
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	20	0.26
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	13	0.26
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	14	0.26
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	17	0.26
(2,994)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	7	0.25
(2,946)	1:109:A:VAL:HG22	1:196:A:LEU:HD21	18	0.25
(2,908)	1:91:A:TYR:HE1	1:109:A:VAL:HG11	18	0.25
(2,908)	1:91:A:TYR:HE1	1:109:A:VAL:HG12	18	0.25
(2,908)	1:91:A:TYR:HE1	1:109:A:VAL:HG13	18	0.25
(2,908)	1:91:A:TYR:HE2	1:109:A:VAL:HG11	18	0.25
(2,908)	1:91:A:TYR:HE2	1:109:A:VAL:HG12	18	0.25
(2,908)	1:91:A:TYR:HE2	1:109:A:VAL:HG13	18	0.25
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG11	7	0.25
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG12	7	0.25
(2,774)	1:39:A:LEU:HD22	1:58:A:VAL:HG13	7	0.25
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG11	7	0.25
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG12	7	0.25
(2,774)	1:39:A:LEU:HD23	1:58:A:VAL:HG13	7	0.25
(2,771)	1:19:A:LEU:HD21	1:22:A:PHE:H	20	0.25
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	7	0.25
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	7	0.25
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	5	0.25
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	6	0.25
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	9	0.25
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	6	0.25
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	9	0.25
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	2	0.25
(2,639)	1:198:A:HIS:H	1:202:A:MET:H	14	0.25
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	17	0.25
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	20	0.25
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	4	0.25
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	18	0.25
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	18	0.25
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	14	0.25
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	9	0.25
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	19	0.25
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	10	0.25
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	18	0.25
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	2	0.25
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	2	0.25
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	18	0.25
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	19	0.25
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	17	0.25
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	3	0.25
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	3	0.25
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	3	0.25
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	5	0.25
(2,243)	1:87:A:LYS:H	1:88:A:VAL:H	8	0.25
(2,241)	1:87:A:LYS:H	1:88:A:VAL:H	8	0.25
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	4	0.25
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	4	0.25
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	4	0.25
(2,153)	1:55:A:ASN:H	1:55:A:ASN:HD21	13	0.25
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	3	0.25
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	8	0.25
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	8	0.25
(2,135)	1:46:A:PHE:H	1:48:A:LEU:H	8	0.25
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	4	0.25
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	16	0.25
(2,108)	1:43:A:GLN:H	1:46:A:PHE:H	16	0.25
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	12	0.25
(1,3)	2:301:A:CA:CA	1:165:A:GLY:O	19	0.25
(1,2)	2:301:A:CA:CA	1:133:A:ASP:O	4	0.25
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	20	0.25
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD22	9	0.24
(2,949)	1:109:A:VAL:HG23	1:196:A:LEU:HD23	9	0.24
(2,758)	1:136:A:ILE:H	1:94:A:VAL:HG11	3	0.24
(2,758)	1:136:A:ILE:H	1:94:A:VAL:HG12	3	0.24
(2,758)	1:136:A:ILE:H	1:94:A:VAL:HG13	3	0.24
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	10	0.24
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	10	0.24
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	2	0.24
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	18	0.24
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	8	0.24
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	9	0.24
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	19	0.24
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	14	0.24
(2,542)	1:170:A:ALA:H	1:137:A:GLY:H	12	0.24
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	13	0.24
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	13	0.24
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	2	0.24
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	18	0.24
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	18	0.24
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD22	4	0.24
(2,236)	1:84:A:TRP:H	1:200:A:LEU:HD23	4	0.24
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	4	0.24
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	4	0.24
(2,204)	1:66:A:ARG:H	1:67:A:CYS:H	13	0.24
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	7	0.24
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	17	0.24
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	17	0.24
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	3	0.24
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	8	0.24
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD11	2	0.24
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD12	2	0.24
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD13	2	0.24
(2,2)	1:200:A:LEU:HD11	1:234:A:ILE:HG13	2	0.24
(2,2)	1:200:A:LEU:HD12	1:234:A:ILE:HG13	2	0.24
(2,2)	1:200:A:LEU:HD13	1:234:A:ILE:HG13	2	0.24
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	6	0.24
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	7	0.24
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	8	0.24
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	14	0.24
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	15	0.24
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	5	0.24
(1,2)	2:301:A:CA:CA	1:133:A:ASP:O	7	0.24
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD22	10	0.23
(2,989)	1:186:A:ILE:HD11	1:156:A:LEU:HD23	10	0.23
(2,988)	1:186:A:ILE:HD11	1:156:A:LEU:HD21	19	0.23
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	13	0.23
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	13	0.23
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	13	0.23
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	13	0.23
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	13	0.23
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	8	0.23
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG11	12	0.23
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG12	12	0.23
(2,902)	1:109:A:VAL:HG11	1:105:A:VAL:HG13	12	0.23
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG11	12	0.23
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG12	12	0.23
(2,902)	1:109:A:VAL:HG12	1:105:A:VAL:HG13	12	0.23
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG11	12	0.23
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG12	12	0.23
(2,902)	1:109:A:VAL:HG13	1:105:A:VAL:HG13	12	0.23
(2,891)	1:105:A:VAL:HG21	1:105:A:VAL:H	7	0.23
(2,891)	1:105:A:VAL:HG22	1:105:A:VAL:H	7	0.23
(2,891)	1:105:A:VAL:HG23	1:105:A:VAL:H	7	0.23
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	12	0.23
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	12	0.23
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	16	0.23
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	16	0.23
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	10	0.23
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	5	0.23
(2,635)	1:116:A:TRP:HE1	1:198:A:HIS:H	18	0.23
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG21	9	0.23
