



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 9PGB / pdb_00009pgb
BMRB ID : 31261
Title : 4-module Cysteine Rich Eggshell Membrane Protein (CREMP)
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Deposited on : 2025-07-07

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
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

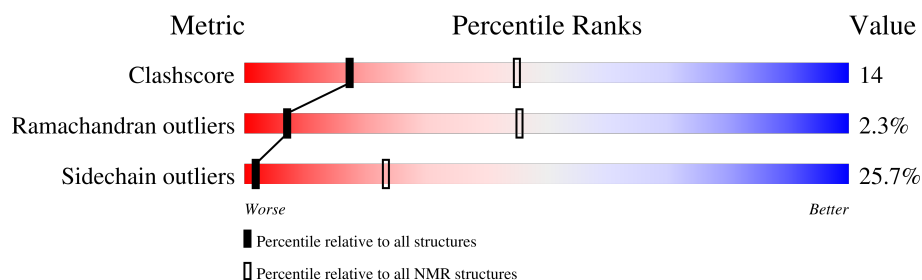
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	121	<div> <div></div> <div>55%</div> <div>33%</div> <div>12%</div> </div>

2 Ensemble composition and analysis

This entry contains 10 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: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:121 (121)	1.81	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 and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1759 atoms, of which 861 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 4-module Cysteine Rich Eggshell Membrane Protein.

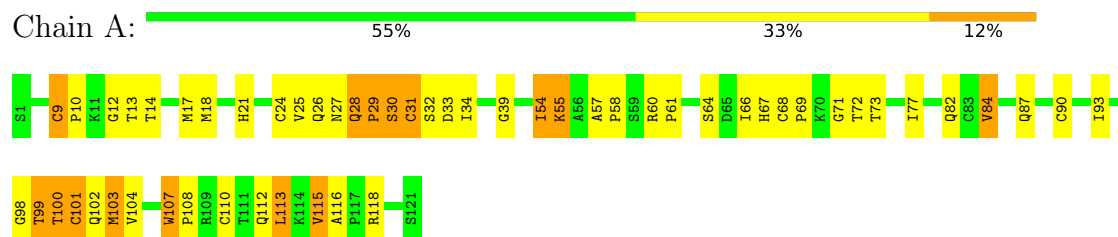
Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1759	536	861	167	174	21	

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: 4-module Cysteine Rich Eggshell Membrane Protein

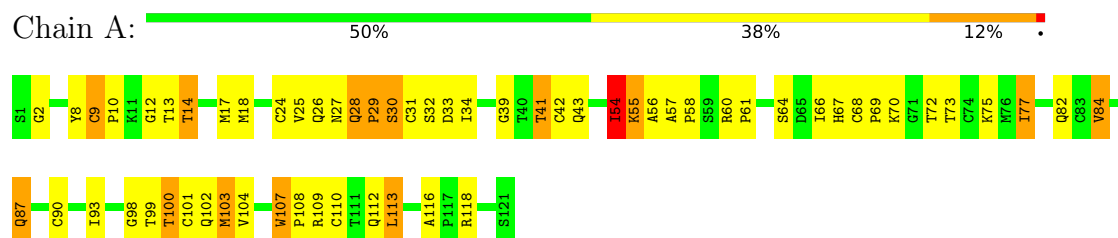


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

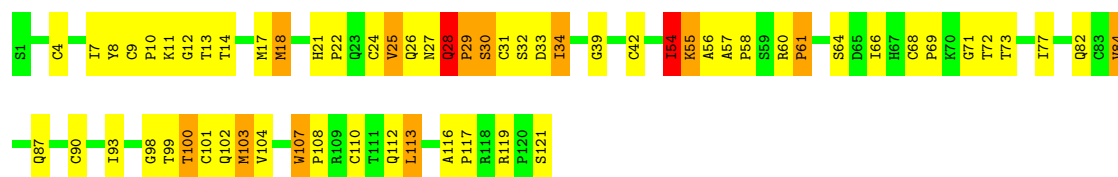
- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein



4.2.2 Score per residue for model 2

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein

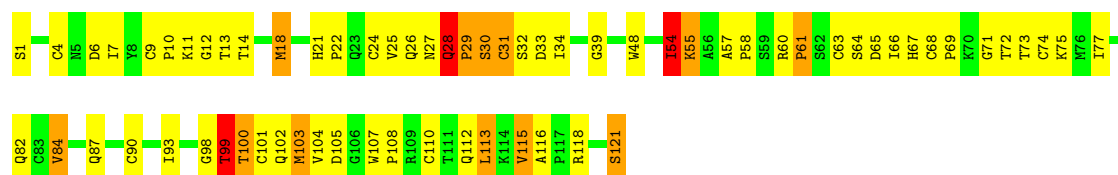




4.2.3 Score per residue for model 3

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein

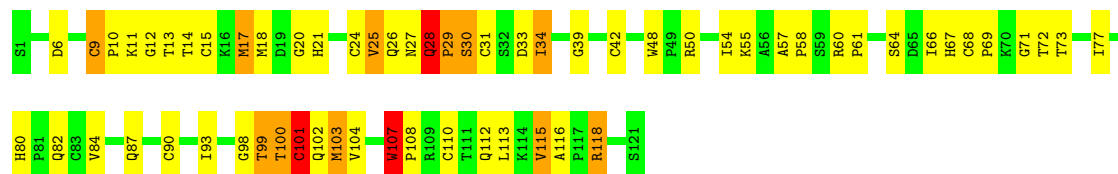
Chain A: 45% 43% 10% .



4.2.4 Score per residue for model 4

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein

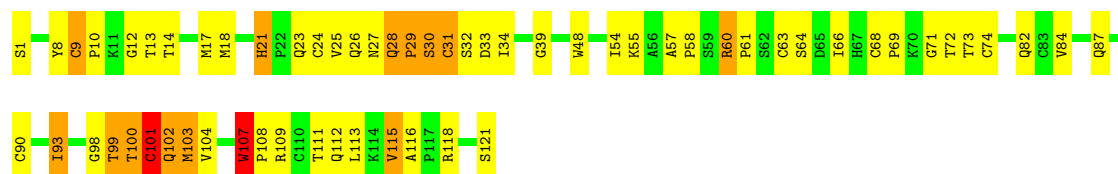
Chain A: 49% 40% 9% .



4.2.5 Score per residue for model 5 (medoid)

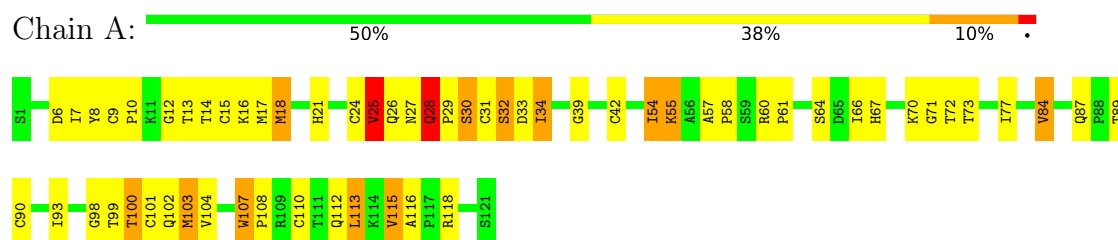
- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein

Chain A: 50% 38% 11% .



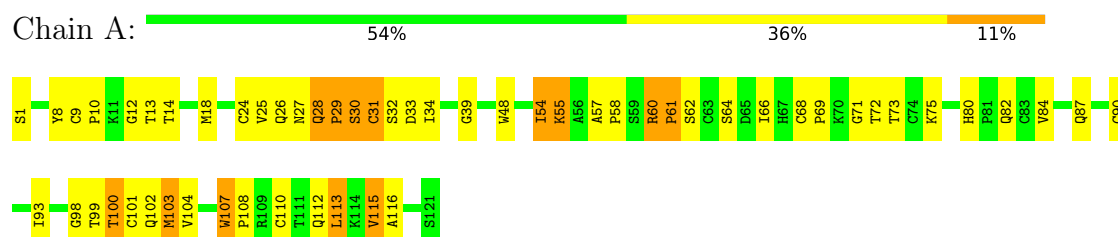
4.2.6 Score per residue for model 6

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein



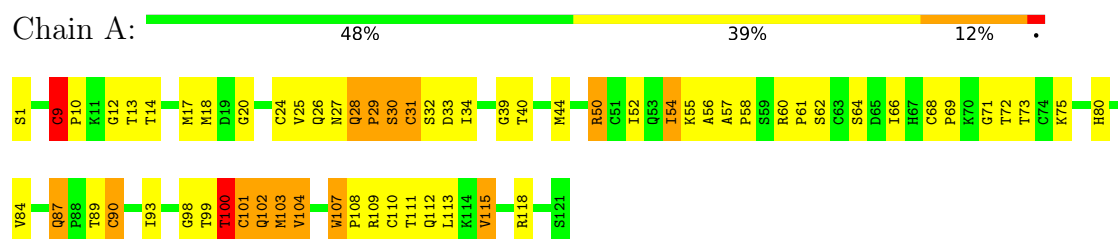
4.2.7 Score per residue for model 7

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein



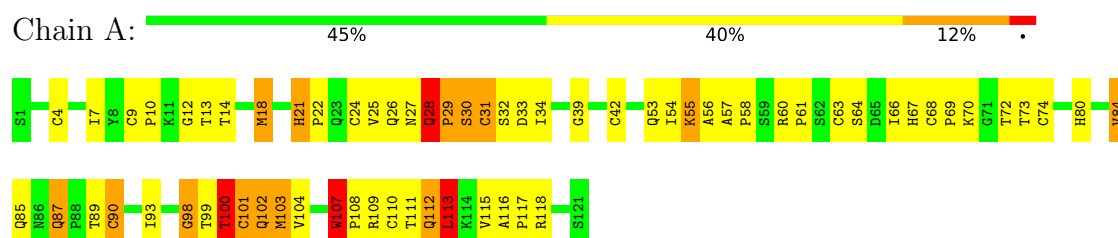
4.2.8 Score per residue for model 8

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein



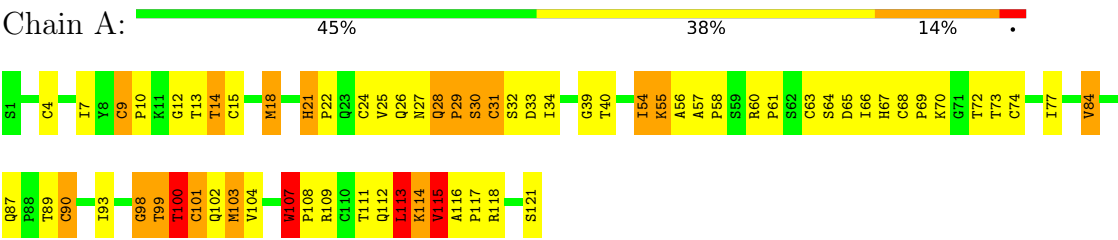
4.2.9 Score per residue for model 9

- Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein



4.2.10 Score per residue for model 10

● Molecule 1: 4-module Cysteine Rich Eggshell Membrane Protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	
PyMOL	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1311
Number of shifts mapped to atoms	1311
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.60±0.02	12±2/917 (1.4± 0.2%)	1.63±0.03	16±2/1240 (1.3± 0.2%)
All	All	1.60	125/9170 (1.4%)	1.63	163/12400 (1.3%)

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
1	A	103	MET	N-CA	-8.12	1.36	1.46	3	10
1	A	84	VAL	CA-C	-7.09	1.47	1.53	6	7
1	A	30	SER	N-CA	-6.90	1.37	1.46	3	9
1	A	101	CYS	N-CA	-6.88	1.37	1.47	8	10
1	A	87	GLN	N-CA	-6.79	1.39	1.46	9	9
1	A	102	GLN	CA-C	-6.74	1.45	1.53	9	10
1	A	30	SER	CA-C	-6.49	1.43	1.52	6	10
1	A	84	VAL	N-CA	-6.22	1.39	1.46	6	7
1	A	25	VAL	CA-C	-6.05	1.47	1.53	7	9
1	A	107	TRP	N-CA	-5.58	1.41	1.46	8	8
1	A	103	MET	CA-C	-5.51	1.46	1.52	3	4
1	A	102	GLN	N-CA	-5.49	1.40	1.46	8	3
1	A	84	VAL	C-N	-5.45	1.26	1.33	9	8
1	A	112	GLN	N-CA	-5.38	1.39	1.46	5	9
1	A	29	PRO	C-N	-5.34	1.26	1.33	3	5
1	A	100	THR	C-N	-5.24	1.26	1.33	9	1
1	A	99	THR	N-CA	-5.24	1.39	1.45	4	3
1	A	100	THR	N-CA	-5.12	1.39	1.45	9	1
1	A	25	VAL	N-CA	-5.09	1.40	1.46	9	1
1	A	85	GLN	N-CA	-5.07	1.39	1.46	9	1

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	65	ASP	N-CA-C	-9.65	100.36	112.72	10	2
1	A	98	GLY	N-CA-C	-9.08	103.17	113.79	3	10
1	A	84	VAL	N-CA-C	-8.45	94.62	106.53	1	10
1	A	39	GLY	N-CA-C	-8.37	104.00	113.79	1	10
1	A	33	ASP	N-CA-C	-8.10	103.23	113.43	1	10
1	A	30	SER	N-CA-C	-7.86	98.25	109.96	6	8
1	A	54	ILE	N-CA-C	-7.54	105.42	112.96	1	3
1	A	87	GLN	N-CA-C	-7.42	92.64	108.66	5	10
1	A	100	THR	N-CA-C	-7.40	99.04	109.69	10	8
1	A	99	THR	N-CA-C	-7.17	99.62	109.95	7	10
1	A	12	GLY	N-CA-C	-6.55	105.56	115.00	2	10
1	A	112	GLN	N-CA-C	-6.36	100.00	109.15	1	10
1	A	114	LYS	N-CA-C	-6.26	104.54	111.36	10	1
1	A	29	PRO	CB-CA-C	-6.25	103.71	111.64	10	6
1	A	67	HIS	CA-CB-CG	-6.08	107.72	113.80	1	6
1	A	103	MET	N-CA-C	-5.97	100.11	109.25	7	7
1	A	71	GLY	N-CA-C	-5.91	107.51	115.36	6	7
1	A	31	CYS	N-CA-C	-5.85	104.09	111.11	8	1
1	A	34	ILE	N-CA-C	-5.80	101.39	109.45	2	1
1	A	90	CYS	CA-C-N	-5.54	113.85	122.16	5	5
1	A	90	CYS	C-N-CA	-5.54	113.85	122.16	5	5
1	A	40	THR	N-CA-C	-5.47	102.10	110.14	8	2
1	A	103	MET	CA-C-N	-5.34	116.33	122.95	7	6
1	A	103	MET	C-N-CA	-5.34	116.33	122.95	7	6
1	A	6	ASP	N-CA-C	-5.31	106.97	113.50	4	3
1	A	28	GLN	N-CA-C	-5.26	98.18	109.81	4	5
1	A	44	MET	N-CA-C	-5.20	98.21	107.98	8	1

There are no chirality outliers.

There are no planarity outliers.

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	898	861	858	24±3
All	All	8980	8610	8580	239

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:HD12	1:A:108:PRO:CB	0.66	2.20	5	1
1:A:113:LEU:CB	1:A:116:ALA:HB2	0.65	2.22	1	7
1:A:68:CYS:CB	1:A:72:THR:HG21	0.62	2.25	3	9
1:A:54:ILE:HD12	1:A:55:LYS:H	0.61	1.55	3	5
1:A:7:ILE:HD12	1:A:22:PRO:HG2	0.61	1.73	10	4
1:A:54:ILE:HD13	1:A:55:LYS:H	0.61	1.55	8	2
1:A:17:MET:HE2	1:A:20:GLY:C	0.60	2.21	8	1
1:A:93:ILE:HD12	1:A:108:PRO:HB2	0.58	1.73	5	1
1:A:68:CYS:HB3	1:A:72:THR:HG21	0.58	1.76	2	9
1:A:109:ARG:O	1:A:111:THR:HG23	0.57	2.00	10	4
1:A:17:MET:HE2	1:A:20:GLY:CA	0.57	2.28	8	1
1:A:17:MET:HE1	1:A:21:HIS:N	0.55	2.16	4	1
1:A:54:ILE:HD12	1:A:55:LYS:N	0.54	2.17	3	5
1:A:54:ILE:HD13	1:A:55:LYS:N	0.54	2.18	8	2
1:A:17:MET:O	1:A:17:MET:HE2	0.54	2.01	5	2
1:A:113:LEU:HB2	1:A:116:ALA:HB2	0.53	1.80	1	2
1:A:107:TRP:CD1	1:A:107:TRP:C	0.53	2.87	6	4
1:A:107:TRP:C	1:A:107:TRP:CD1	0.53	2.87	10	6
1:A:55:LYS:HD2	1:A:57:ALA:HB2	0.53	1.78	2	2
1:A:17:MET:HA	1:A:17:MET:HE3	0.52	1.81	8	1
1:A:30:SER:O	1:A:31:CYS:C	0.52	2.53	4	10
1:A:100:THR:OG1	1:A:113:LEU:HD11	0.52	2.05	8	3
1:A:57:ALA:HB1	1:A:58:PRO:HD2	0.51	1.82	9	9
1:A:18:MET:HE2	1:A:23:GLN:OE1	0.50	2.07	5	1
1:A:103:MET:HA	1:A:108:PRO:HA	0.50	1.84	6	10
1:A:77:ILE:HD11	1:A:84:VAL:CG1	0.49	2.38	3	2
1:A:116:ALA:HB1	1:A:117:PRO:HD2	0.49	1.85	10	3
1:A:28:GLN:O	1:A:29:PRO:C	0.48	2.57	4	10
1:A:98:GLY:O	1:A:113:LEU:HD22	0.47	2.09	9	2
1:A:9:CYS:O	1:A:10:PRO:C	0.47	2.58	5	10
1:A:77:ILE:HD12	1:A:82:GLN:HB3	0.46	1.85	3	3
1:A:60:ARG:O	1:A:61:PRO:C	0.46	2.57	7	10
1:A:18:MET:HE3	1:A:21:HIS:CD2	0.46	2.45	5	1
1:A:99:THR:HG23	1:A:121:SER:O	0.45	2.12	3	1
1:A:17:MET:HE2	1:A:17:MET:HA	0.45	1.88	4	1
1:A:115:VAL:HG13	1:A:115:VAL:O	0.45	2.12	7	3
1:A:41:THR:HG23	1:A:43:GLN:OE1	0.45	2.12	1	1
1:A:115:VAL:O	1:A:115:VAL:HG13	0.45	2.12	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:VAL:HG23	1:A:104:VAL:O	0.44	2.12	5	5
1:A:77:ILE:HD13	1:A:82:GLN:HB3	0.44	1.90	1	1
1:A:100:THR:HG23	1:A:101:CYS:N	0.44	2.27	8	5
1:A:116:ALA:HB3	1:A:119:ARG:HD2	0.44	1.89	2	1
1:A:77:ILE:HD12	1:A:82:GLN:CG	0.43	2.43	3	2
1:A:17:MET:HE1	1:A:20:GLY:CA	0.43	2.42	4	1
1:A:69:PRO:O	1:A:72:THR:HG23	0.43	2.14	10	9
1:A:104:VAL:O	1:A:104:VAL:HG22	0.43	2.12	8	1
1:A:18:MET:O	1:A:21:HIS:CD2	0.43	2.72	3	7
1:A:57:ALA:O	1:A:58:PRO:C	0.42	2.62	5	9
1:A:113:LEU:HB3	1:A:116:ALA:HB2	0.42	1.90	5	5
1:A:55:LYS:O	1:A:57:ALA:N	0.42	2.52	10	3
1:A:8:TYR:C	1:A:9:CYS:O	0.42	2.61	5	5
1:A:77:ILE:HD11	1:A:84:VAL:HG13	0.42	1.91	3	1
1:A:34:ILE:N	1:A:34:ILE:HD13	0.42	2.29	6	2
1:A:48:TRP:C	1:A:48:TRP:CD1	0.42	2.98	3	4
1:A:17:MET:HE1	1:A:20:GLY:C	0.42	2.39	4	1
1:A:84:VAL:HG23	1:A:84:VAL:O	0.42	2.15	3	3
1:A:80:HIS:ND1	1:A:80:HIS:O	0.42	2.53	9	2
1:A:50:ARG:HD2	1:A:52:ILE:HD13	0.42	1.92	8	1
1:A:2:GLY:CA	1:A:17:MET:HE2	0.42	2.44	1	1
1:A:30:SER:C	1:A:32:SER:N	0.41	2.77	6	1
1:A:99:THR:O	1:A:113:LEU:HD11	0.41	2.15	10	1
1:A:84:VAL:O	1:A:84:VAL:HG23	0.41	2.15	6	3
1:A:114:LYS:C	1:A:115:VAL:HG22	0.41	2.39	10	1
1:A:14:THR:O	1:A:14:THR:HG22	0.41	2.16	10	2
1:A:25:VAL:O	1:A:25:VAL:HG12	0.41	2.16	4	2
1:A:112:GLN:O	1:A:113:LEU:C	0.40	2.64	9	1
1:A:80:HIS:O	1:A:80:HIS:ND1	0.40	2.54	7	2
1:A:113:LEU:HD22	1:A:113:LEU:H	0.40	1.76	10	2
1:A:4:CYS:SG	1:A:15:CYS:C	0.40	3.04	10	1
1:A:68:CYS:HB2	1:A:72:THR:HG21	0.40	1.94	3	1
1:A:17:MET:HE2	1:A:17:MET:O	0.40	2.16	6	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/121 (98%)	88±3 (74±2%)	28±3 (24±2%)	3±1 (2±1%)	7	45
All	All	1190/1210 (98%)	881 (74%)	282 (24%)	27 (2%)	7	45