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG22	9	0.23
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG23	9	0.23
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	5	0.23
(2,542)	1:170:A:ALA:H	1:137:A:GLY:H	7	0.23
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	10	0.23
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	10	0.23
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	17	0.23
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	17	0.23
(2,436)	1:133:A:ASP:H	1:92:A:ARG:H	14	0.23
(2,402)	1:122:A:LEU:H	1:200:A:LEU:HD21	20	0.23
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	5	0.23
(2,372)	1:116:A:TRP:HE1	1:198:A:HIS:H	18	0.23
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	16	0.23
(2,313)	1:105:A:VAL:HG21	1:105:A:VAL:H	7	0.23
(2,313)	1:105:A:VAL:HG22	1:105:A:VAL:H	7	0.23
(2,313)	1:105:A:VAL:HG23	1:105:A:VAL:H	7	0.23
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	19	0.23
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	19	0.23
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	20	0.23
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	16	0.23
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	20	0.23
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	7	0.23
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	16	0.23
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	20	0.23
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	16	0.23
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	9	0.23
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	9	0.23
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	4	0.23
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	4	0.23
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	17	0.23
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	20	0.23
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	13	0.23
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	16	0.23
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	2	0.23
(3,83)	1:150:A:ASP:H	4:305:A:PX4:C3	1	0.22
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD22	7	0.22
(2,943)	1:196:A:LEU:HD23	1:200:A:LEU:HD23	7	0.22
(2,905)	1:109:A:VAL:HG21	1:113:A:LEU:HB2	1	0.22
(2,905)	1:109:A:VAL:HG22	1:113:A:LEU:HB2	1	0.22
(2,905)	1:109:A:VAL:HG23	1:113:A:LEU:HB2	1	0.22
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	16	0.22
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	16	0.22
(2,761)	1:19:A:LEU:HD21	1:38:A:LYS:H	2	0.22
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	15	0.22
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	15	0.22
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	16	0.22
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	15	0.22
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	16	0.22
(2,645)	1:199:A:SER:H	1:202:A:MET:H	2	0.22
(2,645)	1:199:A:SER:H	1:202:A:MET:H	15	0.22
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	15	0.22
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	7	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	1	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	1	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	7	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	7	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	15	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	15	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	19	0.22
(2,493)	1:154:A:ASN:HD21	1:154:A:ASN:HD22	19	0.22
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	10	0.22
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	5	0.22
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	20	0.22
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	16	0.22
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	9	0.22
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	9	0.22
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	9	0.22
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	1	0.22
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	12	0.22
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	13	0.22
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	13	0.22
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	13	0.22
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	11	0.22
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	10	0.22
(2,245)	1:88:A:VAL:H	1:123:A:HIS:H	19	0.22
(2,216)	1:74:A:GLU:H	1:24:A:LEU:HD21	17	0.22
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	10	0.22
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	10	0.22
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	2	0.22
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	10	0.22
(2,144)	1:52:A:GLY:H	1:51:A:THR:H	20	0.22
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	1	0.22
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	8	0.22
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	10	0.22
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	10	0.22
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	15	0.22
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	10	0.22
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	10	0.22
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	10	0.22
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	6	0.22
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	8	0.22
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	12	0.22
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	3	0.22
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	16	0.22
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	5	0.22
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	2	0.22
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	10	0.22
(2,990)	1:186:A:ILE:HD12	1:156:A:LEU:HD21	2	0.21
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	17	0.21
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	17	0.21
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	17	0.21
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	1	0.21
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD22	15	0.21
(2,945)	1:109:A:VAL:HG21	1:196:A:LEU:HD23	15	0.21
(2,942)	1:196:A:LEU:HD23	1:200:A:LEU:HD21	16	0.21
(2,815)	1:72:A:VAL:HG11	1:74:A:GLU:H	11	0.21
(2,815)	1:72:A:VAL:HG12	1:74:A:GLU:H	11	0.21
(2,815)	1:72:A:VAL:HG13	1:74:A:GLU:H	11	0.21
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	11	0.21
(2,669)	1:207:A:ASP:H	1:206:A:SER:H	1	0.21
(2,669)	1:207:A:ASP:H	1:206:A:SER:H	1	0.21
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG21	8	0.21
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG22	8	0.21
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG23	8	0.21
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	17	0.21
(2,518)	1:161:A:ALA:H	1:161:A:ALA:HB1	10	0.21
(2,518)	1:161:A:ALA:H	1:161:A:ALA:HB2	10	0.21
(2,518)	1:161:A:ALA:H	1:161:A:ALA:HB3	10	0.21
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	5	0.21
(2,499)	1:156:A:LEU:H	1:157:A:ALA:H	4	0.21
(2,496)	1:156:A:LEU:H	1:157:A:ALA:H	4	0.21
(2,482)	1:140:A:ARG:H	1:141:A:GLY:H	6	0.21
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	3	0.21
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	13	0.21
(2,396)	1:120:A:ILE:H	1:122:A:LEU:H	5	0.21
(2,396)	1:120:A:ILE:H	1:122:A:LEU:H	17	0.21
(2,308)	1:103:A:ILE:H	1:103:A:ILE:HG13	1	0.21
(2,308)	1:103:A:ILE:H	1:103:A:ILE:HG12	1	0.21
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	10	0.21
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	10	0.21
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	6	0.21
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	6	0.21
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	6	0.21
(2,252)	1:89:A:VAL:H	1:123:A:HIS:H	19	0.21
(2,226)	1:75:A:TYR:H	1:73:A:ALA:HA	18	0.21
(2,204)	1:66:A:ARG:H	1:67:A:CYS:H	5	0.21
(2,182)	1:59:A:ILE:HG13	1:60:A:GLU:H	17	0.21
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	5	0.21
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	12	0.21
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	5	0.21
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	12	0.21
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	11	0.21
(2,142)	1:50:A:ILE:H	1:50:A:ILE:HD11	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,142)	1:50:A:ILE:H	1:50:A:ILE:HD12	11	0.21
(2,142)	1:50:A:ILE:H	1:50:A:ILE:HD13	11	0.21
(2,141)	1:50:A:ILE:H	1:50:A:ILE:HG12	14	0.21
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	7	0.21
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	7	0.21
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	14	0.21
(2,111)	1:43:A:GLN:H	1:43:A:GLN:HE21	10	0.21
(2,103)	1:41:A:GLU:H	1:43:A:GLN:H	6	0.21
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	6	0.21
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	20	0.21
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	4	0.21
(2,21)	1:10:A:LEU:H	1:10:A:LEU:HD21	17	0.21
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	3	0.21
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	13	0.21
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	1	0.21
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	7	0.21
(2,1060)	1:126:A:LYS:H	4:348:A:PX4:C1	5	0.2
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	2	0.2
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	16	0.2
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	16	0.2
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	16	0.2
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	20	0.2
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	20	0.2
(2,883)	1:91:A:TYR:HE1	1:93:A:ILE:HD11	18	0.2
(2,883)	1:91:A:TYR:HE1	1:93:A:ILE:HD12	18	0.2
(2,883)	1:91:A:TYR:HE1	1:93:A:ILE:HD13	18	0.2
(2,883)	1:91:A:TYR:HE2	1:93:A:ILE:HD11	18	0.2
(2,883)	1:91:A:TYR:HE2	1:93:A:ILE:HD12	18	0.2
(2,883)	1:91:A:TYR:HE2	1:93:A:ILE:HD13	18	0.2
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	15	0.2
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	15	0.2
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	14	0.2
(2,844)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	14	0.2
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD22	14	0.2
(2,825)	1:89:A:VAL:HG11	1:200:A:LEU:HD23	14	0.2
(2,815)	1:72:A:VAL:HG11	1:74:A:GLU:H	2	0.2
(2,815)	1:72:A:VAL:HG12	1:74:A:GLU:H	2	0.2
(2,815)	1:72:A:VAL:HG13	1:74:A:GLU:H	2	0.2
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	9	0.2
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	17	0.2
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	17	0.2
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,556)	1:158:A:HIS:H	1:173:A:ASP:H	11	0.2
(2,544)	1:136:A:ILE:H	1:170:A:ALA:H	20	0.2
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	18	0.2
(2,412)	1:125:A:ARG:H	1:89:A:VAL:H	9	0.2
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	1	0.2
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	20	0.2
(2,318)	1:104:A:THR:H	1:106:A:ASP:H	11	0.2
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	8	0.2
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD11	7	0.2
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD12	7	0.2
(2,275)	1:92:A:ARG:H	1:136:A:ILE:HD13	7	0.2
(2,253)	1:89:A:VAL:H	1:125:A:ARG:H	9	0.2
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	1	0.2
(2,235)	1:84:A:TRP:H	1:200:A:LEU:HD21	19	0.2
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	11	0.2
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	11	0.2
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	11	0.2
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	4	0.2
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	17	0.2
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	20	0.2
(2,91)	1:37:A:ALA:H	1:36:A:GLU:H	3	0.2
(2,85)	1:34:A:SER:H	1:35:A:LEU:H	3	0.2
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	7	0.2
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	7	0.2
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	7	0.2
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	9	0.2
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	17	0.2
(1,7)	2:302:A:CA:CA	1:151:A:GLY:O	1	0.2
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	13	0.2
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD2	12	0.2
(2,982)	1:69:A:VAL:HG21	1:161:A:ALA:H	8	0.19
(2,982)	1:69:A:VAL:HG22	1:161:A:ALA:H	8	0.19
(2,982)	1:69:A:VAL:HG23	1:161:A:ALA:H	8	0.19
(2,891)	1:105:A:VAL:HG21	1:105:A:VAL:H	20	0.19
(2,891)	1:105:A:VAL:HG22	1:105:A:VAL:H	20	0.19
(2,891)	1:105:A:VAL:HG23	1:105:A:VAL:H	20	0.19
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD22	9	0.19
(2,871)	1:89:A:VAL:HG11	1:122:A:LEU:HD23	9	0.19
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	11	0.19
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	11	0.19
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	11	0.19
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	18	0.19
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	18	0.19
(2,687)	1:213:A:TYR:H	1:211:A:VAL:H	9	0.19
(2,679)	1:213:A:TYR:H	1:211:A:VAL:H	9	0.19
(2,672)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	11	0.19
(2,670)	1:209:A:ASN:HD22	1:209:A:ASN:HD21	11	0.19
(2,590)	1:178:A:TRP:H	1:100:A:LEU:HD21	3	0.19
(2,550)	1:159:A:ALA:H	1:171:A:HIS:H	11	0.19
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG13	12	0.19
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG12	12	0.19
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	5	0.19
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	5	0.19
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	5	0.19
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	15	0.19
(2,498)	1:66:A:ARG:H	1:156:A:LEU:H	10	0.19
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	17	0.19
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	18	0.19
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	12	0.19
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	14	0.19
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	7	0.19
(2,313)	1:105:A:VAL:HG21	1:105:A:VAL:H	20	0.19
(2,313)	1:105:A:VAL:HG22	1:105:A:VAL:H	20	0.19
(2,313)	1:105:A:VAL:HG23	1:105:A:VAL:H	20	0.19
(2,279)	1:136:A:ILE:H	1:93:A:ILE:H	9	0.19
(2,203)	1:66:A:ARG:H	1:156:A:LEU:H	10	0.19
(2,117)	1:44:A:LYS:H	1:47:A:GLY:H	19	0.19
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	7	0.19
(2,112)	1:43:A:GLN:HE21	1:43:A:GLN:HE22	13	0.19
(2,91)	1:37:A:ALA:H	1:36:A:GLU:H	13	0.19
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	17	0.19
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	17	0.19
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	17	0.19
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	5	0.19
(2,1035)	1:72:A:VAL:H	1:72:A:VAL:HG21	2	0.18
(2,1035)	1:72:A:VAL:H	1:72:A:VAL:HG22	2	0.18
(2,1035)	1:72:A:VAL:H	1:72:A:VAL:HG23	2	0.18
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	3	0.18
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	3	0.18
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	3	0.18
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	3	0.18
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	3	0.18
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	3	0.18
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	3	0.18
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	3	0.18
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD22	8	0.18
(2,873)	1:89:A:VAL:HG12	1:122:A:LEU:HD23	8	0.18
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	4	0.18
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	4	0.18
(2,681)	1:212:A:MET:H	1:227:A:SER:H	12	0.18
(2,681)	1:212:A:MET:H	1:227:A:SER:H	20	0.18
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	4	0.18
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	17	0.18
(2,579)	1:178:A:TRP:HE1	1:175:A:ASP:H	9	0.18
(2,550)	1:159:A:ALA:H	1:171:A:HIS:H	16	0.18