All 6 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	118	ARG	8
1	A	115	VAL	8
1	A	56	ALA	5
1	A	61	PRO	3
1	A	113	LEU	2
1	A	9	CYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	108/108 (100%)	80±2 (74±2%)	28±2 (26±2%)	2	23
All	All	1080/1080 (100%)	802 (74%)	278 (26%)	2	23

All 55 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	13	THR	10
1	A	14	THR	10
1	A	24	CYS	10
1	A	26	GLN	10
1	A	27	ASN	10
1	A	28	GLN	10
1	A	34	ILE	10
1	A	54	ILE	10
1	A	64	SER	10
1	A	66	ILE	10
1	A	73	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	93	ILE	10
1	A	100	THR	10
1	A	32	SER	9
1	A	55	LYS	9
1	A	18	MET	8
1	A	90	CYS	8
1	A	110	CYS	8
1	A	113	LEU	7
1	A	9	CYS	5
1	A	42	CYS	5
1	A	104	VAL	5
1	A	31	CYS	5
1	A	107	TRP	5
1	A	70	LYS	4
1	A	75	LYS	4
1	A	121	SER	4
1	A	1	SER	4
1	A	63	CYS	4
1	A	74	CYS	4
1	A	89	THR	4
1	A	77	ILE	3
1	A	87	GLN	3
1	A	4	CYS	3
1	A	11	LYS	3
1	A	25	VAL	3
1	A	99	THR	3
1	A	21	HIS	3
1	A	102	GLN	3
1	A	15	CYS	2
1	A	50	ARG	2
1	A	101	CYS	2
1	A	60	ARG	2
1	A	82	GLN	2
1	A	62	SER	2
1	A	41	THR	1
1	A	109	ARG	1
1	A	105	ASP	1
1	A	17	MET	1
1	A	118	ARG	1
1	A	7	ILE	1
1	A	16	LYS	1
1	A	72	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	53	GLN	1
1	A	115	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 87% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1311
Number of shifts mapped to atoms	1311
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
$^{13}\text{C}_\alpha$	120	0.29 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	110	-0.22 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	120	0.21 ± 0.07	None needed (< 0.5 ppm)
^{15}N	106	-0.69 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1304 atoms were assigned a chemical shift out of a possible 1495. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	583/591 (99%)	237/240 (99%)	240/242 (99%)	106/109 (97%)
Sidechain	676/847 (80%)	454/546 (83%)	221/263 (84%)	1/38 (3%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	45/57 (79%)	24/28 (86%)	19/21 (90%)	2/8 (25%)
Overall	1304/1495 (87%)	715/814 (88%)	480/526 (91%)	109/155 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1304 atoms were assigned a chemical shift out of a possible 1495. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	583/591 (99%)	237/240 (99%)	240/242 (99%)	106/109 (97%)
Sidechain	676/847 (80%)	454/546 (83%)	221/263 (84%)	1/38 (3%)
Aromatic	45/57 (79%)	24/28 (86%)	19/21 (90%)	2/8 (25%)
Overall	1304/1495 (87%)	715/814 (88%)	480/526 (91%)	109/155 (70%)

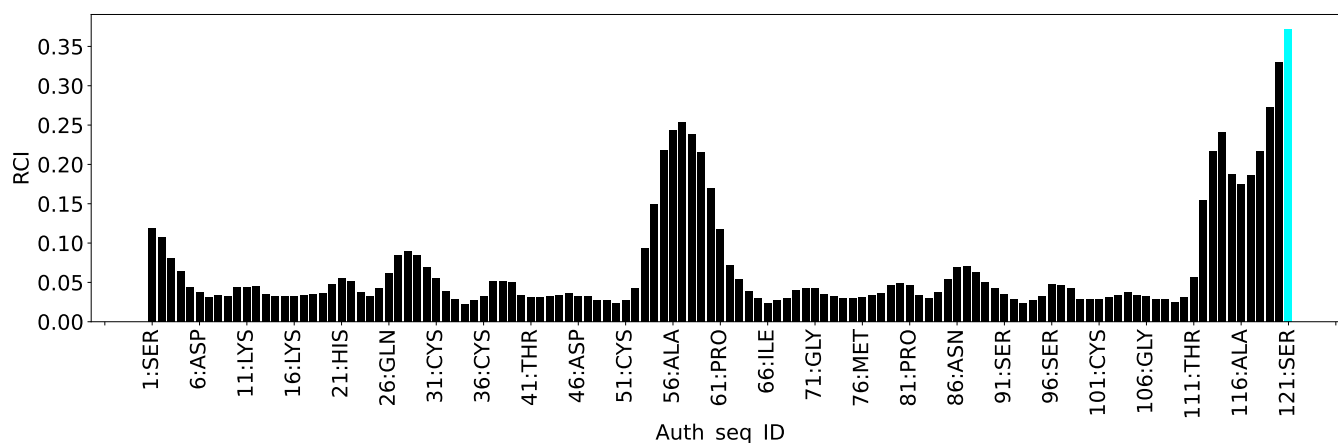
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



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	1448
Intra-residue ($ i-j =0$)	358
Sequential ($ i-j =1$)	551
Medium range ($ i-j >1$ and $ i-j <5$)	335
Long range ($ i-j \geq 5$)	204
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.0
Number of long range restraints per residue ¹	1.7

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)	69.1	0.2
0.2-0.5 (Medium)	139.2	0.5
>0.5 (Large)	160.4	3.31

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 ⓘ

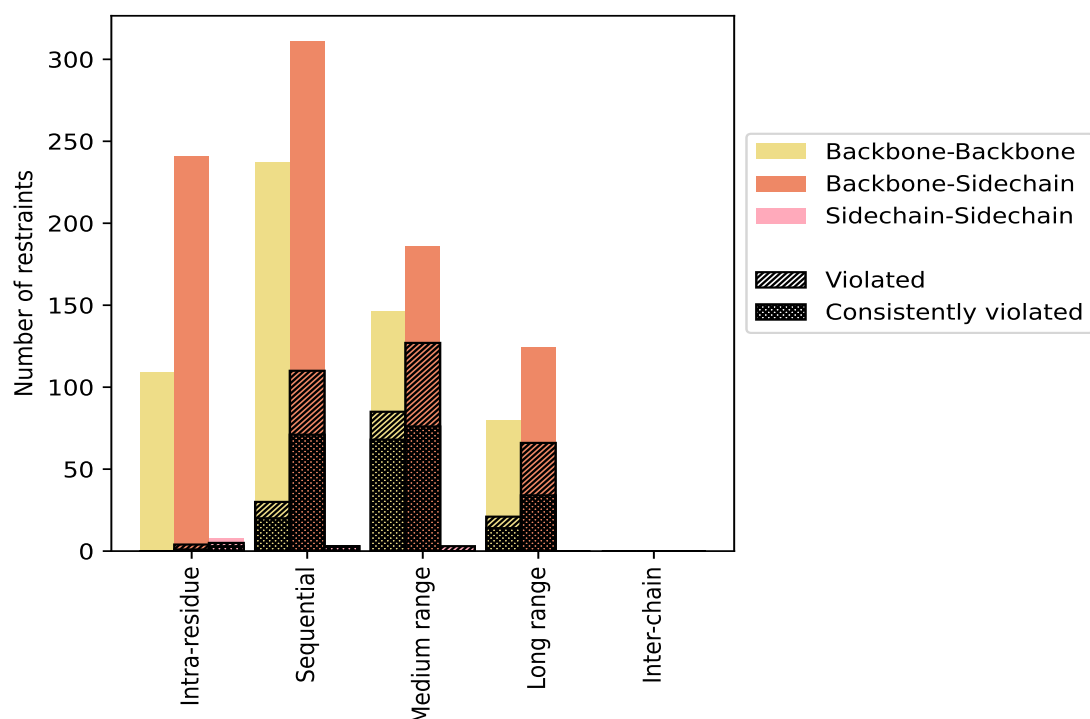
9.1 Summary of distance violations ⓘ

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)	358	24.7	9	2.5	0.6	4	1.1	0.3
Backbone-Backbone	109	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	241	16.6	4	1.7	0.3	1	0.4	0.1
Sidechain-Sidechain	8	0.6	5	62.5	0.3	3	37.5	0.2
Sequential (i-j =1)	551	38.1	143	26.0	9.9	94	17.1	6.5
Backbone-Backbone	237	16.4	30	12.7	2.1	20	8.4	1.4
Backbone-Sidechain	311	21.5	110	35.4	7.6	71	22.8	4.9
Sidechain-Sidechain	3	0.2	3	100.0	0.2	3	100.0	0.2
Medium range (i-j >1 & i-j <5)	335	23.1	215	64.2	14.8	144	43.0	9.9
Backbone-Backbone	146	10.1	85	58.2	5.9	68	46.6	4.7
Backbone-Sidechain	186	12.8	127	68.3	8.8	76	40.9	5.2
Sidechain-Sidechain	3	0.2	3	100.0	0.2	0	0.0	0.0
Long range (i-j ≥5)	204	14.1	87	42.6	6.0	48	23.5	3.3
Backbone-Backbone	80	5.5	21	26.2	1.5	14	17.5	1.0
Backbone-Sidechain	124	8.6	66	53.2	4.6	34	27.4	2.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
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	1448	100.0	454	31.4	31.4	290	20.0	20.0
Backbone-Backbone	572	39.5	136	23.8	9.4	102	17.8	7.0
Backbone-Sidechain	862	59.5	307	35.6	21.2	182	21.1	12.6
Sidechain-Sidechain	14	1.0	11	78.6	0.8	6	42.9	0.4

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

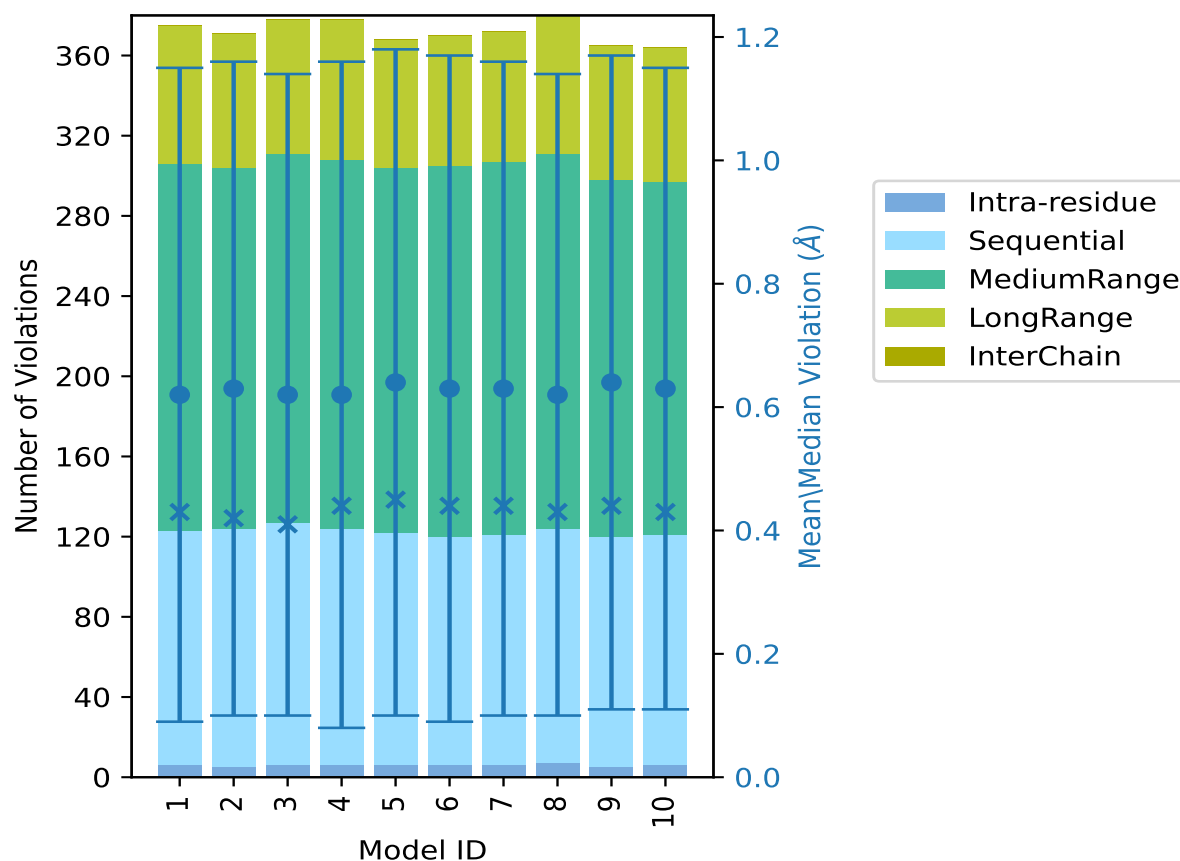
9.2 Distance violation statistics for each model [i](#)

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	6	117	183	69	0	375	0.62	2.92	0.53	0.43
2	5	119	180	67	0	371	0.63	2.96	0.53	0.42
3	6	121	184	67	0	378	0.62	2.81	0.52	0.41
4	6	118	184	70	0	378	0.62	2.87	0.54	0.44
5	6	116	182	64	0	368	0.64	2.83	0.54	0.45
6	6	114	185	65	0	370	0.63	3.31	0.54	0.44
7	6	115	186	65	0	372	0.63	2.87	0.53	0.44
8	7	117	187	69	0	380	0.62	2.95	0.52	0.43
9	5	115	178	67	0	365	0.64	2.89	0.53	0.44
10	6	115	176	67	0	364	0.63	2.79	0.52	0.43

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 [i](#)



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 [i](#)

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, 994(IR:349, SQ:408, MR:120, LR:117, IC:0) 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	%
0	12	12	9	0	33	1	10.0
0	7	8	3	0	18	2	20.0
3	3	5	5	0	16	3	30.0

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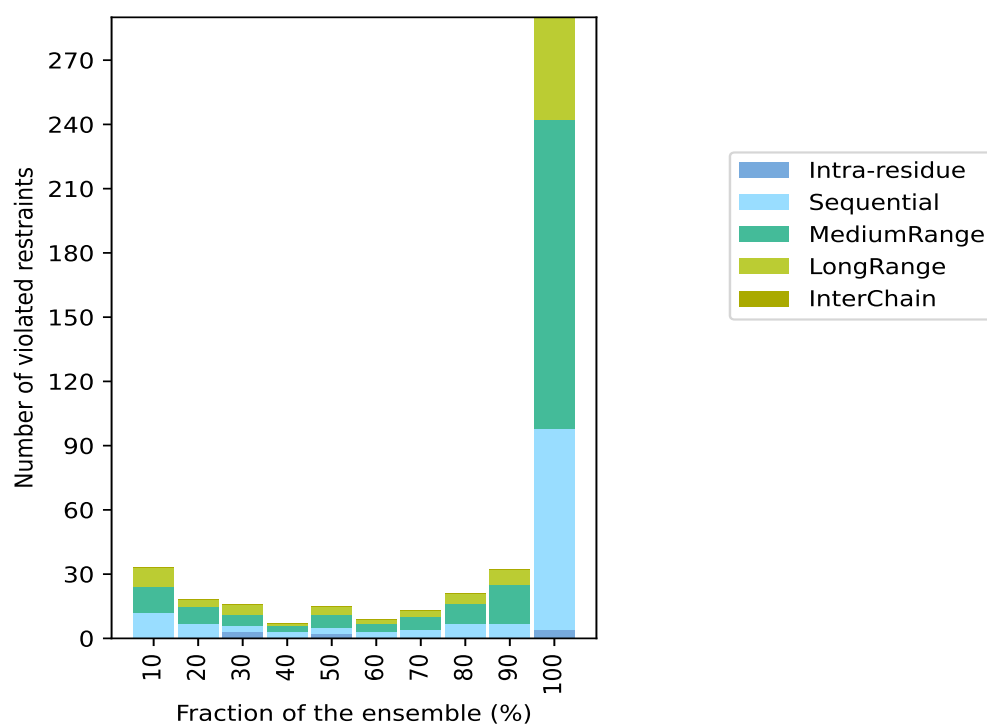
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	3	3	1	0	7	4	40.0
2	3	6	4	0	15	5	50.0
0	3	4	2	0	9	6	60.0
0	4	6	3	0	13	7	70.0
0	7	9	5	0	21	8	80.0
0	7	18	7	0	32	9	90.0
4	94	144	48	0	290	10	100.0