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	15	0.18
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD11	17	0.18
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD12	17	0.18
(2,539)	1:169:A:ASP:H	1:166:A:LEU:HD13	17	0.18
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD11	17	0.18
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD12	17	0.18
(2,538)	1:169:A:ASP:H	1:134:A:ILE:HD13	17	0.18
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD11	20	0.18
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD12	20	0.18
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD13	20	0.18
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	9	0.18
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	7	0.18
(2,319)	1:106:A:ASP:H	1:102:A:HIS:HD2	18	0.18
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	17	0.18
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	1	0.18
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	1	0.18
(2,214)	1:72:A:VAL:H	1:71:A:ASP:H	20	0.18
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	13	0.18
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	13	0.18
(2,191)	1:61:A:ILE:H	1:62:A:MET:H	15	0.18
(2,185)	1:61:A:ILE:H	1:62:A:MET:H	15	0.18
(2,171)	1:55:A:ASN:H	1:58:A:VAL:H	13	0.18
(2,151)	1:55:A:ASN:H	1:58:A:VAL:H	13	0.18
(2,133)	1:47:A:GLY:H	1:206:A:SER:HB3	20	0.18
(2,133)	1:47:A:GLY:H	1:206:A:SER:HB2	20	0.18
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	18	0.18
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	9	0.18
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	18	0.18
(3,26)	1:181:A:GLY:H	4:414:A:PX4:C35	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1027)	1:58:A:VAL:HG13	1:54:A:LEU:HD21	15	0.17
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG13	11	0.17
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG13	11	0.17
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG13	11	0.17
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG12	11	0.17
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG12	11	0.17
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG12	11	0.17
(2,948)	1:109:A:VAL:HG23	1:196:A:LEU:HD21	12	0.17
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	17	0.17
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	17	0.17
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	17	0.17
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	17	0.17
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	17	0.17
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	17	0.17
(2,867)	1:89:A:VAL:HG23	1:200:A:LEU:HD21	20	0.17
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD22	3	0.17
(2,864)	1:89:A:VAL:HG21	1:200:A:LEU:HD23	3	0.17
(2,815)	1:72:A:VAL:HG11	1:74:A:GLU:H	15	0.17
(2,815)	1:72:A:VAL:HG12	1:74:A:GLU:H	15	0.17
(2,815)	1:72:A:VAL:HG13	1:74:A:GLU:H	15	0.17
(2,740)	1:237:A:LEU:H	1:239:A:GLY:H	7	0.17
(2,739)	1:238:A:TYR:H	1:239:A:GLY:H	3	0.17
(2,734)	1:238:A:TYR:H	1:239:A:GLY:H	3	0.17
(2,729)	1:237:A:LEU:H	1:239:A:GLY:H	7	0.17
(2,649)	1:200:A:LEU:HD21	1:199:A:SER:H	6	0.17
(2,639)	1:198:A:HIS:H	1:202:A:MET:H	12	0.17
(2,611)	1:108:A:LEU:HD21	1:188:A:PHE:H	15	0.17
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	13	0.17
(2,588)	1:179:A:THR:H	1:100:A:LEU:HD21	3	0.17
(2,500)	1:68:A:GLY:H	1:157:A:ALA:H	3	0.17
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD11	16	0.17
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD12	16	0.17
(2,469)	1:137:A:GLY:H	1:136:A:ILE:HD13	16	0.17
(2,465)	1:137:A:GLY:H	1:95:A:SER:H	2	0.17
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	18	0.17
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	1	0.17
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	4	0.17
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	4	0.17
(2,318)	1:104:A:THR:H	1:106:A:ASP:H	9	0.17
(2,287)	1:95:A:SER:H	1:137:A:GLY:H	2	0.17
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	7	0.17
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	19	0.17
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	19	0.17
(2,176)	1:59:A:ILE:H	1:59:A:ILE:HG13	9	0.17
(2,176)	1:59:A:ILE:H	1:59:A:ILE:HG12	9	0.17
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	19	0.17
(2,141)	1:50:A:ILE:H	1:50:A:ILE:HG12	11	0.17
(2,139)	1:48:A:LEU:HD22	1:47:A:GLY:H	18	0.17
(2,139)	1:48:A:LEU:HD23	1:47:A:GLY:H	18	0.17
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	10	0.17
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	16	0.17
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD22	19	0.17
(2,22)	1:10:A:LEU:H	1:10:A:LEU:HD23	19	0.17
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	8	0.17
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	8	0.17
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	14	0.17
(1,10)	3:303:A:ZN:ZN	1:171:A:HIS:ND1	19	0.17
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	11	0.17
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	12	0.17
(3,26)	1:181:A:GLY:H	4:308:A:PX4:C35	7	0.16
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	1	0.16
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	1	0.16
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	1	0.16
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	1	0.16
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	1	0.16
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	1	0.16
(2,879)	1:127:A:VAL:HG11	1:91:A:TYR:H	10	0.16
(2,879)	1:127:A:VAL:HG12	1:91:A:TYR:H	10	0.16
(2,879)	1:127:A:VAL:HG13	1:91:A:TYR:H	10	0.16
(2,822)	1:89:A:VAL:HG11	1:122:A:LEU:HG	5	0.16
(2,822)	1:89:A:VAL:HG12	1:122:A:LEU:HG	5	0.16
(2,822)	1:89:A:VAL:HG13	1:122:A:LEU:HG	5	0.16
(2,772)	1:19:A:LEU:HD22	1:22:A:PHE:H	15	0.16
(2,772)	1:19:A:LEU:HD23	1:22:A:PHE:H	15	0.16
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	17	0.16
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	17	0.16
(2,579)	1:178:A:TRP:HE1	1:175:A:ASP:H	12	0.16
(2,550)	1:159:A:ALA:H	1:171:A:HIS:H	17	0.16
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG13	8	0.16
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG12	8	0.16
(2,545)	1:170:A:ALA:H	1:160:A:PHE:H	2	0.16
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	3	0.16
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD11	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD12	7	0.16
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD13	7	0.16
(2,427)	1:132:A:ALA:H	1:131:A:THR:H	17	0.16
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	14	0.16
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	8	0.16
(2,344)	1:109:A:VAL:H	1:112:A:ALA:H	11	0.16
(2,342)	1:189:A:LEU:HD22	1:111:A:LYS:H	5	0.16
(2,342)	1:189:A:LEU:HD23	1:111:A:LYS:H	5	0.16
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	9	0.16
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD11	19	0.16
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD12	19	0.16
(2,298)	1:237:A:LEU:H	1:120:A:ILE:HD13	19	0.16
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	5	0.16
(2,252)	1:89:A:VAL:H	1:123:A:HIS:H	17	0.16
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	2	0.16
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	14	0.16
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	2	0.16
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	14	0.16
(2,171)	1:55:A:ASN:H	1:58:A:VAL:H	15	0.16
(2,167)	1:59:A:ILE:H	1:57:A:ARG:H	17	0.16
(2,165)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	2	0.16
(2,161)	1:55:A:ASN:HD21	1:55:A:ASN:HD22	2	0.16
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG11	12	0.16
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG12	12	0.16
(2,158)	1:55:A:ASN:H	1:58:A:VAL:HG13	12	0.16
(2,151)	1:55:A:ASN:H	1:58:A:VAL:H	15	0.16
(2,123)	1:47:A:GLY:H	1:45:A:PHE:H	3	0.16
(1,12)	3:303:A:ZN:ZN	1:143:A:HIS:NE2	20	0.16
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	9	0.16
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	19	0.16
(1,2)	2:301:A:CA:CA	1:169:A:ASP:OD1	8	0.16
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	3	0.15
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	3	0.15
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	3	0.15
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	3	0.15
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	3	0.15
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	3	0.15
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	18	0.15
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	18	0.15
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	18	0.15
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	18	0.15
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	18	0.15
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG13	8	0.15
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG13	8	0.15
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG13	8	0.15
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG12	8	0.15
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG12	8	0.15
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG12	8	0.15
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	4	0.15
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	4	0.15
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	4	0.15
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	4	0.15
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	4	0.15
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	4	0.15
(2,815)	1:72:A:VAL:HG11	1:74:A:GLU:H	17	0.15
(2,815)	1:72:A:VAL:HG12	1:74:A:GLU:H	17	0.15
(2,815)	1:72:A:VAL:HG13	1:74:A:GLU:H	17	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	12	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	12	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	12	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	12	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	12	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	12	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	13	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	13	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	13	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	13	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	13	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	13	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	17	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	17	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	17	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	17	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	17	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	17	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	19	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	19	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	19	0.15
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	19	0.15
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	19	0.15
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	19	0.15
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG21	16	0.15
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG22	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG23	16	0.15
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	6	0.15
(2,728)	1:236:A:LYS:H	1:237:A:LEU:H	11	0.15
(2,728)	1:236:A:LYS:H	1:237:A:LEU:H	11	0.15
(2,706)	1:231:A:ILE:H	1:231:A:ILE:HG13	3	0.15
(2,706)	1:231:A:ILE:H	1:231:A:ILE:HG12	3	0.15
(2,681)	1:212:A:MET:H	1:227:A:SER:H	4	0.15
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	8	0.15
(2,534)	1:135:A:MET:H	1:169:A:ASP:H	7	0.15
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	14	0.15
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	18	0.15
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	18	0.15
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	4	0.15
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	14	0.15
(2,481)	1:140:A:ARG:H	1:139:A:ALA:H	9	0.15
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	1	0.15
(2,448)	1:135:A:MET:H	1:169:A:ASP:H	7	0.15
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	14	0.15
(2,428)	1:132:A:ALA:H	1:133:A:ASP:H	18	0.15
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	16	0.15
(2,348)	1:189:A:LEU:HD22	1:112:A:ALA:H	17	0.15
(2,348)	1:189:A:LEU:HD23	1:112:A:ALA:H	17	0.15
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	12	0.15
(2,315)	1:106:A:ASP:H	1:108:A:LEU:H	20	0.15
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	10	0.15
(2,285)	1:94:A:VAL:H	1:94:A:VAL:HG21	14	0.15
(2,285)	1:94:A:VAL:H	1:94:A:VAL:HG22	14	0.15
(2,285)	1:94:A:VAL:H	1:94:A:VAL:HG23	14	0.15
(2,285)	1:94:A:VAL:H	1:94:A:VAL:HG11	14	0.15
(2,285)	1:94:A:VAL:H	1:94:A:VAL:HG12	14	0.15
(2,285)	1:94:A:VAL:H	1:94:A:VAL:HG13	14	0.15
(2,226)	1:75:A:TYR:H	1:73:A:ALA:HA	14	0.15
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	15	0.15
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	15	0.15
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	14	0.15
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	14	0.15
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	14	0.15
(2,108)	1:43:A:GLN:H	1:46:A:PHE:H	6	0.15
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	7	0.15
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD11	2	0.15
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD12	2	0.15
(2,6)	1:107:A:ARG:H	1:103:A:ILE:HD13	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	11	0.15
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	11	0.15
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	2	0.15
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	13	0.14
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	13	0.14
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	13	0.14
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	13	0.14
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	13	0.14
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	13	0.14
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	13	0.14
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	13	0.14
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	13	0.14
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	2	0.14
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	2	0.14
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	2	0.14
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	2	0.14
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	2	0.14
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	2	0.14
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG13	13	0.14
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG13	13	0.14
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG13	13	0.14
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG12	13	0.14
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG12	13	0.14
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG12	13	0.14
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG13	19	0.14
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG13	19	0.14
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG13	19	0.14
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG12	19	0.14
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG12	19	0.14
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG12	19	0.14
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD22	5	0.14
(2,939)	1:196:A:LEU:HD21	1:200:A:LEU:HD23	5	0.14
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	15	0.14
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	15	0.14
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD11	1	0.14
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD12	1	0.14
(2,823)	1:89:A:VAL:HG11	1:136:A:ILE:HD13	1	0.14
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD11	1	0.14
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD12	1	0.14
(2,823)	1:89:A:VAL:HG12	1:136:A:ILE:HD13	1	0.14