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 ⓘ

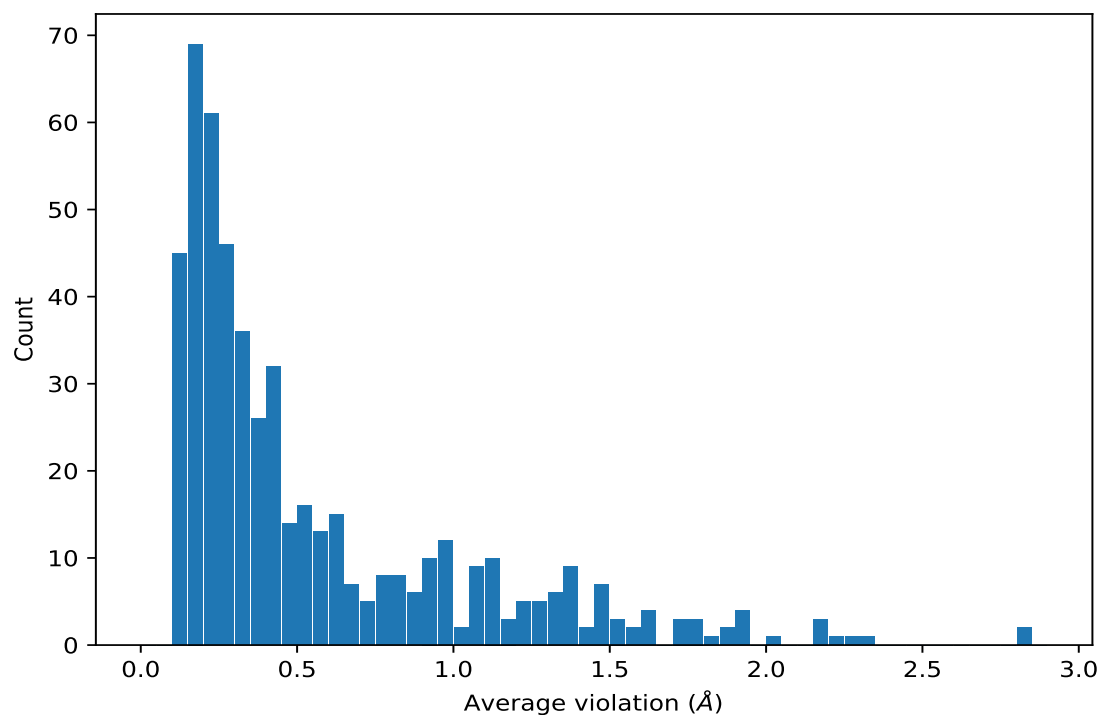


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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)
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	10	2.81	0.08	2.8
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	10	2.8	0.11	2.82
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	10	2.31	0.05	2.32
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	10	2.28	0.06	2.26
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	10	2.2	0.18	2.14
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	10	2.19	0.35	2.19
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	10	2.17	0.44	2.16
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	10	2.16	0.03	2.17
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	10	2.02	0.1	2.02
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	10	1.93	0.06	1.94
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	10	1.91	0.25	1.98
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	10	1.9	0.2	1.86
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	10	1.9	0.39	1.78
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	10	1.86	0.02	1.87
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	10	1.86	0.05	1.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	10	1.84	0.16	1.81
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	10	1.79	0.04	1.78
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	10	1.79	0.04	1.78
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	10	1.79	0.04	1.78
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	10	1.72	0.05	1.73
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	10	1.72	0.23	1.59
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	10	1.71	0.32	1.72
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	10	1.63	0.01	1.63
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	10	1.61	0.04	1.62
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	10	1.6	0.14	1.58
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	10	1.6	0.02	1.59
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	10	1.58	0.05	1.58
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	10	1.56	0.05	1.56
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	10	1.53	0.05	1.53
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	10	1.52	0.3	1.64
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	10	1.51	0.08	1.52
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	10	1.49	0.04	1.5
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	10	1.49	0.04	1.5
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	10	1.49	0.04	1.5
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	10	1.49	0.07	1.48
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	10	1.47	0.21	1.42
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	10	1.46	0.12	1.44
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	10	1.45	0.09	1.44
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	10	1.44	0.31	1.34
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	10	1.4	0.09	1.38
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	10	1.38	0.1	1.38
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	10	1.38	0.27	1.41
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	10	1.38	0.27	1.41
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	10	1.38	0.27	1.41
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	10	1.38	0.1	1.37
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	10	1.37	0.07	1.39
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	10	1.35	0.41	1.6
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	10	1.35	0.41	1.6
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	10	1.35	0.41	1.6
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	10	1.34	0.07	1.33
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	10	1.33	0.04	1.32
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	10	1.33	0.1	1.27
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	10	1.32	0.06	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	10	1.32	0.06	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	10	1.32	0.06	1.31
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	10	1.28	0.03	1.29
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	10	1.28	0.19	1.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	10	1.26	0.03	1.25
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	10	1.26	0.03	1.25
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	10	1.26	0.03	1.25
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	10	1.24	0.01	1.25
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	10	1.24	0.05	1.24
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	10	1.24	0.01	1.24
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	10	1.21	0.12	1.21
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	10	1.2	0.12	1.23
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	10	1.17	0.04	1.15
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	10	1.16	0.09	1.16
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	10	1.16	0.07	1.14
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	10	1.14	0.29	1.28
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	10	1.13	0.34	1.27
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	10	1.13	0.22	1.04
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	10	1.12	0.14	1.06
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	10	1.12	0.14	1.06
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	10	1.12	0.14	1.06
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	10	1.11	0.05	1.11
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	10	1.11	0.08	1.1
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	10	1.1	0.32	1.06
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	10	1.1	0.08	1.11
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	10	1.09	0.08	1.08
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	10	1.09	0.18	1.02
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	10	1.09	0.06	1.1
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	10	1.08	0.09	1.08
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	10	1.06	0.31	0.92
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	10	1.06	0.11	1.08
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	10	1.06	0.11	1.08
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	10	1.06	0.11	1.08
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	10	1.05	0.08	1.04
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	10	1.01	0.14	0.98
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	10	1.0	0.15	1.0
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	10	0.99	0.06	1.0
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	10	0.99	0.06	1.0
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	10	0.99	0.06	1.0
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	10	0.99	0.16	0.92
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	10	0.99	0.04	0.98
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	10	0.98	0.04	0.98
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	10	0.97	0.05	0.98
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	10	0.97	0.59	0.6
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	10	0.97	0.06	0.94
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	10	0.96	0.13	1.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	10	0.95	0.03	0.96
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	10	0.95	0.03	0.96
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	10	0.94	0.41	0.88
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	10	0.93	0.25	1.04
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	10	0.92	0.1	0.92
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	10	0.92	0.09	0.94
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	10	0.92	0.45	0.86
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	10	0.91	0.17	0.94
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	10	0.91	0.11	0.9
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	10	0.91	0.19	1.01
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	10	0.9	0.23	0.89
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	10	0.9	0.1	0.88
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	10	0.87	0.28	0.86
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	10	0.87	0.0	0.87
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	10	0.86	0.01	0.86
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	10	0.86	0.21	0.9
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	10	0.85	0.09	0.82
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	10	0.85	0.04	0.84
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	10	0.84	0.56	0.6
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	10	0.84	0.06	0.84
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	10	0.83	0.02	0.84
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	10	0.81	0.26	0.88
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	10	0.8	0.03	0.8
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	10	0.8	0.22	0.71
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	10	0.8	0.01	0.8
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	10	0.79	0.06	0.78
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	10	0.78	0.17	0.74
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	10	0.77	0.13	0.82
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	10	0.77	0.06	0.76
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	10	0.76	0.02	0.77
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	10	0.76	0.03	0.77
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	10	0.75	0.13	0.78
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	10	0.75	0.06	0.74
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	10	0.74	0.03	0.74
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	10	0.73	0.03	0.74
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	10	0.72	0.08	0.73
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	10	0.72	0.08	0.75
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	10	0.7	0.09	0.72
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	10	0.69	0.25	0.58
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	10	0.69	0.04	0.68
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	10	0.67	0.03	0.68
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	10	0.67	0.16	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	10	0.67	0.07	0.68
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	10	0.67	0.11	0.68
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	10	0.64	0.03	0.62
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	10	0.64	0.18	0.59
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	10	0.62	0.27	0.48
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	10	0.62	0.16	0.57
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	10	0.62	0.05	0.62
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	10	0.61	0.07	0.6
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	10	0.6	0.27	0.54
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	10	0.6	0.02	0.61
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	10	0.6	0.05	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	10	0.6	0.05	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	10	0.6	0.05	0.6
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	10	0.6	0.03	0.58
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	10	0.6	0.03	0.58
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	10	0.6	0.03	0.58
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	10	0.6	0.02	0.6
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	10	0.59	0.03	0.6
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	10	0.59	0.08	0.56
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	10	0.59	0.03	0.58
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	10	0.59	0.06	0.58
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	10	0.59	0.06	0.57
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	10	0.58	0.07	0.59
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	10	0.58	0.08	0.58
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	10	0.58	0.12	0.6
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	10	0.58	0.11	0.6
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	10	0.56	0.06	0.58
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	10	0.55	0.04	0.54
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	10	0.55	0.03	0.56
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	10	0.54	0.03	0.54
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	10	0.53	0.06	0.51
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	10	0.53	0.04	0.54
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	10	0.53	0.01	0.53
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	10	0.53	0.04	0.55
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	10	0.53	0.14	0.46
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	10	0.52	0.05	0.51
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	10	0.51	0.02	0.52
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	10	0.51	0.12	0.5
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	10	0.51	0.01	0.51
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	10	0.51	0.04	0.51
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	10	0.51	0.04	0.5
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	10	0.5	0.2	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	10	0.5	0.07	0.47
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	10	0.5	0.03	0.49
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	10	0.49	0.06	0.5
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	10	0.49	0.08	0.5
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	10	0.49	0.01	0.49
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	10	0.49	0.12	0.5
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	10	0.48	0.04	0.46
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	10	0.47	0.11	0.44
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	10	0.47	0.08	0.44
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	10	0.47	0.09	0.48
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	10	0.47	0.17	0.46
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	10	0.47	0.01	0.46
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	10	0.47	0.1	0.42
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	10	0.46	0.02	0.47
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	10	0.45	0.04	0.46
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	10	0.45	0.13	0.4
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	10	0.44	0.02	0.44
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	10	0.44	0.02	0.44
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	10	0.44	0.08	0.41
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	10	0.44	0.03	0.42
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	10	0.43	0.2	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	10	0.43	0.2	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	10	0.43	0.2	0.36
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	10	0.43	0.04	0.44
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	10	0.43	0.02	0.44
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	10	0.43	0.02	0.44
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	10	0.43	0.02	0.44
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	10	0.43	0.2	0.37
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	10	0.43	0.06	0.43
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	10	0.43	0.05	0.42
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	10	0.43	0.03	0.44
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	10	0.42	0.19	0.42
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	10	0.41	0.02	0.4
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	10	0.41	0.03	0.41
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	10	0.4	0.1	0.39
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	10	0.4	0.07	0.42
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	10	0.4	0.06	0.43
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	10	0.4	0.01	0.4
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	10	0.39	0.04	0.4
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	10	0.39	0.03	0.38
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	10	0.39	0.02	0.39
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	10	0.39	0.03	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	10	0.38	0.08	0.37
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	10	0.38	0.06	0.4
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	10	0.38	0.28	0.29
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	10	0.38	0.13	0.34
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	10	0.38	0.1	0.34
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	10	0.38	0.1	0.34
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	10	0.38	0.1	0.34
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	10	0.37	0.04	0.37
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	10	0.37	0.03	0.36
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	10	0.37	0.03	0.37
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	10	0.37	0.13	0.3
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	10	0.36	0.06	0.36
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	10	0.36	0.06	0.36
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	10	0.36	0.06	0.36
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	10	0.36	0.01	0.36
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	10	0.36	0.02	0.36
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	10	0.36	0.02	0.37
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	10	0.35	0.06	0.36
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	10	0.35	0.04	0.34
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	10	0.35	0.06	0.34
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	10	0.34	0.03	0.35
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	10	0.34	0.07	0.34
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	10	0.33	0.03	0.33
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	10	0.33	0.11	0.3
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	10	0.33	0.11	0.3
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	10	0.33	0.11	0.3
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	10	0.33	0.17	0.26
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	10	0.33	0.02	0.33
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	10	0.33	0.03	0.33
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	10	0.33	0.11	0.3
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	10	0.32	0.05	0.32
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	10	0.32	0.11	0.32
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	10	0.32	0.02	0.32
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	10	0.32	0.03	0.32
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	10	0.32	0.03	0.32
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	10	0.31	0.06	0.32
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	10	0.31	0.07	0.34
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	10	0.31	0.04	0.32
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	10	0.31	0.05	0.3
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	10	0.29	0.02	0.29
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	10	0.29	0.02	0.29
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	10	0.29	0.02	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	10	0.28	0.04	0.3
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	10	0.28	0.06	0.28
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	10	0.28	0.01	0.29
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	10	0.28	0.02	0.28
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	10	0.28	0.04	0.28
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	10	0.28	0.04	0.28
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	10	0.28	0.04	0.28
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	10	0.28	0.03	0.29
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	10	0.28	0.05	0.28
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	10	0.27	0.03	0.29
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	10	0.27	0.07	0.3
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	10	0.27	0.07	0.3
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	10	0.27	0.07	0.3
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	10	0.26	0.03	0.26
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	10	0.26	0.07	0.22
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	10	0.26	0.05	0.28
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	10	0.26	0.06	0.24
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	10	0.26	0.03	0.25
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	10	0.26	0.05	0.27
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	10	0.26	0.01	0.26
(1,466)	1:40:A:THR:H	1:37:A:SER:H	10	0.26	0.06	0.26
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	10	0.25	0.06	0.24
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	10	0.25	0.05	0.24
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	10	0.25	0.05	0.24
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	10	0.25	0.01	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	10	0.25	0.0	0.25
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	10	0.25	0.08	0.24
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	10	0.25	0.05	0.23
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	10	0.24	0.05	0.23
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	10	0.24	0.03	0.24
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	10	0.24	0.02	0.24
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	10	0.24	0.03	0.25
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	10	0.23	0.07	0.22
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	10	0.23	0.03	0.24
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	10	0.23	0.04	0.22
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	10	0.22	0.03	0.22
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	10	0.21	0.04	0.2
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	10	0.21	0.03	0.2
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	10	0.21	0.03	0.21
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	10	0.21	0.02	0.21
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	10	0.21	0.04	0.21
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	10	0.2	0.02	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	10	0.2	0.01	0.2
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	10	0.2	0.03	0.2
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	10	0.2	0.04	0.2
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	10	0.2	0.02	0.2
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	10	0.2	0.08	0.18
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	10	0.2	0.05	0.18
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	10	0.19	0.05	0.2
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	10	0.18	0.02	0.18
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	10	0.18	0.04	0.19
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	10	0.18	0.04	0.18
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	10	0.18	0.01	0.18
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	10	0.18	0.01	0.18
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	10	0.18	0.06	0.16
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	10	0.16	0.02	0.16
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	10	0.16	0.03	0.16
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	10	0.16	0.03	0.16
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	10	0.16	0.02	0.16
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	10	0.13	0.02	0.13
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	10	0.12	0.02	0.12
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	10	0.11	0.01	0.11
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	9	0.84	0.08	0.82
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	9	0.55	0.17	0.49
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	9	0.41	0.23	0.32
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	9	0.4	0.07	0.42
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	9	0.4	0.07	0.42
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	9	0.4	0.07	0.42
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	9	0.4	0.1	0.44
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	9	0.33	0.05	0.3
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	9	0.33	0.05	0.3
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	9	0.33	0.05	0.3
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	9	0.3	0.1	0.33
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	9	0.3	0.1	0.33
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	9	0.3	0.1	0.33
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	9	0.28	0.06	0.29
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	9	0.26	0.05	0.25
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	9	0.24	0.07	0.21
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	9	0.24	0.09	0.24
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	9	0.24	0.09	0.24
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	9	0.24	0.09	0.24
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	9	0.24	0.19	0.19
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	9	0.23	0.05	0.21
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	9	0.23	0.1	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	9	0.22	0.04	0.23
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	9	0.21	0.06	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	9	0.21	0.04	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	9	0.21	0.04	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	9	0.21	0.04	0.21
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	9	0.2	0.03	0.2
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	9	0.2	0.01	0.21
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	9	0.2	0.04	0.2
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	9	0.2	0.02	0.2
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	9	0.2	0.05	0.19
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	9	0.19	0.09	0.16
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	9	0.18	0.03	0.18
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	9	0.17	0.02	0.18
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	9	0.17	0.09	0.14
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	9	0.17	0.09	0.14
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	9	0.17	0.09	0.14
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	9	0.15	0.04	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	9	0.15	0.05	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	9	0.15	0.05	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	9	0.15	0.05	0.13
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	9	0.15	0.05	0.13
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	9	0.15	0.03	0.15
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	9	0.14	0.02	0.14
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	9	0.14	0.02	0.13
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	8	0.69	0.07	0.7
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	8	0.4	0.17	0.4
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	8	0.4	0.02	0.4
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	8	0.29	0.03	0.29
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	8	0.25	0.06	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	8	0.25	0.06	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	8	0.25	0.06	0.26
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	8	0.23	0.09	0.23
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	8	0.23	0.05	0.24
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	8	0.23	0.05	0.24
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	8	0.23	0.05	0.24
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	8	0.23	0.07	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	8	0.23	0.07	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	8	0.23	0.07	0.22
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	8	0.22	0.04	0.22
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	8	0.22	0.04	0.22
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	8	0.22	0.04	0.22
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	8	0.21	0.01	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	8	0.2	0.04	0.19
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	8	0.19	0.05	0.19
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	8	0.18	0.01	0.18
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	8	0.16	0.03	0.17
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	8	0.16	0.02	0.16
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	8	0.16	0.02	0.16
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	8	0.16	0.02	0.16
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	8	0.16	0.02	0.16
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	8	0.15	0.02	0.14
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	8	0.15	0.02	0.14
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	8	0.15	0.02	0.14
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	8	0.14	0.02	0.14
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	8	0.14	0.02	0.14
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	8	0.13	0.02	0.12
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	8	0.12	0.01	0.12
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	7	0.31	0.34	0.15
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	7	0.31	0.08	0.32
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	7	0.26	0.06	0.23
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	7	0.26	0.06	0.23
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	7	0.26	0.06	0.23
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	7	0.22	0.03	0.21
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	7	0.21	0.06	0.22
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	7	0.21	0.06	0.22
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	7	0.21	0.06	0.22
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	7	0.18	0.06	0.16
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	7	0.18	0.06	0.19
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	7	0.18	0.06	0.19
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	7	0.18	0.06	0.19
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	7	0.16	0.04	0.16
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	7	0.14	0.04	0.13
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	7	0.14	0.01	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	7	0.13	0.01	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	7	0.13	0.01	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	7	0.13	0.01	0.13
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	7	0.12	0.02	0.12
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	7	0.11	0.01	0.11
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	6	0.51	0.24	0.52
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	6	0.37	0.43	0.16
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	6	0.28	0.08	0.29
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	6	0.25	0.02	0.24
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	6	0.25	0.02	0.24
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	6	0.25	0.02	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	6	0.22	0.12	0.15
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	6	0.19	0.07	0.18
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	6	0.16	0.05	0.15
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	6	0.14	0.01	0.14
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	6	0.14	0.02	0.14
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG21	5	0.4	0.05	0.39
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG22	5	0.4	0.05	0.39
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG23	5	0.4	0.05	0.39
(1,674)	1:55:A:LYS:HG3	1:41:A:THR:H	5	0.38	0.1	0.36
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG11	5	0.33	0.02	0.33
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG12	5	0.33	0.02	0.33
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG13	5	0.33	0.02	0.33
(1,1276)	1:107:A:TRP:H	1:103:A:MET:HG3	5	0.19	0.07	0.16
(1,57)	1:8:A:TYR:H	1:7:A:ILE:HG13	5	0.19	0.05	0.22
(1,587)	1:48:A:TRP:HE1	1:48:A:TRP:HB3	5	0.17	0.01	0.17
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD11	5	0.16	0.05	0.14
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD12	5	0.16	0.05	0.14
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD13	5	0.16	0.05	0.14
(1,586)	1:48:A:TRP:HE1	1:48:A:TRP:HB2	5	0.15	0.01	0.16
(1,293)	1:25:A:VAL:H	1:16:A:LYS:HD2	5	0.15	0.04	0.12
(1,1325)	1:111:A:THR:H	1:109:A:ARG:HA	5	0.14	0.02	0.13
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD11	5	0.13	0.01	0.13
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD12	5	0.13	0.01	0.13
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD13	5	0.13	0.01	0.13
(1,884)	1:77:A:ILE:H	1:75:A:LYS:H	5	0.13	0.02	0.14
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG11	5	0.13	0.01	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG12	5	0.13	0.01	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG13	5	0.13	0.01	0.13
(1,108)	1:13:A:THR:H	1:24:A:CYS:HB3	5	0.12	0.01	0.12
(1,1264)	1:106:A:GLY:HA2	1:105:A:ASP:H	5	0.11	0.01	0.11
(1,936)	1:79:A:GLY:H	1:81:A:PRO:HD3	4	0.3	0.07	0.28
(1,377)	1:31:A:CYS:HA	1:34:A:ILE:H	4	0.2	0.03	0.18
(1,241)	1:20:A:GLY:H	1:22:A:PRO:HA	4	0.19	0.08	0.16
(1,646)	1:52:A:ILE:HG12	1:53:A:GLN:H	4	0.17	0.04	0.18
(1,1241)	1:104:A:VAL:HG11	1:103:A:MET:H	4	0.16	0.02	0.16
(1,1241)	1:104:A:VAL:HG12	1:103:A:MET:H	4	0.16	0.02	0.16
(1,1241)	1:104:A:VAL:HG13	1:103:A:MET:H	4	0.16	0.02	0.16
(1,677)	1:55:A:LYS:HB2	1:54:A:ILE:H	4	0.13	0.02	0.13
(1,1158)	1:99:A:THR:H	1:110:A:CYS:HB3	4	0.13	0.03	0.12
(1,796)	1:71:A:GLY:H	1:87:A:GLN:HE22	3	0.28	0.04	0.27
(1,144)	1:15:A:CYS:HB3	1:14:A:THR:H	3	0.24	0.13	0.21
(1,617)	1:51:A:CYS:H	1:50:A:ARG:HD2	3	0.24	0.02	0.23