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD11	1	0.14
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD12	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:89:A:VAL:HG13	1:136:A:ILE:HD13	1	0.14
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	1	0.14
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	1	0.14
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	1	0.14
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	1	0.14
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	1	0.14
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	1	0.14
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG21	18	0.14
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG22	18	0.14
(2,784)	1:58:A:VAL:H	1:58:A:VAL:HG23	18	0.14
(2,764)	1:19:A:LEU:HD22	1:40:A:LYS:H	12	0.14
(2,764)	1:19:A:LEU:HD23	1:40:A:LYS:H	12	0.14
(2,754)	1:19:A:LEU:H	1:22:A:PHE:H	13	0.14
(2,650)	1:200:A:LEU:HD22	1:199:A:SER:H	10	0.14
(2,650)	1:200:A:LEU:HD23	1:199:A:SER:H	10	0.14
(2,636)	1:198:A:HIS:H	1:195:A:ALA:H	6	0.14
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	5	0.14
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD22	14	0.14
(2,541)	1:169:A:ASP:H	1:166:A:LEU:HD23	14	0.14
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	11	0.14
(2,505)	1:69:A:VAL:H	1:159:A:ALA:H	18	0.14
(2,455)	1:136:A:ILE:H	1:137:A:GLY:H	11	0.14
(2,279)	1:136:A:ILE:H	1:93:A:ILE:H	13	0.14
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	8	0.14
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	8	0.14
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	20	0.14
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	20	0.14
(2,123)	1:47:A:GLY:H	1:45:A:PHE:H	15	0.14
(2,119)	1:189:A:LEU:H	1:189:A:LEU:HD21	9	0.14
(2,117)	1:44:A:LYS:H	1:47:A:GLY:H	14	0.14
(2,108)	1:43:A:GLN:H	1:46:A:PHE:H	14	0.14
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	17	0.14
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	4	0.14
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	13	0.14
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	13	0.14
(2,1059)	1:129:A:TRP:H	4:321:A:PX4:C1	5	0.13
(2,1012)	1:226:A:LEU:HD21	1:211:A:VAL:HG21	18	0.13
(2,1012)	1:226:A:LEU:HD21	1:211:A:VAL:HG22	18	0.13
(2,1012)	1:226:A:LEU:HD21	1:211:A:VAL:HG23	18	0.13
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	7	0.13
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	7	0.13
(2,987)	1:186:A:ILE:HD11	1:156:A:LEU:HD11	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,987)	1:186:A:ILE:HD11	1:156:A:LEU:HD12	1	0.13
(2,987)	1:186:A:ILE:HD11	1:156:A:LEU:HD13	1	0.13
(2,987)	1:186:A:ILE:HD12	1:156:A:LEU:HD11	1	0.13
(2,987)	1:186:A:ILE:HD12	1:156:A:LEU:HD12	1	0.13
(2,987)	1:186:A:ILE:HD12	1:156:A:LEU:HD13	1	0.13
(2,987)	1:186:A:ILE:HD13	1:156:A:LEU:HD11	1	0.13
(2,987)	1:186:A:ILE:HD13	1:156:A:LEU:HD12	1	0.13
(2,987)	1:186:A:ILE:HD13	1:156:A:LEU:HD13	1	0.13
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	1	0.13
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	1	0.13
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	1	0.13
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	1	0.13
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	1	0.13
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	1	0.13
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	8	0.13
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	8	0.13
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	2	0.13
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	2	0.13
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	2	0.13
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	2	0.13
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	2	0.13
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	2	0.13
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	15	0.13
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	15	0.13
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	15	0.13
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	15	0.13
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	15	0.13
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	15	0.13
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	2	0.13
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	2	0.13
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	2	0.13
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	2	0.13
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	2	0.13
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	2	0.13
(2,788)	1:58:A:VAL:HG21	1:55:A:ASN:H	13	0.13
(2,788)	1:58:A:VAL:HG22	1:55:A:ASN:H	13	0.13
(2,788)	1:58:A:VAL:HG23	1:55:A:ASN:H	13	0.13
(2,745)	1:107:A:ARG:H	1:108:A:LEU:HD21	2	0.13
(2,740)	1:237:A:LEU:H	1:239:A:GLY:H	13	0.13
(2,729)	1:237:A:LEU:H	1:239:A:GLY:H	13	0.13
(2,718)	1:233:A:GLY:H	1:233:A:GLY:HA3	13	0.13
(2,718)	1:233:A:GLY:H	1:233:A:GLY:HA2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	6	0.13
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	2	0.13
(2,632)	1:197:A:GLY:H	1:196:A:LEU:HD21	14	0.13
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG21	7	0.13
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG22	7	0.13
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG23	7	0.13
(2,544)	1:136:A:ILE:H	1:170:A:ALA:H	7	0.13
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	9	0.13
(2,456)	1:136:A:ILE:H	1:92:A:ARG:H	12	0.13
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	1	0.13
(2,413)	1:125:A:ARG:H	1:91:A:TYR:H	10	0.13
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD22	3	0.13
(2,403)	1:122:A:LEU:H	1:200:A:LEU:HD23	3	0.13
(2,339)	1:111:A:LYS:H	1:111:A:LYS:HB3	9	0.13
(2,339)	1:111:A:LYS:H	1:111:A:LYS:HB2	9	0.13
(2,272)	1:135:A:MET:H	1:92:A:ARG:H	4	0.13
(2,269)	1:136:A:ILE:H	1:92:A:ARG:H	12	0.13
(2,230)	1:86:A:SER:H	1:85:A:THR:H	7	0.13
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG21	13	0.13
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG22	13	0.13
(2,156)	1:55:A:ASN:H	1:58:A:VAL:HG23	13	0.13
(2,137)	1:48:A:LEU:HD11	1:48:A:LEU:H	18	0.13
(2,137)	1:48:A:LEU:HD12	1:48:A:LEU:H	18	0.13
(2,137)	1:48:A:LEU:HD13	1:48:A:LEU:H	18	0.13
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	13	0.13
(2,129)	1:46:A:PHE:H	1:47:A:GLY:H	13	0.13
(2,103)	1:41:A:GLU:H	1:43:A:GLN:H	9	0.13
(2,91)	1:37:A:ALA:H	1:36:A:GLU:H	6	0.13
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	11	0.13
(2,13)	1:126:A:LYS:H	1:91:A:TYR:HE1	5	0.13
(2,13)	1:126:A:LYS:H	1:91:A:TYR:HE2	5	0.13
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	9	0.13
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	9	0.13
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	11	0.13
(1,6)	2:302:A:CA:CA	1:173:A:ASP:OD2	10	0.13
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	7	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	7	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	7	0.12
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	7	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	7	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	7	0.12
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	10	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	10	0.12
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	10	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	10	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	10	0.12
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	20	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	20	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	20	0.12
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	20	0.12
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	20	0.12
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	20	0.12
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG13	17	0.12
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG13	17	0.12
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG13	17	0.12
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG12	17	0.12
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG12	17	0.12
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG12	17	0.12
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	5	0.12
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	5	0.12
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	5	0.12
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	5	0.12
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	5	0.12
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	5	0.12
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	11	0.12
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	11	0.12
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	11	0.12
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	11	0.12
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	11	0.12
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	11	0.12
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	2	0.12
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	2	0.12
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD22	14	0.12
(2,746)	1:107:A:ARG:H	1:108:A:LEU:HD23	14	0.12
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	1	0.12
(2,658)	1:200:A:LEU:HD21	1:201:A:GLY:H	19	0.12
(2,636)	1:198:A:HIS:H	1:195:A:ALA:H	20	0.12
(2,612)	1:108:A:LEU:HD22	1:188:A:PHE:H	4	0.12
(2,612)	1:108:A:LEU:HD23	1:188:A:PHE:H	4	0.12
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	9	0.12
(2,610)	1:188:A:PHE:H	1:191:A:ALA:H	10	0.12
(2,602)	1:186:A:ILE:H	1:186:A:ILE:HG13	4	0.12
(2,602)	1:186:A:ILE:H	1:186:A:ILE:HG12	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,580)	1:178:A:TRP:HE1	1:176:A:GLU:H	16	0.12
(2,568)	1:178:A:TRP:HE1	1:176:A:GLU:H	16	0.12
(2,550)	1:159:A:ALA:H	1:171:A:HIS:H	2	0.12
(2,550)	1:159:A:ALA:H	1:171:A:HIS:H	8	0.12
(2,542)	1:170:A:ALA:H	1:137:A:GLY:H	16	0.12
(2,449)	1:135:A:MET:H	1:170:A:ALA:H	9	0.12
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	10	0.12
(2,245)	1:88:A:VAL:H	1:123:A:HIS:H	9	0.12
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	12	0.12
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	12	0.12
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	12	0.12
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	5	0.12
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	5	0.12
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	5	0.12
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG11	15	0.12
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG12	15	0.12
(2,196)	1:194:A:HIS:H	1:211:A:VAL:HG13	15	0.12
(2,103)	1:41:A:GLU:H	1:43:A:GLN:H	3	0.12
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	12	0.12
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	14	0.12
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	15	0.12
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	8	0.12
(2,1061)	1:127:A:VAL:H	4:321:A:PX4:C1	11	0.11
(2,1030)	1:54:A:LEU:HD22	1:39:A:LEU:HD11	10	0.11
(2,1030)	1:54:A:LEU:HD22	1:39:A:LEU:HD12	10	0.11
(2,1030)	1:54:A:LEU:HD22	1:39:A:LEU:HD13	10	0.11
(2,1030)	1:54:A:LEU:HD23	1:39:A:LEU:HD11	10	0.11
(2,1030)	1:54:A:LEU:HD23	1:39:A:LEU:HD12	10	0.11
(2,1030)	1:54:A:LEU:HD23	1:39:A:LEU:HD13	10	0.11
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG21	16	0.11
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG22	16	0.11
(2,1018)	1:231:A:ILE:HD11	1:234:A:ILE:HG23	16	0.11
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG21	16	0.11
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG22	16	0.11
(2,1018)	1:231:A:ILE:HD12	1:234:A:ILE:HG23	16	0.11
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG21	16	0.11
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG22	16	0.11
(2,1018)	1:231:A:ILE:HD13	1:234:A:ILE:HG23	16	0.11
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD22	4	0.11
(2,993)	1:186:A:ILE:HD13	1:156:A:LEU:HD23	4	0.11
(2,992)	1:186:A:ILE:HD13	1:156:A:LEU:HD21	12	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	12	0.11
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	12	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	12	0.11
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	12	0.11
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	12	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	14	0.11
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	14	0.11
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	14	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	14	0.11
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	14	0.11
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	14	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	15	0.11
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	15	0.11
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	15	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	15	0.11
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	15	0.11
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	15	0.11
(2,983)	1:69:A:VAL:HG11	1:159:A:ALA:HB1	19	0.11
(2,983)	1:69:A:VAL:HG11	1:159:A:ALA:HB2	19	0.11
(2,983)	1:69:A:VAL:HG11	1:159:A:ALA:HB3	19	0.11
(2,983)	1:69:A:VAL:HG12	1:159:A:ALA:HB1	19	0.11
(2,983)	1:69:A:VAL:HG12	1:159:A:ALA:HB2	19	0.11
(2,983)	1:69:A:VAL:HG12	1:159:A:ALA:HB3	19	0.11
(2,983)	1:69:A:VAL:HG13	1:159:A:ALA:HB1	19	0.11
(2,983)	1:69:A:VAL:HG13	1:159:A:ALA:HB2	19	0.11
(2,983)	1:69:A:VAL:HG13	1:159:A:ALA:HB3	19	0.11
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG13	20	0.11
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG13	20	0.11
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG13	20	0.11
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG12	20	0.11
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG12	20	0.11
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG12	20	0.11
(2,891)	1:105:A:VAL:HG21	1:105:A:VAL:H	3	0.11
(2,891)	1:105:A:VAL:HG22	1:105:A:VAL:H	3	0.11
(2,891)	1:105:A:VAL:HG23	1:105:A:VAL:H	3	0.11
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG13	10	0.11
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG13	10	0.11
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG13	10	0.11
(2,889)	1:103:A:ILE:HD11	1:103:A:ILE:HG12	10	0.11
(2,889)	1:103:A:ILE:HD12	1:103:A:ILE:HG12	10	0.11
(2,889)	1:103:A:ILE:HD13	1:103:A:ILE:HG12	10	0.11
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	3	0.11
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	3	0.11
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	3	0.11
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	3	0.11
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	3	0.11
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	6	0.11
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	6	0.11
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	6	0.11
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	6	0.11
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	6	0.11
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	6	0.11
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	7	0.11
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	7	0.11
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	7	0.11
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	7	0.11
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	7	0.11
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	7	0.11
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	3	0.11
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	3	0.11
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD22	20	0.11
(2,866)	1:89:A:VAL:HG22	1:200:A:LEU:HD23	20	0.11
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	17	0.11
(2,848)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	17	0.11
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD22	17	0.11
(2,829)	1:89:A:VAL:HG13	1:200:A:LEU:HD23	17	0.11
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	6	0.11