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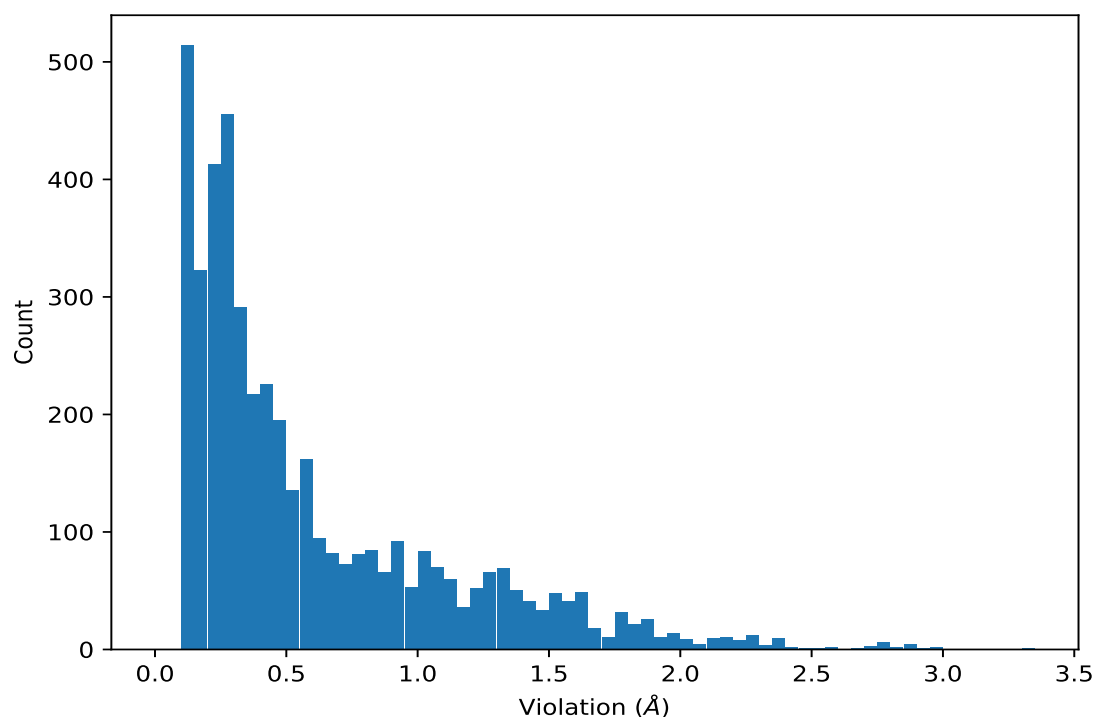
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,983)	1:84:A:VAL:H	1:75:A:LYS:HG2	3	0.21	0.06	0.2
(1,784)	1:70:A:LYS:H	1:70:A:LYS:HE2	3	0.2	0.03	0.19
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG21	3	0.18	0.06	0.15
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG22	3	0.18	0.06	0.15
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG23	3	0.18	0.06	0.15
(1,1052)	1:89:A:THR:H	1:83:A:CYS:HB2	3	0.16	0.05	0.13
(1,1382)	1:116:A:ALA:H	1:113:A:LEU:HA	3	0.16	0.04	0.17
(1,1055)	1:89:A:THR:HG21	1:87:A:GLN:H	3	0.12	0.02	0.11
(1,1055)	1:89:A:THR:HG22	1:87:A:GLN:H	3	0.12	0.02	0.11
(1,1055)	1:89:A:THR:HG23	1:87:A:GLN:H	3	0.12	0.02	0.11
(1,1312)	1:110:A:CYS:H	1:109:A:ARG:HG2	3	0.12	0.01	0.13
(1,424)	1:36:A:CYS:HB2	1:34:A:ILE:H	3	0.12	0.02	0.12
(1,177)	1:16:A:LYS:H	1:23:A:GLN:HG2	3	0.12	0.01	0.11
(1,161)	1:16:A:LYS:H	1:16:A:LYS:HE2	3	0.11	0.0	0.11
(1,721)	1:60:A:ARG:H	1:60:A:ARG:HH11	3	0.1	0.0	0.1
(1,835)	1:73:A:THR:H	1:86:A:ASN:HB2	3	0.1	0.0	0.1
(1,23)	1:6:A:ASP:HB2	1:3:A:GLY:H	3	0.1	0.0	0.1
(1,1314)	1:110:A:CYS:H	1:109:A:ARG:HD2	2	0.34	0.2	0.34
(1,1353)	1:113:A:LEU:HD21	1:112:A:GLN:H	2	0.32	0.01	0.32
(1,1353)	1:113:A:LEU:HD22	1:112:A:GLN:H	2	0.32	0.01	0.32
(1,1353)	1:113:A:LEU:HD23	1:112:A:GLN:H	2	0.32	0.01	0.32
(1,1293)	1:107:A:TRP:HE1	1:109:A:ARG:HD2	2	0.31	0.03	0.31
(1,700)	1:57:A:ALA:H	1:55:A:LYS:HD2	2	0.26	0.08	0.26
(1,215)	1:19:A:ASP:H	1:18:A:MET:HG3	2	0.2	0.05	0.2
(1,1239)	1:104:A:VAL:H	1:103:A:MET:HG3	2	0.2	0.04	0.2
(1,612)	1:51:A:CYS:HB3	1:36:A:CYS:H	2	0.18	0.02	0.18
(1,498)	1:43:A:GLN:HG2	1:41:A:THR:H	2	0.17	0.06	0.17
(1,1051)	1:88:A:PRO:HG2	1:89:A:THR:H	2	0.16	0.01	0.16
(1,1)	1:3:A:GLY:H	1:1:A:SER:HG	2	0.16	0.06	0.16
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD11	2	0.16	0.04	0.16
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD12	2	0.16	0.04	0.16
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD13	2	0.16	0.04	0.16
(1,1179)	1:100:A:THR:HG21	1:113:A:LEU:H	2	0.16	0.02	0.16
(1,1179)	1:100:A:THR:HG22	1:113:A:LEU:H	2	0.16	0.02	0.16
(1,1179)	1:100:A:THR:HG23	1:113:A:LEU:H	2	0.16	0.02	0.16
(1,908)	1:78:A:ASP:H	1:77:A:ILE:HG12	2	0.15	0.04	0.15
(1,656)	1:53:A:GLN:HG3	1:55:A:LYS:H	2	0.14	0.02	0.14
(1,185)	1:17:A:MET:H	1:1:A:SER:HA	2	0.12	0.02	0.12
(1,800)	1:72:A:THR:H	1:70:A:LYS:HD2	2	0.12	0.02	0.12
(1,1356)	1:113:A:LEU:HA	1:112:A:GLN:H	2	0.12	0.02	0.12
(1,277)	1:23:A:GLN:HG2	1:26:A:GLN: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)
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	6	3.31
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	2	2.96
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	8	2.95
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	1	2.92
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	6	2.9
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	9	2.89
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	4	2.87
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	7	2.87
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	4	2.86
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	5	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	3	2.81
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	4	2.8
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	9	2.8
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	10	2.79
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	2	2.79
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	5	2.78
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	8	2.78
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	7	2.73
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	6	2.71
(1,443)	1:37:A:SER:HG	1:35:A:GLN:H	1	2.7
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	3	2.68
(1,33)	1:7:A:ILE:HA	1:3:A:GLY:H	10	2.58
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	9	2.56
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	6	2.54
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	5	2.45
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	9	2.43
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	4	2.42
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	1	2.4
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	4	2.38
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	1	2.37
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	4	2.37
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	8	2.37
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	10	2.36
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	9	2.36
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	5	2.35
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	10	2.35
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	4	2.35
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	2	2.32
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	5	2.32
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	1	2.31
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	3	2.31
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	9	2.3
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	3	2.3
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	1	2.3
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	2	2.27
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	10	2.27
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	5	2.27
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	6	2.26
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	10	2.26
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	4	2.26
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	7	2.26
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	1	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	7	2.25
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	3	2.24
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	7	2.24
(1,1223)	1:103:A:MET:HA	1:101:A:CYS:H	8	2.22
(1,63)	1:8:A:TYR:H	1:11:A:LYS:H	6	2.21
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	8	2.21
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	5	2.2
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	7	2.2
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	1	2.2
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	4	2.19
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	9	2.19
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	10	2.19
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	6	2.18
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	2	2.18
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	1	2.18
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	8	2.17
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	4	2.17
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	7	2.17
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	8	2.17
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	5	2.16
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	8	2.14
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	6	2.14
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	3	2.13
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	4	2.13
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	6	2.13
(1,802)	1:72:A:THR:HA	1:70:A:LYS:H	2	2.12
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	2	2.12
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	10	2.12
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	8	2.11
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	5	2.1
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	7	2.09
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	5	2.09
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	3	2.08
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	9	2.07
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	8	2.06
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	3	2.05
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	6	2.05
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	9	2.05
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	10	2.04
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	4	2.04
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	5	2.02
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	2	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	7	2.02
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	1	2.0
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	7	1.99
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	2	1.99
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	9	1.99
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	3	1.99
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	4	1.99
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	3	1.98
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	2	1.98
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	3	1.98
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	5	1.98
(1,1308)	1:110:A:CYS:H	1:101:A:CYS:H	1	1.97
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	7	1.97
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	8	1.97
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	5	1.96
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	10	1.96
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	9	1.95
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	5	1.95
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	6	1.93
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	3	1.92
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	8	1.92
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	10	1.92
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	2	1.92
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	6	1.91
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	1	1.91
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	7	1.91
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	10	1.91
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	9	1.9
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	4	1.9
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	4	1.9
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	4	1.9
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	7	1.89
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	6	1.89
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	5	1.89
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	5	1.88
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	6	1.88
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	7	1.88
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	7	1.88
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	3	1.87
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	8	1.87
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	8	1.87
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	9	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	6	1.87
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	2	1.87
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	4	1.86
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	6	1.86
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	9	1.86
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	3	1.86
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	10	1.86
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	4	1.85
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	8	1.85
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	7	1.85
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	1	1.85
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	2	1.84
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	1	1.84
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	4	1.84
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	5	1.84
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	2	1.83
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	2	1.83
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	2	1.83
(1,1348)	1:113:A:LEU:HA	1:99:A:THR:H	10	1.83
(1,344)	1:27:A:ASN:H	1:29:A:PRO:HD2	2	1.83
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	1	1.82
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	10	1.82
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	3	1.82
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	5	1.82
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	5	1.82
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	5	1.82
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	1	1.81
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	5	1.81
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	9	1.81
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	9	1.8
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	3	1.8
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	3	1.8
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	3	1.8
(1,954)	1:82:A:GLN:H	1:80:A:HIS:HE2	5	1.79
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	2	1.79
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	1	1.79
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	1	1.79
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	1	1.79
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	9	1.79
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	9	1.79
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	9	1.79
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	3	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	10	1.78
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	10	1.78
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	10	1.78
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	4	1.78
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	1	1.77
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	4	1.77
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	3	1.77
(1,867)	1:75:A:LYS:H	1:85:A:GLN:H	9	1.76
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	9	1.76
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	6	1.76
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	6	1.76
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	6	1.76
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	8	1.76
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	8	1.76
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	8	1.76
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	3	1.76
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	7	1.75
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	7	1.75
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	10	1.75
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	3	1.75
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	2	1.75
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	2	1.75
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	2	1.75
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	2	1.73
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	3	1.73
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	5	1.73
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	10	1.73
(1,114)	1:13:A:THR:HG21	1:30:A:SER:H	7	1.73
(1,114)	1:13:A:THR:HG22	1:30:A:SER:H	7	1.73
(1,114)	1:13:A:THR:HG23	1:30:A:SER:H	7	1.73
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	8	1.72
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	7	1.71
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	4	1.71
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	2	1.71
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	6	1.7
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	9	1.7
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	9	1.7
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	9	1.7
(1,22)	1:5:A:ASN:H	1:17:A:MET:HA	9	1.7
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	1	1.69
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	1	1.69
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	1	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	10	1.69
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	3	1.68
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	7	1.68
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	2	1.68
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	5	1.67
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	5	1.67
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	2	1.66
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	1	1.66
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	3	1.66
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	8	1.66
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	2	1.65
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	7	1.65
(1,226)	1:20:A:GLY:H	1:16:A:LYS:HB2	9	1.65
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	6	1.65
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	2	1.64
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	7	1.64
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	6	1.64
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	1	1.64
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	7	1.64
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	1	1.63
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	7	1.63
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	8	1.63
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	9	1.63
(1,413)	1:35:A:GLN:HB2	1:33:A:ASP:H	8	1.63
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	10	1.63
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	10	1.63
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	10	1.63
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	2	1.63
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	3	1.63
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	4	1.63
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	7	1.63
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	10	1.63
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	9	1.63
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	2	1.62
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	8	1.62
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	3	1.62
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	8	1.62
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	2	1.62
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	1	1.62
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	8	1.62
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	10	1.61
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	4	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	5	1.61
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	3	1.61
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	3	1.61
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	3	1.61
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	7	1.61
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	7	1.61
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	7	1.61
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	5	1.61
(1,75)	1:9:A:CYS:H	1:10:A:PRO:HB2	9	1.61
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	1	1.6
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	5	1.6
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	3	1.6
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	8	1.6
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	1	1.6
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	2	1.6
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	2	1.6
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	2	1.6
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	6	1.59
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	2	1.59
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	4	1.59
(1,774)	1:68:A:CYS:H	1:69:A:PRO:HB2	10	1.59
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	6	1.59
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	10	1.59
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	6	1.59
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	6	1.59
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	6	1.59
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	4	1.59
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	8	1.59
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	9	1.58
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	10	1.58
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	10	1.58
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	9	1.58
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	4	1.58
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	5	1.58
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	6	1.58
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	10	1.58
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	10	1.58
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	5	1.58
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	7	1.58
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	5	1.58
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	5	1.58
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	5	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	4	1.57
(1,1284)	1:107:A:TRP:H	1:107:A:TRP:HE1	9	1.57
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	1	1.57
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	3	1.57
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	6	1.57
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	9	1.57
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	9	1.56
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	3	1.56
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	1	1.56
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	2	1.56
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	4	1.56
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	9	1.56
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	7	1.55
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	9	1.55
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	7	1.55
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	8	1.55
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	3	1.54
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	8	1.54
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	1	1.54
(1,1297)	1:108:A:PRO:HA	1:105:A:ASP:H	5	1.54
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	2	1.54
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	8	1.54
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	10	1.54
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	10	1.53
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	4	1.53
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	1	1.53
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	1	1.53
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	1	1.53
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	2	1.53
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	5	1.53
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	2	1.53
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	1	1.53
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	2	1.53
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	4	1.52
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	5	1.52
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	5	1.52
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	5	1.52
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	7	1.52
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	7	1.52
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	7	1.52
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	1	1.52
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	6	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	9	1.51
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	1	1.51
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	8	1.51
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	9	1.51
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	9	1.51
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	9	1.51
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	9	1.51
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	10	1.51
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	4	1.51
(1,194)	1:18:A:MET:HB2	1:3:A:GLY:H	8	1.51
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	5	1.51
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	10	1.5
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	7	1.5
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	3	1.5
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	3	1.5
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	3	1.5
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	1	1.5
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	4	1.5
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	7	1.5
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	6	1.5
(1,319)	1:26:A:GLN:H	1:29:A:PRO:HB2	4	1.5
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	3	1.5
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	3	1.49
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	3	1.49
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	3	1.49
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	6	1.49
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	8	1.49
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	8	1.49
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	8	1.49
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	1	1.49
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	1	1.48
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	9	1.48
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	4	1.48
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	4	1.48
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	4	1.48
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	4	1.48
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	10	1.48
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	10	1.48
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	10	1.48
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	9	1.48
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	7	1.48
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	6	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	8	1.47
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	3	1.47
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	6	1.47
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	5	1.47
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	2	1.47
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	2	1.47
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	2	1.47
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	2	1.47
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	1	1.46
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	6	1.46
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	10	1.46
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	7	1.46
(1,472)	1:41:A:THR:H	1:39:A:GLY:HA2	8	1.46
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	1	1.46
(1,1254)	1:105:A:ASP:H	1:109:A:ARG:H	9	1.45
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	5	1.45
(1,883)	1:77:A:ILE:H	1:74:A:CYS:HB2	8	1.45
(1,64)	1:8:A:TYR:HA	1:11:A:LYS:H	6	1.45
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	3	1.44
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	6	1.44
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	6	1.44
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	6	1.44
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	10	1.44
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	10	1.44
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	10	1.44
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	4	1.44
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	8	1.44
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	2	1.44
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	2	1.44
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	8	1.44
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	2	1.44
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	3	1.44
(1,968)	1:83:A:CYS:H	1:64:A:SER:HB2	10	1.44
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	9	1.44
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	10	1.44
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	4	1.44
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	9	1.44
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	9	1.44
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	9	1.44
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	2	1.44
(1,378)	1:31:A:CYS:HB2	1:34:A:ILE:H	6	1.44
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	8	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	8	1.43
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	10	1.43
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	6	1.43
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	7	1.42
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	1	1.42
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	2	1.42
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	1	1.42
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	6	1.42
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	10	1.41
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	4	1.41
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	2	1.41
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	2	1.41
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	2	1.41
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	5	1.4
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	4	1.4
(1,1435)	1:89:A:THR:H	1:92:A:ASP:H	5	1.4
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	6	1.4
(1,817)	1:73:A:THR:HG21	1:72:A:THR:H	6	1.4
(1,817)	1:73:A:THR:HG22	1:72:A:THR:H	6	1.4
(1,817)	1:73:A:THR:HG23	1:72:A:THR:H	6	1.4
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	6	1.4
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	7	1.4
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	7	1.4
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	6	1.4
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	6	1.4
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	6	1.4
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	7	1.4
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	4	1.4
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	7	1.39
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	7	1.39
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	7	1.39
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	8	1.39
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	7	1.39
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	3	1.39
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	9	1.39
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	10	1.39
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	4	1.39
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	4	1.39
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	4	1.39
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	7	1.38
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	7	1.38
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:109:A:ARG:H	1:107:A:TRP:HB2	7	1.38
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	8	1.38
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	1	1.38
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	4	1.38
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	9	1.38
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	4	1.38
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	8	1.38
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	2	1.37
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	5	1.37
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	1	1.37
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	6	1.37
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	3	1.36
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	6	1.36
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	3	1.36
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	6	1.36
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	5	1.36
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	2	1.35
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	5	1.35
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	3	1.35
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	10	1.35
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	5	1.35
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	3	1.35
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	8	1.34
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	8	1.34
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	8	1.34
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	7	1.34
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	8	1.34
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	2	1.34
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	10	1.34
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	9	1.34
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	3	1.34
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	5	1.34
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	7	1.34
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	2	1.34
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	9	1.34
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	6	1.33
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	1	1.33
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	1	1.33
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	2	1.33
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	4	1.33
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	6	1.33
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	2	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	3	1.33
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	10	1.32
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	6	1.32
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	6	1.32
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	8	1.32
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	5	1.32
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	5	1.32
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	5	1.32
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	6	1.32
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	4	1.31
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	1	1.31
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	3	1.31
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	5	1.31
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	9	1.31
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	10	1.31
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	5	1.31
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	9	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	7	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	7	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	7	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	8	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	8	1.31
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	8	1.31
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	5	1.31
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	10	1.31
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	4	1.31
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	4	1.31
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	4	1.31
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	9	1.3
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	9	1.3
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	9	1.3
(1,1423)	1:31:A:CYS:HB3	1:30:A:SER:H	6	1.3
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	9	1.3
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	2	1.3
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	8	1.3
(1,919)	1:79:A:GLY:H	1:75:A:LYS:HB3	3	1.3
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	9	1.3
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	5	1.3
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	1	1.3
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	1	1.3
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	1	1.3
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	10	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	10	1.3
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	10	1.3
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	8	1.3
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	8	1.3
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	8	1.3
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	2	1.3
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	10	1.3
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	10	1.29
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	8	1.29
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	4	1.29
(1,1337)	1:111:A:THR:H	1:112:A:GLN:HB2	9	1.29
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	6	1.29
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	7	1.29
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	9	1.29
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	3	1.29
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	4	1.29
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	5	1.29
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	7	1.29
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	8	1.29
(1,592)	1:48:A:TRP:HE1	1:49:A:PRO:HB2	10	1.29
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	10	1.29
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	6	1.28
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	1	1.28
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	3	1.28
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	5	1.28
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	5	1.28
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	5	1.28
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	10	1.28
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	10	1.28
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	10	1.28
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	3	1.27
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	5	1.27
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	9	1.27
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	2	1.27
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	7	1.27
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	10	1.27
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	3	1.27
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	3	1.27
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	3	1.27
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	3	1.27
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	1	1.26
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	6	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:101:A:CYS:HB2	1:111:A:THR:H	1	1.26
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	5	1.26
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	4	1.26
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	1	1.26
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	4	1.26
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	6	1.26
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	6	1.26
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	6	1.26
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	9	1.26
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	2	1.25
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	3	1.25
(1,1355)	1:113:A:LEU:HB2	1:112:A:GLN:H	7	1.25
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	2	1.25
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	7	1.25
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	9	1.25
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	8	1.25
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	1	1.25
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	3	1.25
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	5	1.25
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	6	1.25
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	9	1.25
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	1	1.25
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	1	1.25
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	1	1.25
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	3	1.25
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	3	1.25
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	3	1.25
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	5	1.25
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	5	1.25
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	5	1.25
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	3	1.25
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	9	1.24
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	4	1.24
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	7	1.24
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	2	1.24
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	7	1.24
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	8	1.24
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	7	1.24
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	7	1.24
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	7	1.24
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	9	1.24
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	9	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	9	1.24
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	1	1.24
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	2	1.24
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	6	1.24
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	7	1.24
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	10	1.24
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	9	1.24
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	3	1.23
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	5	1.23
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	2	1.23
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	8	1.23
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	7	1.23
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	7	1.23
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	7	1.23
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	6	1.23
(1,601)	1:50:A:ARG:H	1:48:A:TRP:HB2	9	1.23
(1,515)	1:43:A:GLN:HA	1:51:A:CYS:H	1	1.23
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	10	1.23
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	8	1.23
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	4	1.23
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	5	1.23
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	1	1.22
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	3	1.22
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	6	1.22
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	8	1.22
(1,373)	1:31:A:CYS:H	1:33:A:ASP:HA	1	1.22
(1,116)	1:14:A:THR:HG21	1:13:A:THR:H	2	1.22
(1,116)	1:14:A:THR:HG22	1:13:A:THR:H	2	1.22
(1,116)	1:14:A:THR:HG23	1:13:A:THR:H	2	1.22
(1,91)	1:12:A:GLY:HA2	1:11:A:LYS:H	8	1.22
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	7	1.21
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	5	1.21
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	6	1.21
(1,790)	1:71:A:GLY:HA2	1:70:A:LYS:H	6	1.21
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	9	1.21
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	6	1.21
(1,433)	1:36:A:CYS:H	1:37:A:SER:HB2	2	1.21
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG11	9	1.21
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG12	9	1.21
(1,290)	1:24:A:CYS:H	1:25:A:VAL:HG13	9	1.21
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	8	1.21
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	10	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:101:A:CYS:H	1:90:A:CYS:H	4	1.2
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	3	1.2
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	8	1.2
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	6	1.2
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	9	1.19
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	2	1.19
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	10	1.19
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	5	1.19
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	1	1.19
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	4	1.18
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	5	1.18
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	1	1.18
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	5	1.18
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	7	1.18
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	5	1.17
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	2	1.17
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	7	1.17
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	10	1.17
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	3	1.17
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	5	1.17
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	2	1.17
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	2	1.17
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	2	1.17
(1,624)	1:51:A:CYS:H	1:52:A:ILE:HB	10	1.17
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	3	1.17
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	8	1.17
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	2	1.16
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	7	1.16
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	10	1.16
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	5	1.16
(1,539)	1:44:A:MET:HA	1:51:A:CYS:H	8	1.16
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	9	1.16
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	4	1.16
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	4	1.16
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	7	1.16
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	3	1.15
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	3	1.15
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	4	1.15
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	5	1.15
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	8	1.15
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	2	1.15
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	4	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	4	1.15
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	4	1.15
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	1	1.15
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	10	1.15
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	3	1.15
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	2	1.15
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	4	1.15
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	4	1.15
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	5	1.15
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	6	1.15
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	5	1.15
(1,1422)	1:31:A:CYS:HB2	1:30:A:SER:H	7	1.14
(1,1407)	1:30:A:SER:H	1:32:A:SER:HA	1	1.14
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	7	1.14
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	3	1.14
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	1	1.14
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	6	1.14
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	1	1.14
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	3	1.14
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	5	1.14
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	2	1.14
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	7	1.14
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	9	1.14
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	8	1.14
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	7	1.13
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	3	1.13
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	2	1.13
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	10	1.13
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	7	1.13
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	4	1.13
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	1	1.13
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	8	1.12
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	5	1.12
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	8	1.12
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	3	1.12
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	1	1.12
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	1	1.12
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	6	1.12
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	3	1.11
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	3	1.11
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	3	1.11
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	5	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	2	1.11
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	6	1.11
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	7	1.11
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	9	1.11
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	5	1.11
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	1	1.1
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	1	1.1
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	1	1.1
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	2	1.1
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	8	1.1
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	3	1.1
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	3	1.09
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	1	1.09
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	1	1.09
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	1	1.09
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	6	1.09
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	6	1.09
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	6	1.09
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	10	1.09
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	7	1.09
(1,98)	1:13:A:THR:H	1:11:A:LYS:HG3	8	1.09
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	7	1.08
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	2	1.08
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	2	1.08
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	2	1.08
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	9	1.08
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	3	1.08
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	8	1.08
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	10	1.08
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	1	1.08
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	4	1.08
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	5	1.07
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	5	1.07
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	5	1.07
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	4	1.07
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	4	1.07
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	4	1.07
(1,1012)	1:85:A:GLN:H	1:88:A:PRO:HD2	9	1.07
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	4	1.07
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	8	1.07
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	10	1.07
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	8	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	8	1.07
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	8	1.07
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	1	1.07
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	2	1.07
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	3	1.07
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	4	1.07
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	1	1.06
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	4	1.06
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	8	1.06
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	8	1.06
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	8	1.06
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	9	1.06
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	10	1.06
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	7	1.06
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	7	1.06
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	7	1.06
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	4	1.06
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	2	1.06
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	2	1.06
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	2	1.06
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	10	1.06
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	6	1.05
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	10	1.05
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	9	1.05
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	4	1.05
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	4	1.05
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	4	1.05
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	4	1.05
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	5	1.05
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	10	1.05
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	8	1.05
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	3	1.05
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	5	1.05
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	7	1.05
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	1	1.05
(1,417)	1:35:A:GLN:HB2	1:34:A:ILE:H	8	1.05
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	4	1.05
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	9	1.05
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	2	1.05
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	8	1.04
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	8	1.04
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	5	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	6	1.04
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	7	1.04
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	1	1.04
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	1	1.04
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	1	1.04
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	3	1.04
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	3	1.04
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	3	1.04
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	1	1.04
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	9	1.04
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	8	1.04
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	3	1.04
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	3	1.04
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	3	1.04
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	3	1.04
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	6	1.04
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	7	1.04
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	4	1.04
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	10	1.04
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	10	1.04
(1,41)	1:7:A:ILE:HG13	1:6:A:ASP:H	6	1.04
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	3	1.03
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	4	1.03
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	5	1.03
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	4	1.03
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	1	1.03
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	8	1.03
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	4	1.03
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	5	1.03
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	2	1.03
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	10	1.03
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	10	1.03
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	10	1.03
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	6	1.03
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	6	1.03
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	6	1.03
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	6	1.03
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	10	1.03
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	1	1.03
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	9	1.03
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	4	1.02
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	4	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	2	1.02
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	9	1.02
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	7	1.02
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	3	1.02
(1,422)	1:35:A:GLN:HA	1:38:A:LYS:H	2	1.02
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	6	1.02
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	3	1.02
(1,1216)	1:102:A:GLN:HA	1:105:A:ASP:H	6	1.01
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	10	1.01
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	2	1.01
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	2	1.01
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	2	1.01
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	6	1.01
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	6	1.01
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	6	1.01
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	7	1.01
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	10	1.01
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	2	1.01
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	3	1.01
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	10	1.01
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	7	1.01
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	1	1.0
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	7	1.0
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	7	1.0
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	7	1.0
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	5	1.0
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	5	1.0
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	6	1.0
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	5	1.0
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	3	1.0
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	9	1.0
(1,751)	1:65:A:ASP:H	1:63:A:CYS:H	1	1.0
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	2	1.0
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	6	1.0
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	6	1.0
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	9	1.0
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	10	1.0
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	9	1.0
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	9	1.0
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	5	0.99
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	5	0.99
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	5	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	4	0.99
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	1	0.99
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	3	0.99
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	10	0.99
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	7	0.99
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	7	0.99
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	9	0.99
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	5	0.99
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	2	0.99
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	8	0.99
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	5	0.98
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	5	0.98
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	5	0.98
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	1	0.98
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	1	0.98
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	6	0.98
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	2	0.98
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	2	0.98
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	8	0.98
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	2	0.98
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	6	0.98
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	3	0.98
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	4	0.98
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	7	0.98
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	8	0.97
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	5	0.97
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	7	0.97
(1,978)	1:84:A:VAL:H	1:72:A:THR:HB	6	0.97
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	8	0.97
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	1	0.97
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	10	0.97
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	3	0.97
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	5	0.97
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	2	0.97
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	8	0.97
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	9	0.97
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	7	0.96
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	3	0.96
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	10	0.96
(1,1035)	1:86:A:ASN:H	1:88:A:PRO:HD2	1	0.96
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	4	0.96
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	1	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:60:A:ARG:H	1:61:A:PRO:HB2	3	0.96
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	4	0.96
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	4	0.96
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	7	0.96
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	8	0.96
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	9	0.96
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	10	0.96
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	1	0.96
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	5	0.95
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	2	0.95
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	8	0.95
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	3	0.95
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	2	0.95
(1,225)	1:19:A:ASP:H	1:23:A:GLN:H	6	0.95
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	9	0.95
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	3	0.95
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	8	0.95
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	7	0.95
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	10	0.95
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	2	0.94
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	6	0.94
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	8	0.94
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	8	0.94
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	8	0.94
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	7	0.94
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	9	0.94
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	9	0.94
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	5	0.94
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	4	0.94
(1,471)	1:41:A:THR:H	1:38:A:LYS:HA	1	0.94
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	1	0.94
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	5	0.94
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	4	0.94
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	5	0.94
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	10	0.93
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	4	0.93
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	8	0.93
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	5	0.93
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	1	0.93
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	6	0.93
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	4	0.93
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	5	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:54:A:ILE:HD11	1:57:A:ALA:H	10	0.93
(1,673)	1:54:A:ILE:HD12	1:57:A:ALA:H	10	0.93
(1,673)	1:54:A:ILE:HD13	1:57:A:ALA:H	10	0.93
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	5	0.93
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	1	0.93
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	5	0.93
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	7	0.93
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	8	0.93
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	2	0.92
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	3	0.92
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	9	0.92
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	8	0.92
(1,1054)	1:89:A:THR:HA	1:87:A:GLN:H	10	0.92
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	7	0.92
(1,1044)	1:88:A:PRO:HB2	1:87:A:GLN:H	4	0.92
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	3	0.92
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	1	0.92
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	3	0.92
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	7	0.92
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	4	0.92
(1,156)	1:16:A:LYS:H	1:14:A:THR:H	10	0.92
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	2	0.92
(1,65)	1:9:A:CYS:H	1:7:A:ILE:H	6	0.92
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	5	0.92
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG21	4	0.91
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG22	4	0.91
(1,1436)	1:89:A:THR:H	1:93:A:ILE:HG23	4	0.91
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	6	0.91
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	9	0.91
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	9	0.91
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	9	0.91
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	6	0.91
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	10	0.91
(1,810)	1:72:A:THR:H	1:83:A:CYS:HB3	7	0.91
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	9	0.91
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	7	0.91
(1,255)	1:22:A:PRO:HB2	1:21:A:HIS:H	6	0.91
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	1	0.91
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	1	0.91
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	1	0.91
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	3	0.91
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	1	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	1	0.9
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	4	0.9
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	5	0.9
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	4	0.9
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	8	0.9
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	10	0.9
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	10	0.9
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	10	0.9
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	9	0.9
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	7	0.9
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	6	0.9
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	7	0.9
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	10	0.9
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	4	0.9
(1,151)	1:15:A:CYS:H	1:24:A:CYS:H	6	0.9
(1,52)	1:8:A:TYR:H	1:6:A:ASP:HB2	10	0.9
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	2	0.89
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	2	0.89
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	1	0.89
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	1	0.89
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	6	0.89
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	9	0.89
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	8	0.89
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	9	0.89
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	7	0.89
(1,356)	1:29:A:PRO:HB2	1:28:A:GLN:H	6	0.89
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	8	0.89
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	4	0.89
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	5	0.88
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	6	0.88
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	10	0.88
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	3	0.88
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	7	0.88
(1,1162)	1:100:A:THR:HG21	1:99:A:THR:H	9	0.88
(1,1162)	1:100:A:THR:HG22	1:99:A:THR:H	9	0.88
(1,1162)	1:100:A:THR:HG23	1:99:A:THR:H	9	0.88
(1,1109)	1:93:A:ILE:HG12	1:100:A:THR:H	4	0.88
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	1	0.88
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	4	0.88
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	7	0.88
(1,549)	1:45:A:VAL:H	1:47:A:GLY:HA3	1	0.88
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	10	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:27:A:ASN:H	1:24:A:CYS:HB3	6	0.88
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	5	0.88
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	1	0.87
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	8	0.87
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	8	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	1	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	2	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	3	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	4	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	5	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	6	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	7	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	8	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	9	0.87
(1,1286)	1:107:A:TRP:HE1	1:107:A:TRP:HZ3	10	0.87
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	2	0.87
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	4	0.87
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	9	0.87
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	2	0.87
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	2	0.87
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	2	0.87
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	5	0.87
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	10	0.87
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	2	0.87
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	3	0.87
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	4	0.87
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	5	0.87
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	7	0.87
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	9	0.86
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	1	0.86
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	5	0.86
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	1	0.86
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	6	0.86
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	8	0.86
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	9	0.86
(1,582)	1:48:A:TRP:HE1	1:48:A:TRP:HZ3	10	0.86
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	6	0.86
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	1	0.86
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	5	0.86
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	7	0.86
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	7	0.85
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	6	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	9	0.85
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	2	0.85
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	5	0.85
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	10	0.85
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	2	0.85
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	6	0.85
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	3	0.84
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	5	0.84
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	6	0.84
(1,1188)	1:101:A:CYS:HB2	1:100:A:THR:H	10	0.84
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	2	0.84
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	10	0.84
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	2	0.84
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	6	0.84
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	9	0.84
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	10	0.84
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	8	0.84
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	7	0.83
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	3	0.83
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	9	0.83
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	7	0.83
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	10	0.83
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	3	0.83
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	2	0.83
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	1	0.83
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	3	0.83
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	4	0.83
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	8	0.83
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	3	0.83
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	8	0.82
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	2	0.82
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	5	0.82
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	10	0.82
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	10	0.82
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD11	10	0.82
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD12	10	0.82
(1,1222)	1:102:A:GLN:H	1:113:A:LEU:HD13	10	0.82
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	1	0.82
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	6	0.82
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	6	0.82
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	3	0.82
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	4	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	2	0.82
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	3	0.82
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	8	0.82
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	2	0.82
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	3	0.82
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	5	0.82
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	2	0.82
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	2	0.81
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	9	0.81
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	10	0.81
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	6	0.81
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	3	0.81
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	10	0.81
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	2	0.81
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	9	0.81
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	10	0.81
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	5	0.8
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	3	0.8
(1,1178)	1:100:A:THR:H	1:112:A:GLN:HB2	8	0.8
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	5	0.8
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	8	0.8
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	9	0.8
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	10	0.8
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	7	0.8
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	6	0.8
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	3	0.8
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	4	0.8
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	5	0.8
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	7	0.8
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	8	0.8
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	9	0.8
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	8	0.8
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	2	0.8
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	10	0.8
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	5	0.8
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	6	0.8
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	7	0.8
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	3	0.8
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	4	0.8
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	7	0.8
(1,70)	1:9:A:CYS:HB2	1:8:A:TYR:H	4	0.8
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	1	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	1	0.79
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	4	0.79
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	10	0.79
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	1	0.79
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	3	0.79
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	4	0.79
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	5	0.79
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	6	0.79
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	10	0.79
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	4	0.79
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	6	0.79
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	6	0.79
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	4	0.79
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	10	0.79
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	6	0.78
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	8	0.78
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	8	0.78
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	5	0.78
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	1	0.78
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	7	0.78
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	7	0.78
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	8	0.78
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	9	0.78
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	7	0.78
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	4	0.78
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	2	0.77
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	9	0.77
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	3	0.77
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	4	0.77
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	8	0.77
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	7	0.77
(1,1196)	1:101:A:CYS:H	1:103:A:MET:HG3	1	0.77
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	3	0.77
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	5	0.77
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	9	0.77
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	4	0.77
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	1	0.77
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	4	0.77
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	8	0.77
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	1	0.77
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	8	0.77
(1,548)	1:45:A:VAL:H	1:46:A:ASP:HB2	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	5	0.77
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	2	0.77
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	4	0.77
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	9	0.77
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	2	0.77
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	9	0.77
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	4	0.76
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	5	0.76
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	6	0.76
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	4	0.76
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	1	0.76
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	2	0.76
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	8	0.76
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	1	0.76
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	9	0.76
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	2	0.76
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	7	0.76
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	2	0.76
(1,880)	1:76:A:MET:H	1:79:A:GLY:HA2	6	0.76
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	1	0.76
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	3	0.76
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	8	0.76
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	8	0.76
(1,540)	1:45:A:VAL:H	1:43:A:GLN:HG3	9	0.76
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	1	0.76
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	4	0.76
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	3	0.75
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	2	0.75
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	5	0.75
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	9	0.75
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	4	0.75
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	6	0.75
(1,860)	1:75:A:LYS:H	1:82:A:GLN:HB2	3	0.75
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	5	0.75
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	1	0.75
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	3	0.75
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	9	0.75
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	3	0.75
(1,1441)	1:62:A:SER:H	1:63:A:CYS:HB2	1	0.74
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	9	0.74
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	8	0.74
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	8	0.74
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	7	0.74
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	6	0.74
(1,776)	1:69:A:PRO:HB3	1:72:A:THR:H	2	0.74
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	4	0.74
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	6	0.74
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	10	0.74
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	2	0.74
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	4	0.74
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	5	0.74
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	7	0.74
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	6	0.74
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	5	0.73
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	7	0.73
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	10	0.73
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	5	0.73
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	8	0.73
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	8	0.73
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	3	0.73
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	5	0.73
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	6	0.73
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	7	0.73
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	3	0.73
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	9	0.73
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	10	0.73
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	8	0.73
(1,291)	1:24:A:CYS:H	1:26:A:GLN:H	10	0.73
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	1	0.73
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	5	0.73
(1,207)	1:18:A:MET:H	1:21:A:HIS:HB3	1	0.73
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	3	0.72
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	10	0.72
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	3	0.72
(1,1290)	1:107:A:TRP:HE1	1:108:A:PRO:HB2	7	0.72
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	7	0.72
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	9	0.72
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	6	0.72
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	5	0.72
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	4	0.72
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	2	0.72
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	6	0.72
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	5	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:27:A:ASN:H	1:25:A:VAL:H	5	0.72
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	5	0.71
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	6	0.71
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	7	0.71
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	2	0.71
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	7	0.71
(1,1339)	1:111:A:THR:HA	1:114:A:LYS:H	10	0.71
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	6	0.71
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	10	0.71
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	1	0.71
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	5	0.71
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	7	0.71
(1,1046)	1:88:A:PRO:HG2	1:87:A:GLN:H	4	0.71
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	1	0.71
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	7	0.71
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	4	0.71
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	2	0.71
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	5	0.71
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	9	0.71
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	6	0.71
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	9	0.71
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	3	0.71
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	7	0.71
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	10	0.71
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	4	0.71
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	4	0.71
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	4	0.71
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	6	0.7
(1,1210)	1:102:A:GLN:H	1:103:A:MET:HB2	5	0.7
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	9	0.7
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	1	0.7
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	2	0.7
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	8	0.7
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	6	0.7
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	3	0.7
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	7	0.7
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	3	0.7
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	4	0.7
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	8	0.7
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	8	0.69
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	10	0.69
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	10	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	10	0.69
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	8	0.69
(1,932)	1:79:A:GLY:H	1:80:A:HIS:HE1	9	0.69
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	10	0.69
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	6	0.69
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	4	0.69
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	9	0.69
(1,512)	1:43:A:GLN:HA	1:46:A:ASP:H	8	0.69
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	9	0.68
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	2	0.68
(1,1014)	1:85:A:GLN:H	1:88:A:PRO:HG2	5	0.68
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	1	0.68
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	5	0.68
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	3	0.68
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	7	0.68
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	7	0.68
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	10	0.68
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	10	0.67
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	3	0.67
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	9	0.67
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	9	0.67
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	9	0.67
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	3	0.67
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	1	0.67
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	2	0.67
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	6	0.67
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	8	0.67
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	8	0.67
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	2	0.67
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	1	0.67
(1,594)	1:48:A:TRP:H	1:49:A:PRO:HB2	9	0.67
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	5	0.67
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	6	0.67
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	9	0.67
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	4	0.66
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	4	0.66
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	9	0.66
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	2	0.66
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	9	0.66
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	4	0.66
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	8	0.66
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	5	0.66
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	8	0.66
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	9	0.66
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	4	0.66
(1,547)	1:45:A:VAL:H	1:46:A:ASP:HB3	1	0.66
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	1	0.65
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	8	0.65
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	10	0.65
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	1	0.65
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	7	0.65
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	3	0.65
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	7	0.65
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	6	0.65
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	4	0.65
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	4	0.65
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	4	0.65
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	6	0.65
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	6	0.65
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	6	0.65
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	9	0.65
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	7	0.65
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	9	0.65
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	8	0.65
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	9	0.65
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	7	0.65
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	7	0.64
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	6	0.64
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	8	0.64
(1,1195)	1:101:A:CYS:H	1:102:A:GLN:HG3	8	0.64
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	8	0.64
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	5	0.64
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	5	0.64