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	6	0.11
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	6	0.11
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	6	0.11
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	6	0.11
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	6	0.11
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	7	0.11
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	7	0.11
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	7	0.11
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	7	0.11
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	7	0.11
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	7	0.11
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	14	0.11
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	14	0.11
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	14	0.11
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	14	0.11
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	14	0.11
(2,787)	1:58:A:VAL:HG21	1:43:A:GLN:HE21	14	0.11
(2,787)	1:58:A:VAL:HG22	1:43:A:GLN:HE21	14	0.11
(2,787)	1:58:A:VAL:HG23	1:43:A:GLN:HE21	14	0.11
(2,706)	1:231:A:ILE:H	1:231:A:ILE:HG13	11	0.11
(2,706)	1:231:A:ILE:H	1:231:A:ILE:HG12	11	0.11
(2,645)	1:199:A:SER:H	1:202:A:MET:H	20	0.11
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD22	13	0.11
(2,605)	1:186:A:ILE:H	1:156:A:LEU:HD23	13	0.11
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG21	2	0.11
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG22	2	0.11
(2,597)	1:185:A:GLY:H	1:179:A:THR:HG23	2	0.11
(2,580)	1:178:A:TRP:HE1	1:176:A:GLU:H	2	0.11
(2,568)	1:178:A:TRP:HE1	1:176:A:GLU:H	2	0.11
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG13	15	0.11
(2,549)	1:170:A:ALA:H	1:136:A:ILE:HG12	15	0.11
(2,526)	1:160:A:PHE:H	1:168:A:GLY:H	17	0.11
(2,483)	1:139:A:ALA:HB1	1:140:A:ARG:H	17	0.11
(2,483)	1:139:A:ALA:HB2	1:140:A:ARG:H	17	0.11
(2,483)	1:139:A:ALA:HB3	1:140:A:ARG:H	17	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD11	3	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD12	3	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD13	3	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD11	6	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD12	6	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD13	6	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD11	12	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD12	12	0.11
(2,443)	1:134:A:ILE:H	1:136:A:ILE:HD13	12	0.11
(2,406)	1:123:A:HIS:H	1:122:A:LEU:HD21	20	0.11
(2,337)	1:111:A:LYS:H	1:109:A:VAL:H	8	0.11
(2,313)	1:105:A:VAL:HG21	1:105:A:VAL:H	3	0.11
(2,313)	1:105:A:VAL:HG22	1:105:A:VAL:H	3	0.11
(2,313)	1:105:A:VAL:HG23	1:105:A:VAL:H	3	0.11
(2,293)	1:98:A:ARG:H	1:100:A:LEU:H	8	0.11
(2,279)	1:136:A:ILE:H	1:93:A:ILE:H	17	0.11
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG13	13	0.11
(2,276)	1:92:A:ARG:H	1:93:A:ILE:HG12	13	0.11
(2,246)	1:88:A:VAL:H	1:86:A:SER:H	14	0.11
(2,230)	1:86:A:SER:H	1:85:A:THR:H	16	0.11
(2,214)	1:72:A:VAL:H	1:71:A:ASP:H	14	0.11
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG21	14	0.11
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG22	14	0.11
(2,210)	1:68:A:GLY:H	1:155:A:THR:HG23	14	0.11
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	18	0.11
(2,159)	1:55:A:ASN:H	1:54:A:LEU:HD21	7	0.11
(2,153)	1:55:A:ASN:H	1:55:A:ASN:HD21	4	0.11
(2,152)	1:55:A:ASN:H	1:56:A:SER:H	1	0.11
(2,135)	1:46:A:PHE:H	1:48:A:LEU:H	19	0.11
(2,123)	1:47:A:GLY:H	1:45:A:PHE:H	5	0.11
(2,108)	1:43:A:GLN:H	1:46:A:PHE:H	8	0.11
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	5	0.11
(2,51)	1:183:A:SER:H	1:185:A:GLY:H	9	0.11
(2,42)	1:16:A:GLN:H	1:18:A:TYR:H	9	0.11
(1,13)	3:304:A:ZN:ZN	1:198:A:HIS:NE2	14	0.11
(1,11)	3:303:A:ZN:ZN	1:145:A:ASP:OD2	10	0.11
(1,10)	3:303:A:ZN:ZN	1:158:A:HIS:NE2	5	0.11
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG13	5	0.1
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG13	5	0.1
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG13	5	0.1
(2,986)	1:186:A:ILE:HD11	1:186:A:ILE:HG12	5	0.1
(2,986)	1:186:A:ILE:HD12	1:186:A:ILE:HG12	5	0.1
(2,986)	1:186:A:ILE:HD13	1:186:A:ILE:HG12	5	0.1
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG13	15	0.1
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG13	15	0.1
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG13	15	0.1
(2,958)	1:120:A:ILE:HD11	1:120:A:ILE:HG12	15	0.1
(2,958)	1:120:A:ILE:HD12	1:120:A:ILE:HG12	15	0.1
(2,958)	1:120:A:ILE:HD13	1:120:A:ILE:HG12	15	0.1
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD22	14	0.1
(2,947)	1:109:A:VAL:HG22	1:196:A:LEU:HD23	14	0.1
(2,944)	1:109:A:VAL:HG21	1:196:A:LEU:HD21	8	0.1
(2,886)	1:94:A:VAL:H	1:94:A:VAL:HG21	14	0.1
(2,886)	1:94:A:VAL:H	1:94:A:VAL:HG22	14	0.1
(2,886)	1:94:A:VAL:H	1:94:A:VAL:HG23	14	0.1
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	8	0.1
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	8	0.1
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	8	0.1
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	8	0.1
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	8	0.1
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	8	0.1
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG13	16	0.1
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG13	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG13	16	0.1
(2,884)	1:93:A:ILE:HD11	1:93:A:ILE:HG12	16	0.1
(2,884)	1:93:A:ILE:HD12	1:93:A:ILE:HG12	16	0.1
(2,884)	1:93:A:ILE:HD13	1:93:A:ILE:HG12	16	0.1
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD22	10	0.1
(2,868)	1:89:A:VAL:HG23	1:200:A:LEU:HD23	10	0.1
(2,833)	1:134:A:ILE:HD11	1:89:A:VAL:HG11	5	0.1
(2,833)	1:134:A:ILE:HD11	1:89:A:VAL:HG12	5	0.1
(2,833)	1:134:A:ILE:HD11	1:89:A:VAL:HG13	5	0.1
(2,833)	1:134:A:ILE:HD12	1:89:A:VAL:HG11	5	0.1
(2,833)	1:134:A:ILE:HD12	1:89:A:VAL:HG12	5	0.1
(2,833)	1:134:A:ILE:HD12	1:89:A:VAL:HG13	5	0.1
(2,833)	1:134:A:ILE:HD13	1:89:A:VAL:HG11	5	0.1
(2,833)	1:134:A:ILE:HD13	1:89:A:VAL:HG12	5	0.1
(2,833)	1:134:A:ILE:HD13	1:89:A:VAL:HG13	5	0.1
(2,830)	1:134:A:ILE:HD11	1:89:A:VAL:HG11	5	0.1
(2,830)	1:134:A:ILE:HD11	1:89:A:VAL:HG12	5	0.1
(2,830)	1:134:A:ILE:HD11	1:89:A:VAL:HG13	5	0.1
(2,830)	1:134:A:ILE:HD12	1:89:A:VAL:HG11	5	0.1
(2,830)	1:134:A:ILE:HD12	1:89:A:VAL:HG12	5	0.1
(2,830)	1:134:A:ILE:HD12	1:89:A:VAL:HG13	5	0.1
(2,830)	1:134:A:ILE:HD13	1:89:A:VAL:HG11	5	0.1
(2,830)	1:134:A:ILE:HD13	1:89:A:VAL:HG12	5	0.1
(2,830)	1:134:A:ILE:HD13	1:89:A:VAL:HG13	5	0.1
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG13	4	0.1
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG13	4	0.1
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG13	4	0.1
(2,793)	1:59:A:ILE:HD11	1:59:A:ILE:HG12	4	0.1
(2,793)	1:59:A:ILE:HD12	1:59:A:ILE:HG12	4	0.1
(2,793)	1:59:A:ILE:HD13	1:59:A:ILE:HG12	4	0.1
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG11	6	0.1
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG12	6	0.1
(2,773)	1:39:A:LEU:HD21	1:58:A:VAL:HG13	6	0.1
(2,748)	1:23:A:TYR:H	1:25:A:TYR:H	13	0.1
(2,676)	1:210:A:ALA:H	1:213:A:TYR:H	8	0.1
(2,650)	1:200:A:LEU:HD22	1:199:A:SER:H	11	0.1
(2,650)	1:200:A:LEU:HD23	1:199:A:SER:H	11	0.1
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB3	4	0.1
(2,513)	1:160:A:PHE:H	1:199:A:SER:HB2	4	0.1
(2,490)	1:154:A:ASN:HD22	1:154:A:ASN:H	11	0.1
(2,347)	1:189:A:LEU:HD21	1:112:A:ALA:H	9	0.1
(2,212)	1:68:A:GLY:H	1:69:A:VAL:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,208)	1:68:A:GLY:H	1:69:A:VAL:H	9	0.1
(2,93)	1:37:A:ALA:H	1:39:A:LEU:H	2	0.1
(2,79)	1:25:A:TYR:H	1:26:A:ASP:H	13	0.1
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD11	6	0.1
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD12	6	0.1
(2,20)	1:10:A:LEU:H	1:10:A:LEU:HD13	6	0.1
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	4	0.1
(2,3)	1:128:A:VAL:H	1:129:A:TRP:H	4	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found