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	5	0.64
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	3	0.64
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	9	0.64
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	6	0.64
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	9	0.64
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	7	0.64
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	4	0.64
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	1	0.64
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	9	0.64
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	7	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	9	0.63
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	9	0.63
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	10	0.63
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	4	0.63
(1,1136)	1:96:A:SER:H	1:99:A:THR:H	3	0.63
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	4	0.63
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	10	0.63
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	7	0.63
(1,935)	1:79:A:GLY:H	1:81:A:PRO:HD2	4	0.63
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	10	0.63
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	3	0.63
(1,816)	1:73:A:THR:HB	1:72:A:THR:H	10	0.63
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	2	0.63
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	1	0.63
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	1	0.63
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	1	0.63
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	9	0.63
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	4	0.63
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	3	0.63
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	5	0.63
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	2	0.63
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	6	0.63
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	4	0.62
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	7	0.62
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	7	0.62
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	7	0.62
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	10	0.62
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	3	0.62
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	8	0.62
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	9	0.62
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	5	0.62
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	10	0.62
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	2	0.62
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	2	0.62
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	7	0.62
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	5	0.62
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	1	0.62
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	3	0.62
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	2	0.62
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	10	0.62
(1,511)	1:43:A:GLN:H	1:45:A:VAL:H	8	0.62
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	4	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	8	0.62
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	4	0.62
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	10	0.61
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	4	0.61
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	9	0.61
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	1	0.61
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	9	0.61
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	9	0.61
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	4	0.61
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	5	0.61
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	5	0.61
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	5	0.61
(1,1236)	1:103:A:MET:HA	1:110:A:CYS:H	4	0.61
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	4	0.61
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	8	0.61
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	4	0.61
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	10	0.61
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	5	0.61
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	8	0.61
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	5	0.61
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	7	0.61
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	9	0.61
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	3	0.61
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	9	0.61
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	1	0.61
(1,705)	1:57:A:ALA:H	1:58:A:PRO:HG2	2	0.61
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	10	0.61
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	4	0.61
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	5	0.61
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	6	0.61
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	10	0.61
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	10	0.61
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	7	0.61
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	7	0.61
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	1	0.61
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	8	0.61
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	7	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	1	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	1	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	1	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	2	0.6
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	2	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	2	0.6
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	3	0.6
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	10	0.6
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	5	0.6
(1,1009)	1:85:A:GLN:H	1:86:A:ASN:HA	2	0.6
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	2	0.6
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	1	0.6
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	8	0.6
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	9	0.6
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	1	0.6
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	4	0.6
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	7	0.6
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	8	0.6
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	3	0.6
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	5	0.6
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	3	0.6
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	9	0.59
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	4	0.59
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	6	0.59
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	6	0.59
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	6	0.59
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	5	0.59
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	3	0.59
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	6	0.59
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	10	0.59
(1,1045)	1:88:A:PRO:HG3	1:87:A:GLN:H	10	0.59
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	3	0.59
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	4	0.59
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	8	0.59
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	9	0.59
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	9	0.59
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	9	0.59
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	4	0.59
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	5	0.59
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	5	0.59
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	5	0.59
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	7	0.59
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	7	0.59
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	7	0.59
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	8	0.59
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	7	0.59
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	1	0.59
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	7	0.59
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	1	0.59
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	8	0.59
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	5	0.59
(1,258)	1:22:A:PRO:HA	1:24:A:CYS:H	8	0.59
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	7	0.59
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	9	0.59
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	8	0.58
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	8	0.58
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	3	0.58
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	3	0.58
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	3	0.58
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	2	0.58
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	10	0.58
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	7	0.58
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	8	0.58
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	3	0.58
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	3	0.58
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	9	0.58
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	2	0.58
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	10	0.58
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	2	0.58
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	2	0.58
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	2	0.58
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	8	0.58
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	8	0.58
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	8	0.58
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	10	0.58
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	10	0.58
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	10	0.58
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	4	0.58
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	8	0.58
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	1	0.58
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	10	0.58
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	2	0.58
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	4	0.58
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	6	0.58
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE1	8	0.58
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE2	8	0.58
(1,166)	1:16:A:LYS:H	1:17:A:MET:HE3	8	0.58
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	6	0.57
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	5	0.57
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	2	0.57
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	6	0.57
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	2	0.57
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	9	0.57
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	5	0.57
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	10	0.57
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	3	0.57
(1,933)	1:79:A:GLY:H	1:80:A:HIS:HB3	6	0.57
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	3	0.57
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	9	0.57
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	9	0.57
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	9	0.57
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	9	0.57
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	10	0.57
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	5	0.57
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	8	0.57
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	1	0.57
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	2	0.57
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	3	0.57
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	7	0.57
(1,460)	1:39:A:GLY:HA3	1:38:A:LYS:H	2	0.57
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	8	0.57
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	6	0.56
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	3	0.56
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	6	0.56
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	1	0.56
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	1	0.56
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	10	0.56
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	3	0.56
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	6	0.56
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	8	0.56
(1,767)	1:66:A:ILE:HD11	1:65:A:ASP:H	3	0.56
(1,767)	1:66:A:ILE:HD12	1:65:A:ASP:H	3	0.56
(1,767)	1:66:A:ILE:HD13	1:65:A:ASP:H	3	0.56
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	1	0.56
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	4	0.56
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	8	0.56
(1,674)	1:55:A:LYS:HG3	1:41:A:THR:H	10	0.56
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	10	0.56
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	2	0.56
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	6	0.56
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	8	0.56
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	9	0.56
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	2	0.56
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	10	0.56
(1,1416)	1:31:A:CYS:H	1:28:A:GLN:H	6	0.55
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	6	0.55
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	6	0.55
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	4	0.55
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	2	0.55
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	4	0.55
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	4	0.55
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	1	0.55
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	4	0.55
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	5	0.55
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	9	0.55
(1,750)	1:64:A:SER:H	1:66:A:ILE:H	6	0.55
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	2	0.55
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	3	0.55
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	8	0.55
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	5	0.55
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	9	0.55
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	4	0.55
(1,375)	1:31:A:CYS:HB2	1:33:A:ASP:H	6	0.55
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	9	0.55
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	2	0.55
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	3	0.55
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	5	0.55
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	8	0.55
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	4	0.54
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	4	0.54
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	9	0.54
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	8	0.54
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	8	0.54
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	8	0.54
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	1	0.54
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	5	0.54
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	6	0.54
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	7	0.54
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	5	0.54
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:85:A:GLN:H	1:83:A:CYS:H	7	0.54
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	1	0.54
(1,909)	1:78:A:ASP:H	1:77:A:ILE:HG13	5	0.54
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	2	0.54
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	8	0.54
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	10	0.54
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	1	0.54
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	6	0.54
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	2	0.54
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	3	0.54
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	4	0.54
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	7	0.54
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	7	0.54
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	9	0.54
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	10	0.54
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	7	0.54
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	10	0.54
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	3	0.54
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	4	0.54
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	6	0.54
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	1	0.53
(1,1314)	1:110:A:CYS:H	1:109:A:ARG:HD2	1	0.53
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	8	0.53
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	8	0.53
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	1	0.53
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	7	0.53
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	2	0.53
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	9	0.53
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	10	0.53
(1,997)	1:84:A:VAL:H	1:89:A:THR:H	6	0.53
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	1	0.53
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	8	0.53
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	2	0.53
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	7	0.53
(1,809)	1:72:A:THR:H	1:83:A:CYS:HB2	7	0.53
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	6	0.53
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	5	0.53
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	1	0.53
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	10	0.53
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	7	0.53
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	4	0.53
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	10	0.53
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	3	0.53
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	4	0.53
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	9	0.53
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	3	0.53
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	9	0.53
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	7	0.52
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	10	0.52
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	7	0.52
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG21	4	0.52
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG22	4	0.52
(1,1237)	1:103:A:MET:H	1:111:A:THR:HG23	4	0.52
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	10	0.52
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	1	0.52
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	1	0.52
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	2	0.52
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	1	0.52
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	3	0.52
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	6	0.52
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	2	0.52
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	5	0.52
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	5	0.52
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	2	0.52
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	1	0.52
(1,598)	1:49:A:PRO:HA	1:46:A:ASP:H	6	0.52
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	3	0.52
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	5	0.52
(1,327)	1:27:A:ASN:H	1:24:A:CYS:HB2	5	0.52
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	1	0.52
(1,198)	1:18:A:MET:H	1:17:A:MET:HG2	7	0.52
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	8	0.52
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	1	0.52
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	7	0.52
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	9	0.51
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	10	0.51
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	1	0.51
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	7	0.51
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	7	0.51
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	6	0.51
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	5	0.51
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	7	0.51
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	2	0.51
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	7	0.51
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	8	0.51
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	4	0.51
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	8	0.51
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	3	0.51
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	6	0.51
(1,316)	1:26:A:GLN:H	1:28:A:GLN:HG2	1	0.51
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	2	0.51
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	5	0.51
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	6	0.51
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	10	0.51
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	6	0.5
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	4	0.5
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	2	0.5
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	1	0.5
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	7	0.5
(1,1194)	1:101:A:CYS:H	1:102:A:GLN:HE21	6	0.5
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	2	0.5
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	2	0.5
(1,1145)	1:98:A:GLY:HA3	1:97:A:LYS:H	8	0.5
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	8	0.5
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	9	0.5
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	4	0.5
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	8	0.5
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	10	0.5
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	1	0.5
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	2	0.5
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	1	0.5
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	6	0.5
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	5	0.5
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	7	0.5
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	10	0.5
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	10	0.5
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	10	0.5
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	2	0.5
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	5	0.5
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	1	0.5
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	5	0.5
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	4	0.5
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	5	0.49
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	8	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	6	0.49
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	9	0.49
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	3	0.49
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	1	0.49
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	2	0.49
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	3	0.49
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	4	0.49
(1,1053)	1:89:A:THR:H	1:87:A:GLN:HB2	5	0.49
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	3	0.49
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	5	0.49
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	10	0.49
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	3	0.49
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	3	0.49
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	5	0.49
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	9	0.49
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	5	0.49
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	9	0.49
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	2	0.49
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	9	0.49
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	2	0.49
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	7	0.49
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG21	8	0.49
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG22	8	0.49
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG23	8	0.49
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	6	0.49
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	8	0.49
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	8	0.49
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	7	0.49
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	3	0.49
(1,92)	1:12:A:GLY:HA3	1:11:A:LYS:H	8	0.49
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	1	0.48
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	7	0.48
(1,1405)	1:29:A:PRO:HB3	1:33:A:ASP:H	4	0.48
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	5	0.48
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	10	0.48
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	9	0.48
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	3	0.48
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	7	0.48
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	2	0.48
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	7	0.48
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	5	0.48
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:93:A:ILE:H	1:94:A:GLN:HB2	10	0.48
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	9	0.48
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	5	0.48
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	2	0.48
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	10	0.48
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	6	0.48
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	5	0.48
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	9	0.48
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	5	0.48
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	10	0.48
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	1	0.48
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	3	0.48
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	7	0.48
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	1	0.48
(1,473)	1:41:A:THR:H	1:39:A:GLY:H	1	0.48
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	5	0.48
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	6	0.48
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	1	0.48
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	2	0.48
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	8	0.48
(1,357)	1:29:A:PRO:HD2	1:30:A:SER:H	2	0.48
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	5	0.48
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	5	0.48
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	8	0.48
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	9	0.48
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	1	0.48
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	4	0.48
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	2	0.48
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	2	0.48
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	2	0.48
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	9	0.48
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	9	0.48
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	9	0.48
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	3	0.47
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	7	0.47
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	8	0.47
(1,1183)	1:101:A:CYS:H	1:99:A:THR:HB	3	0.47
(1,1034)	1:86:A:ASN:H	1:88:A:PRO:HB3	4	0.47
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	7	0.47
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	1	0.47
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	6	0.47
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	6	0.47
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	6	0.47
(1,898)	1:77:A:ILE:H	1:79:A:GLY:HA3	5	0.47
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	5	0.47
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	6	0.47
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	10	0.47
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	10	0.47
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	6	0.47
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	2	0.47
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	9	0.47
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	3	0.47
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	5	0.47
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	10	0.47
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	4	0.47
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	4	0.47
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	5	0.47
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	2	0.47
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	10	0.47
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	2	0.47
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	6	0.47
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	2	0.47
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	5	0.47
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	4	0.47
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	6	0.46
(1,1415)	1:31:A:CYS:H	1:28:A:GLN:HB2	6	0.46
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	3	0.46
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	4	0.46
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	6	0.46
(1,1306)	1:110:A:CYS:HA	1:99:A:THR:H	9	0.46
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	2	0.46
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	5	0.46
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	4	0.46
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	3	0.46
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	6	0.46
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	7	0.46
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	8	0.46
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	1	0.46
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	4	0.46
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	8	0.46
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	10	0.46
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	5	0.46
(1,704)	1:57:A:ALA:H	1:58:A:PRO:HA	9	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	9	0.46
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	2	0.46
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	4	0.46
(1,517)	1:44:A:MET:H	1:34:A:ILE:HB	8	0.46
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	7	0.46
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	7	0.46
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	7	0.46
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	3	0.46
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	6	0.46
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	7	0.46
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	10	0.46
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	4	0.46
(1,264)	1:23:A:GLN:H	1:22:A:PRO:HD2	6	0.46
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	8	0.46
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	1	0.46
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	6	0.46
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	9	0.46
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	9	0.46
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	9	0.46
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	4	0.46
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	1	0.46
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	4	0.46
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	10	0.46
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	3	0.46
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	7	0.46
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	10	0.46
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	7	0.46
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	7	0.46
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	7	0.46
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	7	0.45
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	5	0.45
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	8	0.45
(1,1346)	1:112:A:GLN:H	1:114:A:LYS:HB2	10	0.45
(1,1273)	1:106:A:GLY:H	1:108:A:PRO:HD2	1	0.45
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	3	0.45
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	4	0.45
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	6	0.45
(1,1161)	1:100:A:THR:HB	1:99:A:THR:H	8	0.45
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	6	0.45
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	4	0.45
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	4	0.45
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	4	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	8	0.45
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	6	0.45
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	10	0.45
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	6	0.45
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	5	0.45
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	1	0.45
(1,715)	1:60:A:ARG:HA	1:59:A:SER:H	4	0.45
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	3	0.45
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	5	0.45
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	2	0.45
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	10	0.45
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	6	0.45
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	4	0.45
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	6	0.45
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	9	0.45
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	9	0.45
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	9	0.45
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	9	0.45
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	9	0.45
(1,361)	1:29:A:PRO:HG3	1:30:A:SER:H	9	0.45
(1,205)	1:18:A:MET:H	1:19:A:ASP:HA	7	0.45
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	3	0.45
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	1	0.45
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	1	0.45
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	1	0.45
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	9	0.44
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	9	0.44
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	1	0.44
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	10	0.44
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	3	0.44
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	8	0.44
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	4	0.44
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	8	0.44
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	1	0.44
(1,1036)	1:86:A:ASN:H	1:89:A:THR:H	9	0.44
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	4	0.44
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	1	0.44
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	10	0.44
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	1	0.44
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	3	0.44
(1,946)	1:81:A:PRO:HB2	1:83:A:CYS:H	4	0.44
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	1	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	1	0.44
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	1	0.44
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	6	0.44
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	6	0.44
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	6	0.44
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	1	0.44
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	5	0.44
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	9	0.44
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	1	0.44
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	4	0.44
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	6	0.44
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	6	0.44
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	3	0.44
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	8	0.44
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	5	0.44
(1,631)	1:52:A:ILE:H	1:43:A:GLN:HA	8	0.44
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	3	0.44
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	5	0.44
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	7	0.44
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	2	0.44
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	2	0.44
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	2	0.44
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	4	0.44
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	2	0.44
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	7	0.44
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	6	0.44
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	2	0.44
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	2	0.44
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	2	0.44
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	3	0.44
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	3	0.44
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	3	0.44
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	6	0.44
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	6	0.44
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	6	0.44
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	8	0.44
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	8	0.44
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	8	0.44
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	1	0.44
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	3	0.44
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	4	0.44
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:13:A:THR:H	1:11:A:LYS:HG2	7	0.44
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	10	0.43
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	2	0.43
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	8	0.43
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	4	0.43
(1,1309)	1:110:A:CYS:H	1:108:A:PRO:HG2	10	0.43
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	2	0.43
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	3	0.43
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	3	0.43
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	4	0.43
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	9	0.43
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	10	0.43
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	1	0.43
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	2	0.43
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	3	0.43
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	8	0.43
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	9	0.43
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	10	0.43
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	5	0.43
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	10	0.43
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	1	0.43
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	4	0.43
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	3	0.43
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	7	0.43
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	8	0.43
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	9	0.43
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	7	0.43
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	2	0.43
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	6	0.43
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	3	0.43
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	9	0.43
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	10	0.43
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	8	0.43
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	5	0.43
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	5	0.43
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	5	0.43
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	7	0.43
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	7	0.43
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	7	0.43
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	8	0.43
(1,62)	1:8:A:TYR:H	1:11:A:LYS:HD2	6	0.43
(1,27)	1:6:A:ASP:HB3	1:5:A:ASN:H	6	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	6	0.42
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	7	0.42
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	6	0.42
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	4	0.42
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	5	0.42
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	8	0.42
(1,994)	1:84:A:VAL:H	1:85:A:GLN:HB3	6	0.42
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	1	0.42
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	1	0.42
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	1	0.42
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	2	0.42
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	10	0.42
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	10	0.42
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	3	0.42
(1,761)	1:65:A:ASP:H	1:66:A:ILE:HG13	2	0.42
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	2	0.42
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	7	0.42
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	8	0.42
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	2	0.42
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	8	0.42
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	8	0.42
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	8	0.42
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	8	0.42
(1,304)	1:26:A:GLN:HG3	1:13:A:THR:H	4	0.42
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	2	0.42
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	5	0.42
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	1	0.42
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	1	0.42
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	1	0.42
(1,107)	1:13:A:THR:H	1:24:A:CYS:HB2	6	0.42
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	8	0.42
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	8	0.42
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	8	0.42
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	8	0.41
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	3	0.41
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	9	0.41
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	9	0.41
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	1	0.41
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	6	0.41
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	6	0.41
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	6	0.41
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	9	0.41
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	3	0.41
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	1	0.41
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	7	0.41
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	10	0.41
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	10	0.41
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	10	0.41
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	1	0.41
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	6	0.41
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	9	0.41
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	2	0.41
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	2	0.41
(1,768)	1:68:A:CYS:H	1:66:A:ILE:HA	9	0.41
(1,736)	1:62:A:SER:H	1:61:A:PRO:HD2	3	0.41
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	3	0.41
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	8	0.41
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	9	0.41
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	7	0.41
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	7	0.41
(1,628)	1:51:A:CYS:HB2	1:53:A:GLN:H	8	0.41
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	1	0.41
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG21	3	0.41
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG22	3	0.41
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG23	3	0.41
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	8	0.41
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	3	0.41
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	6	0.41
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	2	0.41
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	6	0.41
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	1	0.41
(1,144)	1:15:A:CYS:HB3	1:14:A:THR:H	10	0.41
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	10	0.41
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	10	0.41
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	10	0.41
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	4	0.41
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	4	0.41
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	4	0.41
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	10	0.41
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	10	0.41
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	10	0.41
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	10	0.4
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	5	0.4
(1,1411)	1:30:A:SER:HA	1:33:A:ASP:H	5	0.4
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	3	0.4
(1,1320)	1:111:A:THR:H	1:95:A:CYS:HB2	9	0.4
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	1	0.4
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	4	0.4
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	9	0.4
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	4	0.4
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	1	0.4
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	2	0.4
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	9	0.4
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	9	0.4
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	9	0.4
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	9	0.4
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	7	0.4
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	2	0.4
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	5	0.4
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	2	0.4
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	3	0.4
(1,936)	1:79:A:GLY:H	1:81:A:PRO:HD3	6	0.4
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	8	0.4
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	2	0.4
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	2	0.4
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	2	0.4
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	3	0.4
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	2	0.4
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	4	0.4
(1,725)	1:60:A:ARG:H	1:61:A:PRO:HG2	7	0.4
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	1	0.4
(1,674)	1:55:A:LYS:HG3	1:41:A:THR:H	7	0.4
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	8	0.4
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	10	0.4
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	4	0.4
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	6	0.4
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	10	0.4
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	2	0.4
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	1	0.4
(1,535)	1:44:A:MET:H	1:48:A:TRP:H	2	0.4
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	5	0.4
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	9	0.4
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	3	0.4
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	3	0.39
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	7	0.39
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	9	0.39
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	6	0.39
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	10	0.39
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	10	0.39
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	9	0.39
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	9	0.39
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	9	0.39
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	1	0.39
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	1	0.39
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	10	0.39
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	2	0.39
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	3	0.39
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	3	0.39
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	3	0.39
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	3	0.39
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	5	0.39
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	5	0.39
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	5	0.39
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	9	0.39
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	4	0.39
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	5	0.39
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	7	0.39
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	8	0.39
(1,945)	1:81:A:PRO:HD2	1:82:A:GLN:H	10	0.39
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	8	0.39
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	9	0.39
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	1	0.39
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	7	0.39
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	5	0.39
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	10	0.39
(1,709)	1:57:A:ALA:H	1:62:A:SER:HB2	2	0.39
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	8	0.39
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	9	0.39
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	9	0.39
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	9	0.39
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	1	0.39
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	3	0.39
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	5	0.39
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	2	0.39
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	5	0.39
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	8	0.39
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG21	4	0.39
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG22	4	0.39
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG23	4	0.39
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	7	0.39
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	4	0.39
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	6	0.39
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	10	0.39
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	10	0.39
(1,140)	1:14:A:THR:HG21	1:28:A:GLN:H	4	0.39
(1,140)	1:14:A:THR:HG22	1:28:A:GLN:H	4	0.39
(1,140)	1:14:A:THR:HG23	1:28:A:GLN:H	4	0.39
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	10	0.39
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	3	0.39
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	3	0.39
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	3	0.39
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	1	0.38
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	10	0.38
(1,1389)	1:116:A:ALA:H	1:118:A:ARG:H	10	0.38
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	10	0.38
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	10	0.38
(1,1291)	1:107:A:TRP:H	1:108:A:PRO:HG2	5	0.38
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	10	0.38
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	3	0.38
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	4	0.38
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	5	0.38
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	9	0.38
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	4	0.38
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	2	0.38
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	8	0.38
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	10	0.38
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	6	0.38
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	3	0.38
(1,967)	1:82:A:GLN:HG2	1:85:A:GLN:H	9	0.38
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	4	0.38
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	8	0.38
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	7	0.38
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	9	0.38
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	9	0.38
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	9	0.38
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	3	0.38
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	10	0.38
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	6	0.38
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	6	0.38
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	8	0.38
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	6	0.38
(1,600)	1:50:A:ARG:H	1:48:A:TRP:HA	9	0.38
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG21	6	0.38
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG22	6	0.38
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG23	6	0.38
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	7	0.38
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	1	0.38
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	4	0.38
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	5	0.38
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	9	0.38
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	7	0.38
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	9	0.38
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	4	0.38
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	9	0.38
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	9	0.38
(1,159)	1:16:A:LYS:HA	1:15:A:CYS:H	4	0.38
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	10	0.38
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	1	0.38
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	3	0.38
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	6	0.38
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	9	0.38
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	9	0.38
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	9	0.38
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	1	0.37
(1,1425)	1:88:A:PRO:HG2	1:90:A:CYS:H	9	0.37
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	7	0.37
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	3	0.37
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	4	0.37
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	6	0.37
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	10	0.37
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	3	0.37
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	6	0.37
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	7	0.37
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	8	0.37
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	10	0.37
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	6	0.37
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	8	0.37
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	8	0.37
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	2	0.37
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	8	0.37
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	5	0.37
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	3	0.37
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	9	0.37
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	10	0.37
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	9	0.37
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	10	0.37
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	10	0.37
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	10	0.37
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	2	0.37
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	2	0.37
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	2	0.37
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	5	0.37
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	1	0.37
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	2	0.37
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	7	0.37
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	3	0.37
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	7	0.37
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	9	0.37
(1,522)	1:44:A:MET:H	1:43:A:GLN:HG3	8	0.37
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	1	0.37
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	4	0.37
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	6	0.37
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	10	0.37
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	9	0.37
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	3	0.37
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	10	0.37
(1,209)	1:18:A:MET:H	1:21:A:HIS:HE2	1	0.37
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	3	0.37
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	4	0.37
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	5	0.37
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	2	0.37
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	10	0.37
(1,1381)	1:116:A:ALA:H	1:113:A:LEU:H	2	0.36
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	3	0.36
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	4	0.36
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG11	6	0.36
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG12	6	0.36
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG13	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	6	0.36
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	9	0.36
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	10	0.36
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	3	0.36
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	8	0.36
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	1	0.36
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	7	0.36
(1,1157)	1:99:A:THR:H	1:110:A:CYS:HB2	4	0.36
(1,1086)	1:93:A:ILE:H	1:91:A:SER:HB3	6	0.36
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	1	0.36
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	2	0.36
(1,1015)	1:85:A:GLN:H	1:88:A:PRO:HG3	9	0.36
(1,953)	1:82:A:GLN:H	1:80:A:HIS:HB2	7	0.36
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	9	0.36
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	4	0.36
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	2	0.36
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	10	0.36
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	2	0.36
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	10	0.36
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	3	0.36
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	3	0.36
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	3	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	4	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	4	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	4	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	9	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	9	0.36
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	9	0.36
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	4	0.36
(1,674)	1:55:A:LYS:HG3	1:41:A:THR:H	9	0.36
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	5	0.36
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	1	0.36
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	3	0.36
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	5	0.36
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	10	0.36
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	4	0.36
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	1	0.36
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	2	0.36
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	6	0.36
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	8	0.36
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	5	0.36
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	2	0.36
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	9	0.36
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	5	0.36
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	5	0.36
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	5	0.36
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	6	0.36
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	5	0.35
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	2	0.35
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	4	0.35
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	1	0.35
(1,1260)	1:106:A:GLY:H	1:104:A:VAL:HB	5	0.35
(1,1160)	1:100:A:THR:H	1:97:A:LYS:HD2	5	0.35
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	3	0.35
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	1	0.35
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	2	0.35
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	10	0.35
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	10	0.35
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	10	0.35
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	5	0.35
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	3	0.35
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	7	0.35
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	10	0.35
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	4	0.35
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	3	0.35
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	5	0.35
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	8	0.35
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	7	0.35
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	7	0.35
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	7	0.35
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	9	0.35
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	6	0.35
(1,674)	1:55:A:LYS:HG3	1:41:A:THR:H	8	0.35
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	10	0.35
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	10	0.35
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	10	0.35
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	8	0.35
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	6	0.35
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	4	0.35
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	10	0.35
(1,442)	1:36:A:CYS:HB2	1:40:A:THR:H	1	0.35
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	3	0.35
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	4	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	7	0.35
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	3	0.35
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	1	0.35
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	2	0.35
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	7	0.35
(1,174)	1:16:A:LYS:HA	1:18:A:MET:H	9	0.35
(1,115)	1:14:A:THR:HB	1:13:A:THR:H	7	0.35
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	9	0.35
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	3	0.35
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	3	0.35
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	3	0.35
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	2	0.34
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	7	0.34
(1,1417)	1:31:A:CYS:H	1:29:A:PRO:HG2	6	0.34
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	8	0.34
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	2	0.34
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	9	0.34
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	5	0.34
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	8	0.34
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	7	0.34
(1,1293)	1:107:A:TRP:HE1	1:109:A:ARG:HD2	2	0.34
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG11	10	0.34
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG12	10	0.34
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG13	10	0.34
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	2	0.34
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	3	0.34
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	3	0.34
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	3	0.34
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	7	0.34
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	1	0.34
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	1	0.34
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	1	0.34
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	5	0.34
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	5	0.34
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	5	0.34
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	2	0.34
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	2	0.34
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	2	0.34
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	7	0.34
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	8	0.34
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	1	0.34
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:77:A:ILE:H	1:78:A:ASP:HB2	6	0.34
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	3	0.34
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	5	0.34
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	8	0.34
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	4	0.34
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	10	0.34
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	8	0.34
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	8	0.34
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	8	0.34
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	2	0.34
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	1	0.34
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	6	0.34
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	8	0.34
(1,700)	1:57:A:ALA:H	1:55:A:LYS:HD2	7	0.34
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	7	0.34
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	3	0.34
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	9	0.34
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	10	0.34
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	8	0.34
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	8	0.34
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	2	0.34
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	8	0.34
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	6	0.34
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	1	0.34
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	2	0.34
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	6	0.34
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	6	0.34
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	1	0.34
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	1	0.34
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	1	0.34
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	8	0.34
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	8	0.34
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	8	0.34
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	8	0.34
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	7	0.34
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	8	0.34
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	1	0.34
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	2	0.33
(1,1413)	1:30:A:SER:H	1:34:A:ILE:H	8	0.33
(1,1353)	1:113:A:LEU:HD21	1:112:A:GLN:H	9	0.33
(1,1353)	1:113:A:LEU:HD22	1:112:A:GLN:H	9	0.33
(1,1353)	1:113:A:LEU:HD23	1:112:A:GLN:H	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	5	0.33
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	9	0.33
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	10	0.33
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	7	0.33
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG11	4	0.33
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG12	4	0.33
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG13	4	0.33
(1,1276)	1:107:A:TRP:H	1:103:A:MET:HG3	3	0.33
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	5	0.33
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	9	0.33
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	8	0.33
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	7	0.33
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	7	0.33
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	7	0.33
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	9	0.33
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	3	0.33
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	4	0.33
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	4	0.33
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	4	0.33
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	10	0.33
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	2	0.33
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	10	0.33
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	4	0.33
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	6	0.33
(1,796)	1:71:A:GLY:H	1:87:A:GLN:HE22	9	0.33
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	3	0.33
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	3	0.33
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	3	0.33
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	7	0.33
(1,699)	1:57:A:ALA:H	1:54:A:ILE:H	10	0.33
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	4	0.33
(1,593)	1:48:A:TRP:H	1:49:A:PRO:HG2	9	0.33
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	5	0.33
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	6	0.33
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	10	0.33
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	9	0.33
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG21	5	0.33
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG22	5	0.33
(1,497)	1:43:A:GLN:H	1:41:A:THR:HG23	5	0.33
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	6	0.33
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	6	0.33
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	3	0.33
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	3	0.33
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	3	0.33
(1,236)	1:20:A:GLY:H	1:21:A:HIS:HD2	1	0.33
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	6	0.33
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	2	0.33
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	2	0.33
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	2	0.33
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	2	0.33
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	10	0.33
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	10	0.33
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	10	0.33
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	8	0.32
(1,1353)	1:113:A:LEU:HD21	1:112:A:GLN:H	10	0.32
(1,1353)	1:113:A:LEU:HD22	1:112:A:GLN:H	10	0.32
(1,1353)	1:113:A:LEU:HD23	1:112:A:GLN:H	10	0.32
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	2	0.32
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	4	0.32
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	6	0.32
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	10	0.32
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	5	0.32
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	3	0.32
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	6	0.32
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	6	0.32
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	6	0.32
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	4	0.32
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	7	0.32
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	9	0.32
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	5	0.32
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	8	0.32
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	8	0.32
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	8	0.32
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	10	0.32
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	10	0.32
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	10	0.32
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	1	0.32
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	2	0.32
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	9	0.32
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	1	0.32
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	4	0.32
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	7	0.32
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	9	0.32
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	7	0.32
(1,689)	1:56:A:ALA:H	1:54:A:ILE:H	10	0.32
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	1	0.32
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	6	0.32
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	3	0.32
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	7	0.32
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	7	0.32
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	7	0.32
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	4	0.32
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	2	0.32
(1,485)	1:42:A:CYS:H	1:40:A:THR:HG21	1	0.32
(1,485)	1:42:A:CYS:H	1:40:A:THR:HG22	1	0.32
(1,485)	1:42:A:CYS:H	1:40:A:THR:HG23	1	0.32
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	1	0.32
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	1	0.32
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	1	0.32
(1,466)	1:40:A:THR:H	1:37:A:SER:H	9	0.32
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	2	0.32
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	7	0.32
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	8	0.32
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	10	0.32
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	2	0.32
(1,353)	1:28:A:GLN:HB2	1:30:A:SER:H	8	0.32
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	4	0.32
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	4	0.32
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	3	0.32
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	2	0.32
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	3	0.32
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	10	0.32
(1,220)	1:19:A:ASP:H	1:20:A:GLY:HA3	5	0.32
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	5	0.32
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	8	0.32
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	7	0.32
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	7	0.31
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	4	0.31
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	6	0.31
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	1	0.31
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	6	0.31
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	9	0.31
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	5	0.31
(1,1170)	1:100:A:THR:H	1:102:A:GLN:HB3	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	8	0.31
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	9	0.31
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	2	0.31
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	1	0.31
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	1	0.31
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	1	0.31
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	9	0.31
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	9	0.31
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	9	0.31
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	9	0.31
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	9	0.31
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	9	0.31
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	8	0.31
(1,936)	1:79:A:GLY:H	1:81:A:PRO:HD3	3	0.31
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	7	0.31
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG21	5	0.31
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG22	5	0.31
(1,769)	1:68:A:CYS:H	1:66:A:ILE:HG23	5	0.31
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	2	0.31
(1,701)	1:57:A:ALA:H	1:55:A:LYS:HG2	8	0.31
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	7	0.31
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	2	0.31
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	10	0.31
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	3	0.31
(1,533)	1:44:A:MET:HB2	1:46:A:ASP:H	1	0.31
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	2	0.31
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	10	0.31
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	3	0.31
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	5	0.31
(1,466)	1:40:A:THR:H	1:37:A:SER:H	10	0.31
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	3	0.31
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	9	0.31
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	9	0.31
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	9	0.31
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	8	0.31
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	5	0.31
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	5	0.31
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	5	0.31
(1,242)	1:20:A:GLY:H	1:22:A:PRO:HD2	10	0.31
(1,241)	1:20:A:GLY:H	1:22:A:PRO:HA	1	0.31
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	1	0.31
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	3	0.31
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	4	0.31
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	7	0.31
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	7	0.3
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	3	0.3
(1,1372)	1:115:A:VAL:HB	1:114:A:LYS:H	1	0.3
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	3	0.3
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	3	0.3
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	3	0.3
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	7	0.3
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	7	0.3
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	7	0.3
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	1	0.3
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	1	0.3
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	6	0.3
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	4	0.3
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	2	0.3
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	5	0.3
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG11	5	0.3
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG12	5	0.3
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG13	5	0.3
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG11	9	0.3
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG12	9	0.3
(1,1278)	1:107:A:TRP:HE1	1:104:A:VAL:HG13	9	0.3
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	8	0.3
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	6	0.3
(1,1127)	1:95:A:CYS:H	1:97:A:LYS:H	9	0.3
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	5	0.3
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	7	0.3
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	1	0.3
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	1	0.3
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	1	0.3
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	6	0.3
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	6	0.3
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	6	0.3
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	10	0.3
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	3	0.3
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	6	0.3
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	4	0.3
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	4	0.3
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	4	0.3
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	3	0.3
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	3	0.3
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	1	0.3
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	6	0.3
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	10	0.3
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	8	0.3
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	8	0.3
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	8	0.3
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	2	0.3
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	7	0.3
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	9	0.3
(1,878)	1:76:A:MET:H	1:77:A:ILE:HG13	5	0.3
(1,866)	1:75:A:LYS:HB3	1:84:A:VAL:H	4	0.3
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	1	0.3
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	3	0.3
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	1	0.3
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	5	0.3
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	4	0.3
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	4	0.3
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	4	0.3
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	8	0.3
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	8	0.3
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	8	0.3
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	3	0.3
(1,734)	1:62:A:SER:H	1:60:A:ARG:HA	3	0.3
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	3	0.3
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	4	0.3
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	6	0.3
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	1	0.3
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	7	0.3
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	8	0.3
(1,466)	1:40:A:THR:H	1:37:A:SER:H	8	0.3
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	4	0.3
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	10	0.3
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	1	0.3
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	9	0.3
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	9	0.3
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	9	0.3
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	9	0.3
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	9	0.3
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	6	0.3
(1,186)	1:17:A:MET:HB2	1:3:A:GLY:H	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	3	0.3
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	9	0.3
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	5	0.3
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	8	0.3
(1,38)	1:7:A:ILE:HG21	1:6:A:ASP:H	4	0.3
(1,38)	1:7:A:ILE:HG22	1:6:A:ASP:H	4	0.3
(1,38)	1:7:A:ILE:HG23	1:6:A:ASP:H	4	0.3
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	8	0.29
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	8	0.29
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	1	0.29
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	3	0.29
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	10	0.29
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	4	0.29
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	5	0.29
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	8	0.29
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	10	0.29
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	8	0.29
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	9	0.29
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	10	0.29
(1,1124)	1:95:A:CYS:H	1:96:A:SER:HB2	3	0.29
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	6	0.29
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	10	0.29
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	1	0.29
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	1	0.29
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	1	0.29
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	10	0.29
(1,1094)	1:93:A:ILE:HD11	1:92:A:ASP:H	2	0.29
(1,1094)	1:93:A:ILE:HD12	1:92:A:ASP:H	2	0.29
(1,1094)	1:93:A:ILE:HD13	1:92:A:ASP:H	2	0.29
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	8	0.29
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	10	0.29
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	8	0.29
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	9	0.29
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	6	0.29
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	5	0.29
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	10	0.29
(1,999)	1:85:A:GLN:H	1:68:A:CYS:HB2	6	0.29
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	9	0.29
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	9	0.29
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	9	0.29
(1,995)	1:84:A:VAL:H	1:86:A:ASN:H	6	0.29
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	2	0.29
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	2	0.29
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	6	0.29
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	6	0.29
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	6	0.29
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	2	0.29
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	3	0.29
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG21	7	0.29
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG22	7	0.29
(1,965)	1:82:A:GLN:H	1:84:A:VAL:HG23	7	0.29
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	3	0.29
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	3	0.29
(1,836)	1:73:A:THR:H	1:87:A:GLN:H	6	0.29
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	2	0.29
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	1	0.29
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	1	0.29
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	1	0.29
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	5	0.29
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	5	0.29
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	5	0.29
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	8	0.29
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	1	0.29
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	10	0.29
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	1	0.29
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	1	0.29
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	1	0.29
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	10	0.29
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	7	0.29
(1,575)	1:47:A:GLY:H	1:49:A:PRO:HB3	1	0.29
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	2	0.29
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	5	0.29
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	2	0.29
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	5	0.29
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	7	0.29
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	7	0.29
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	7	0.29
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	7	0.29
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	10	0.29
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	10	0.29
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	10	0.29
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	2	0.29
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	8	0.29
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	2	0.29
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	7	0.29
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	1	0.29
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	2	0.29
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	5	0.29
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	9	0.29
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	10	0.29
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	1	0.29
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	10	0.29
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	5	0.28
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	9	0.28
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	7	0.28
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	2	0.28
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	1	0.28
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	1	0.28
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	1	0.28
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	3	0.28
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	3	0.28
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	3	0.28
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	7	0.28
(1,1293)	1:107:A:TRP:HE1	1:109:A:ARG:HD2	1	0.28
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	4	0.28
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	3	0.28
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	7	0.28
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	2	0.28
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	6	0.28
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	6	0.28
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	6	0.28
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	4	0.28
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	5	0.28
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	5	0.28
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	5	0.28
(1,983)	1:84:A:VAL:H	1:75:A:LYS:HG2	10	0.28
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	5	0.28
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	7	0.28
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	4	0.28
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	5	0.28
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	8	0.28
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	8	0.28
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	8	0.28
(1,903)	1:77:A:ILE:H	1:82:A:GLN:HG2	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	8	0.28
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	8	0.28
(1,827)	1:73:A:THR:HB	1:85:A:GLN:H	9	0.28
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	5	0.28
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	4	0.28
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	2	0.28
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	2	0.28
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	2	0.28
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	8	0.28
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	8	0.28
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	8	0.28
(1,634)	1:52:A:ILE:H	1:50:A:ARG:H	9	0.28
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	5	0.28
(1,495)	1:42:A:CYS:H	1:43:A:GLN:HG3	9	0.28
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	4	0.28
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	4	0.28
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	4	0.28
(1,466)	1:40:A:THR:H	1:37:A:SER:H	5	0.28
(1,466)	1:40:A:THR:H	1:37:A:SER:H	6	0.28
(1,439)	1:36:A:CYS:HA	1:38:A:LYS:H	9	0.28
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	4	0.28
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	6	0.28
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	7	0.28
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	3	0.28
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	1	0.28
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	2	0.28
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	3	0.28
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	5	0.28
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	7	0.28
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	8	0.28
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	9	0.28
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	10	0.28
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	10	0.28
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	10	0.28
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	10	0.28
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	10	0.28
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	3	0.28
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	6	0.28
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	5	0.28
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	10	0.28
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	4	0.28
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	2	0.27
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	6	0.27
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	6	0.27
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	6	0.27
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	3	0.27
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	7	0.27
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	2	0.27
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	7	0.27
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	4	0.27
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	8	0.27
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	3	0.27
(1,1137)	1:96:A:SER:HG	1:99:A:THR:H	3	0.27
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	4	0.27
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	7	0.27
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	3	0.27
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	3	0.27
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	3	0.27
(1,1048)	1:88:A:PRO:HD2	1:89:A:THR:H	7	0.27
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	6	0.27
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	3	0.27
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	3	0.27
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	3	0.27
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	4	0.27
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	4	0.27
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	4	0.27
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	8	0.27
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	8	0.27
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	8	0.27
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	8	0.27
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	4	0.27
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	4	0.27
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	4	0.27
(1,897)	1:77:A:ILE:H	1:78:A:ASP:HB3	6	0.27
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	10	0.27
(1,811)	1:72:A:THR:HG21	1:83:A:CYS:H	7	0.27
(1,811)	1:72:A:THR:HG22	1:83:A:CYS:H	7	0.27
(1,811)	1:72:A:THR:HG23	1:83:A:CYS:H	7	0.27
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	6	0.27
(1,796)	1:71:A:GLY:H	1:87:A:GLN:HE22	8	0.27
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	3	0.27
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	2	0.27
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	2	0.27
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	5	0.27
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	9	0.27
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	8	0.27
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	5	0.27
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	9	0.27
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	3	0.27
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	9	0.27
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	10	0.27
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	3	0.27
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	3	0.27
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	9	0.27
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	8	0.27
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	8	0.27
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	8	0.27
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	10	0.27
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	8	0.27
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	2	0.27
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	2	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	2	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	2	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	5	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	5	0.26
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	5	0.26
(1,1363)	1:113:A:LEU:H	1:115:A:VAL:H	6	0.26
(1,1349)	1:113:A:LEU:H	1:111:A:THR:HA	7	0.26
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	2	0.26
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	5	0.26
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	7	0.26
(1,1256)	1:106:A:GLY:H	1:103:A:MET:HG3	9	0.26
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	5	0.26
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	1	0.26
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	3	0.26
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	2	0.26
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	4	0.26
(1,1123)	1:95:A:CYS:H	1:96:A:SER:HG	1	0.26
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	2	0.26
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	2	0.26
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	2	0.26
(1,1072)	1:91:A:SER:HA	1:94:A:GLN:H	5	0.26
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	2	0.26
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	2	0.26
(1,984)	1:84:A:VAL:HG21	1:83:A:CYS:H	7	0.26
(1,984)	1:84:A:VAL:HG22	1:83:A:CYS:H	7	0.26
(1,984)	1:84:A:VAL:HG23	1:83:A:CYS:H	7	0.26
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	4	0.26
(1,975)	1:83:A:CYS:H	1:84:A:VAL:HA	9	0.26
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD11	9	0.26
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD12	9	0.26
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD13	9	0.26
(1,707)	1:57:A:ALA:H	1:59:A:SER:HB2	10	0.26
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	2	0.26
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	9	0.26
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	10	0.26
(1,617)	1:51:A:CYS:H	1:50:A:ARG:HD2	2	0.26
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	7	0.26
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	10	0.26
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	10	0.26
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	10	0.26
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG21	10	0.26
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG22	10	0.26
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG23	10	0.26
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	1	0.26
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	2	0.26
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	6	0.26
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	10	0.26
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	8	0.26
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	2	0.26
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	2	0.26
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	5	0.26
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	7	0.26
(1,377)	1:31:A:CYS:HA	1:34:A:ILE:H	1	0.26
(1,355)	1:29:A:PRO:HG2	1:28:A:GLN:H	4	0.26
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	1	0.26
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	1	0.26
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	8	0.26
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	8	0.26
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	9	0.26
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	3	0.26
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	10	0.26
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	1	0.26
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	3	0.26
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	6	0.26
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	8	0.26
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	1	0.25
(1,1439)	1:60:A:ARG:HG2	1:63:A:CYS:H	10	0.25
(1,1433)	1:89:A:THR:HA	1:91:A:SER:H	5	0.25
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	1	0.25
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	4	0.25
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	4	0.25
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	4	0.25
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	4	0.25
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	10	0.25
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	2	0.25
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	6	0.25
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	1	0.25
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	9	0.25
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	2	0.25
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	1	0.25
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	6	0.25
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	2	0.25
(1,936)	1:79:A:GLY:H	1:81:A:PRO:HD3	1	0.25
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	3	0.25
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	6	0.25
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	9	0.25
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	7	0.25
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	7	0.25
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	7	0.25
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	7	0.25
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	9	0.25
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	3	0.25
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	7	0.25
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	8	0.25
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	2	0.25
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	1	0.25
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	8	0.25
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	3	0.25
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	4	0.25
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	9	0.25
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	9	0.25
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	9	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	1	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	2	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	4	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	5	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	6	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	7	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	8	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	9	0.25
(1,583)	1:48:A:TRP:HE1	1:48:A:TRP:HE3	10	0.25
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	3	0.25
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	4	0.25
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	5	0.25
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	7	0.25
(1,566)	1:47:A:GLY:HA3	1:46:A:ASP:H	8	0.25
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	10	0.25
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	5	0.25
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	5	0.25
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	5	0.25
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	6	0.25
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	6	0.25
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	6	0.25
(1,466)	1:40:A:THR:H	1:37:A:SER:H	2	0.25
(1,466)	1:40:A:THR:H	1:37:A:SER:H	3	0.25
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	9	0.25
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	7	0.25
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	10	0.25
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	5	0.25
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	5	0.25
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	2	0.25
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	3	0.25
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	5	0.25
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	9	0.25
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	5	0.25
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	5	0.25
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	5	0.25
(1,253)	1:22:A:PRO:HB2	1:4:A:CYS:H	6	0.25
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	6	0.25
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	7	0.25
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	8	0.25
(1,215)	1:19:A:ASP:H	1:18:A:MET:HG3	4	0.25
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	9	0.25
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	8	0.24
(1,1406)	1:30:A:SER:H	1:31:A:CYS:HA	9	0.24
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	5	0.24
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	8	0.24
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	8	0.24
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	1	0.24
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	6	0.24
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	9	0.24
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	7	0.24
(1,1214)	1:102:A:GLN:HA	1:104:A:VAL:H	7	0.24
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	5	0.24
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	4	0.24
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	3	0.24
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	3	0.24
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	3	0.24
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	4	0.24
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	7	0.24
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	10	0.24
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	10	0.24
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	10	0.24
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	1	0.24
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	6	0.24
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	2	0.24
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	3	0.24
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	3	0.24
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	3	0.24
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	3	0.24
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	9	0.24
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	6	0.24
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	8	0.24
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	10	0.24
(1,796)	1:71:A:GLY:H	1:87:A:GLN:HE22	1	0.24
(1,784)	1:70:A:LYS:H	1:70:A:LYS:HE2	7	0.24
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	1	0.24
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	6	0.24
(1,674)	1:55:A:LYS:HG3	1:41:A:THR:H	5	0.24
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	2	0.24
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	2	0.24
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	2	0.24
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	5	0.24
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	5	0.24
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	5	0.24
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	1	0.24
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	1	0.24
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	8	0.24
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	9	0.24
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	10	0.24
(1,466)	1:40:A:THR:H	1:37:A:SER:H	4	0.24
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	9	0.24
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	9	0.24
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	2	0.24
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	2	0.24
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	2	0.24
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	10	0.24
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	10	0.24
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	10	0.24
(1,423)	1:36:A:CYS:H	1:34:A:ILE:HG12	9	0.24
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	4	0.24
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	5	0.24
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	3	0.24
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	4	0.24
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	6	0.24
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	7	0.24
(1,279)	1:24:A:CYS:H	1:13:A:THR:HB	10	0.24
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	7	0.24
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	7	0.24
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	7	0.24
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	2	0.24
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	4	0.24
(1,223)	1:19:A:ASP:H	1:21:A:HIS:HE1	5	0.24
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	1	0.24
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	10	0.24
(1,141)	1:15:A:CYS:H	1:9:A:CYS:HB2	9	0.24
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	5	0.24
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	5	0.24
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	5	0.24
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	6	0.23
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	3	0.23
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	7	0.23
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	3	0.23
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	8	0.23
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	2	0.23
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	10	0.23
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	2	0.23
(1,1239)	1:104:A:VAL:H	1:103:A:MET:HG3	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	7	0.23
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	7	0.23
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	7	0.23
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	7	0.23
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	10	0.23
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	10	0.23
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	10	0.23
(1,1052)	1:89:A:THR:H	1:83:A:CYS:HB2	6	0.23
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	5	0.23
(1,1033)	1:86:A:ASN:H	1:87:A:GLN:HB2	3	0.23
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	9	0.23
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	7	0.23
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	7	0.23
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	7	0.23
(1,936)	1:79:A:GLY:H	1:81:A:PRO:HD3	2	0.23
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	2	0.23
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	2	0.23
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	2	0.23
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD11	9	0.23
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD12	9	0.23
(1,907)	1:78:A:ASP:H	1:77:A:ILE:HD13	9	0.23
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	1	0.23
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	6	0.23
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	4	0.23
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	7	0.23
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	3	0.23
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	5	0.23
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	4	0.23
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	4	0.23
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	2	0.23
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	5	0.23
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	4	0.23
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	4	0.23
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	4	0.23
(1,617)	1:51:A:CYS:H	1:50:A:ARG:HD2	8	0.23
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	2	0.23
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	1	0.23
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	3	0.23
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	6	0.23
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	8	0.23
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	8	0.23
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	2	0.23
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	4	0.23
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	9	0.23
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	10	0.23
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	1	0.23
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	4	0.23
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	6	0.23
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	6	0.23
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	7	0.23
(1,498)	1:43:A:GLN:HG2	1:41:A:THR:H	1	0.23
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	7	0.23
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	7	0.23
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	8	0.23
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	5	0.23
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	3	0.23
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	4	0.23
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	2	0.23
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	5	0.23
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	1	0.23
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	1	0.23
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	9	0.23
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	9	0.23
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	4	0.23
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	4	0.23
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	4	0.23
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	5	0.23
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	5	0.23
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	5	0.23
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	4	0.23
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	8	0.23
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	6	0.23
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	2	0.23
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	9	0.23
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	10	0.23
(1,57)	1:8:A:TYR:H	1:7:A:ILE:HG13	8	0.23
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	5	0.23
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	2	0.22
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	10	0.22
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	2	0.22
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	3	0.22
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	2	0.22
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	9	0.22
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	4	0.22
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	10	0.22
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	2	0.22
(1,1247)	1:105:A:ASP:H	1:102:A:GLN:HE21	8	0.22
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	1	0.22
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	3	0.22
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	8	0.22
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	8	0.22
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	8	0.22
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	3	0.22
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	4	0.22
(1,977)	1:84:A:VAL:H	1:68:A:CYS:HB2	6	0.22
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	2	0.22
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	2	0.22
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	3	0.22
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	7	0.22
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	8	0.22
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	4	0.22
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	10	0.22
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	7	0.22
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	4	0.22
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	4	0.22
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	4	0.22
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	7	0.22
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	7	0.22
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	7	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	6	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	6	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	6	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	8	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	8	0.22
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	8	0.22
(1,617)	1:51:A:CYS:H	1:50:A:ARG:HD2	4	0.22
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	6	0.22
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	3	0.22
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	4	0.22
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	5	0.22
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	5	0.22
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	6	0.22
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	1	0.22
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	2	0.22
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	3	0.22
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	4	0.22
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	1	0.22
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	1	0.22
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	1	0.22
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	1	0.22
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	1	0.22
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	5	0.22
(1,230)	1:20:A:GLY:H	1:18:A:MET:HG2	1	0.22
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	1	0.22
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	6	0.22
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	5	0.22
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	1	0.22
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	6	0.22
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	6	0.22
(1,57)	1:8:A:TYR:H	1:7:A:ILE:HG13	1	0.22
(1,57)	1:8:A:TYR:H	1:7:A:ILE:HG13	7	0.22
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	8	0.22
(1,1)	1:3:A:GLY:H	1:1:A:SER:HG	4	0.22
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	4	0.21
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	5	0.21
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	10	0.21
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	3	0.21
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	10	0.21
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	6	0.21
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	7	0.21
(1,1364)	1:113:A:LEU:H	1:121:A:SER:H	8	0.21
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	7	0.21
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	10	0.21
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	5	0.21
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	8	0.21
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	9	0.21
(1,1292)	1:107:A:TRP:H	1:108:A:PRO:HB3	1	0.21
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	1	0.21
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	4	0.21
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	6	0.21
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	7	0.21
(1,1263)	1:106:A:GLY:HA3	1:105:A:ASP:H	3	0.21
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	5	0.21
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	2	0.21
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	1	0.21
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	2	0.21
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	7	0.21
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	7	0.21
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	7	0.21
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	2	0.21
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	9	0.21
(1,996)	1:84:A:VAL:HG21	1:86:A:ASN:H	6	0.21
(1,996)	1:84:A:VAL:HG22	1:86:A:ASN:H	6	0.21
(1,996)	1:84:A:VAL:HG23	1:86:A:ASN:H	6	0.21
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	1	0.21
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	3	0.21
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	8	0.21
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	3	0.21
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	8	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	1	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	1	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	1	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	6	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	6	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	6	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	9	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	9	0.21
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	9	0.21
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	5	0.21
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	7	0.21
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	7	0.21
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	7	0.21
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	4	0.21
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	7	0.21
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	2	0.21
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	7	0.21
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	3	0.21
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	7	0.21
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	3	0.21
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	4	0.21
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	9	0.21
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	3	0.21
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	3	0.21
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	3	0.21
(1,438)	1:36:A:CYS:H	1:37:A:SER:HB3	10	0.21
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	6	0.21
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	8	0.21
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	10	0.21
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	9	0.21
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	10	0.21
(1,388)	1:32:A:SER:HB3	1:34:A:ILE:H	6	0.21
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	7	0.21
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	7	0.21
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	7	0.21
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	4	0.21
(1,293)	1:25:A:VAL:H	1:16:A:LYS:HD2	10	0.21
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	4	0.21
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	4	0.21
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	1	0.21
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	1	0.21
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	1	0.21
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	9	0.21
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	9	0.21
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	9	0.21
(1,199)	1:18:A:MET:H	1:17:A:MET:HG3	4	0.21
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	3	0.21
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	5	0.21
(1,144)	1:15:A:CYS:HB3	1:14:A:THR:H	6	0.21
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	5	0.21
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	6	0.21
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	7	0.21
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	10	0.21
(1,80)	1:10:A:PRO:HB2	1:13:A:THR:H	8	0.21
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	7	0.21
(1,51)	1:8:A:TYR:H	1:5:A:ASN:HA	6	0.21
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	4	0.21
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	9	0.21
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	1	0.21
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	3	0.21
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	6	0.2
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	5	0.2
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	7	0.2
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD11	6	0.2
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD12	6	0.2
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD13	6	0.2
(1,1382)	1:116:A:ALA:H	1:113:A:LEU:HA	2	0.2
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	8	0.2
(1,1295)	1:108:A:PRO:HB3	1:103:A:MET:H	8	0.2
(1,1275)	1:107:A:TRP:H	1:103:A:MET:H	4	0.2
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	3	0.2
(1,1110)	1:93:A:ILE:HD11	1:100:A:THR:H	1	0.2
(1,1110)	1:93:A:ILE:HD12	1:100:A:THR:H	1	0.2
(1,1110)	1:93:A:ILE:HD13	1:100:A:THR:H	1	0.2
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	1	0.2
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	6	0.2
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	6	0.2
(1,1067)	1:90:A:CYS:H	1:97:A:LYS:HG2	1	0.2
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	1	0.2
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	3	0.2
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	8	0.2
(1,983)	1:84:A:VAL:H	1:75:A:LYS:HG2	4	0.2
(1,949)	1:82:A:GLN:H	1:66:A:ILE:HG12	10	0.2
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	5	0.2
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	7	0.2
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	9	0.2
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	10	0.2
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	7	0.2
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	1	0.2
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	2	0.2
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	3	0.2
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	7	0.2
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	2	0.2
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	2	0.2
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	2	0.2
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	9	0.2
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	3	0.2
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	3	0.2
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	3	0.2
(1,646)	1:52:A:ILE:HG12	1:53:A:GLN:H	8	0.2
(1,646)	1:52:A:ILE:HG12	1:53:A:GLN:H	10	0.2
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	1	0.2
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	3	0.2
(1,612)	1:51:A:CYS:HB3	1:36:A:CYS:H	8	0.2
(1,611)	1:51:A:CYS:H	1:36:A:CYS:HB3	2	0.2
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	9	0.2
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	3	0.2
(1,513)	1:43:A:GLN:H	1:49:A:PRO:HA	8	0.2
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	5	0.2
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	8	0.2
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	2	0.2
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	1	0.2
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	6	0.2
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	5	0.2
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	3	0.2
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	5	0.2
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	6	0.2
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	8	0.2
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	6	0.2
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	8	0.2
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	8	0.2
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	6	0.2
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	7	0.2
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	9	0.2
(1,241)	1:20:A:GLY:H	1:22:A:PRO:HA	8	0.2
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	7	0.2
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	9	0.2
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	6	0.2
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	7	0.2
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	2	0.2
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	5	0.2
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	2	0.2
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	3	0.2
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	10	0.2
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	1	0.2
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	10	0.2
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	1	0.2
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	1	0.2
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	1	0.2
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	9	0.2
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	4	0.19
(1,1371)	1:115:A:VAL:HA	1:114:A:LYS:H	5	0.19
(1,1350)	1:113:A:LEU:H	1:111:A:THR:HB	3	0.19
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	3	0.19
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	2	0.19
(1,1276)	1:107:A:TRP:H	1:103:A:MET:HG3	4	0.19
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	8	0.19
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	3	0.19
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	7	0.19
(1,1241)	1:104:A:VAL:HG11	1:103:A:MET:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:104:A:VAL:HG12	1:103:A:MET:H	1	0.19
(1,1241)	1:104:A:VAL:HG13	1:103:A:MET:H	1	0.19
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	5	0.19
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	7	0.19
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	9	0.19
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	10	0.19
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	10	0.19
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	10	0.19
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	10	0.19
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	7	0.19
(1,1050)	1:88:A:PRO:HG3	1:89:A:THR:H	10	0.19
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	3	0.19
(1,908)	1:78:A:ASP:H	1:77:A:ILE:HG12	10	0.19
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	7	0.19
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	8	0.19
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	1	0.19
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	1	0.19
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	2	0.19
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	9	0.19
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	9	0.19
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	9	0.19
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	2	0.19
(1,784)	1:70:A:LYS:H	1:70:A:LYS:HE2	5	0.19
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	4	0.19
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	5	0.19
(1,770)	1:68:A:CYS:H	1:67:A:HIS:HE1	9	0.19
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	2	0.19
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	3	0.19
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	4	0.19
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	9	0.19
(1,764)	1:65:A:ASP:H	1:67:A:HIS:HB3	6	0.19
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	4	0.19
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	8	0.19
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	5	0.19
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	6	0.19
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	10	0.19
(1,657)	1:53:A:GLN:H	1:55:A:LYS:HE2	4	0.19
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	8	0.19
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	5	0.19
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	5	0.19
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	5	0.19
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:47:A:GLY:H	1:49:A:PRO:HD2	1	0.19
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	3	0.19
(1,466)	1:40:A:THR:H	1:37:A:SER:H	7	0.19
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	2	0.19
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	3	0.19
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	3	0.19
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	3	0.19
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	1	0.19
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	2	0.19
(1,401)	1:33:A:ASP:H	1:34:A:ILE:H	7	0.19
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	6	0.19
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	1	0.19
(1,377)	1:31:A:CYS:HA	1:34:A:ILE:H	7	0.19
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	3	0.19
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE1	2	0.19
(1,320)	1:27:A:ASN:H	1:8:A:TYR:HE2	2	0.19
(1,293)	1:25:A:VAL:H	1:16:A:LYS:HD2	7	0.19
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	4	0.19
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	4	0.19
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	1	0.19
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	3	0.19
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	4	0.19
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	3	0.19
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	1	0.19
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	4	0.19
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	7	0.19
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	5	0.19
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	3	0.19
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	1	0.18
(1,1440)	1:61:A:PRO:HB3	1:63:A:CYS:H	4	0.18
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	4	0.18
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	8	0.18
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	1	0.18
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	3	0.18
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	9	0.18
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	5	0.18
(1,1324)	1:111:A:THR:H	1:109:A:ARG:H	8	0.18
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	5	0.18
(1,1272)	1:106:A:GLY:H	1:108:A:PRO:HA	9	0.18
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	1	0.18
(1,1176)	1:100:A:THR:HB	1:112:A:GLN:H	8	0.18
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	6	0.18
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	8	0.18
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	8	0.18
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	8	0.18
(1,1111)	1:94:A:GLN:HB2	1:92:A:ASP:H	5	0.18
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	1	0.18
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	2	0.18
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	3	0.18
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	9	0.18
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	10	0.18
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	1	0.18
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	2	0.18
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	8	0.18
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	4	0.18
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	5	0.18
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	9	0.18
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD11	3	0.18
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD12	3	0.18
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD13	3	0.18
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	2	0.18
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	2	0.18
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	2	0.18
(1,784)	1:70:A:LYS:H	1:70:A:LYS:HE2	8	0.18
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	1	0.18
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	8	0.18
(1,700)	1:57:A:ALA:H	1:55:A:LYS:HD2	8	0.18
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	2	0.18
(1,650)	1:52:A:ILE:H	1:54:A:ILE:H	1	0.18
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	6	0.18
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	8	0.18
(1,587)	1:48:A:TRP:HE1	1:48:A:TRP:HB3	1	0.18
(1,587)	1:48:A:TRP:HE1	1:48:A:TRP:HB3	10	0.18
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	1	0.18
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	9	0.18
(1,518)	1:44:A:MET:HB2	1:34:A:ILE:H	9	0.18
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	7	0.18
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	9	0.18
(1,510)	1:43:A:GLN:H	1:44:A:MET:HA	10	0.18
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	7	0.18
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	5	0.18
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	4	0.18
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:36:A:CYS:H	1:37:A:SER:HG	7	0.18
(1,387)	1:32:A:SER:HB2	1:34:A:ILE:H	10	0.18
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	6	0.18
(1,377)	1:31:A:CYS:HA	1:34:A:ILE:H	3	0.18
(1,377)	1:31:A:CYS:HA	1:34:A:ILE:H	5	0.18
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	8	0.18
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	10	0.18
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	6	0.18
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	6	0.18
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	6	0.18
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	10	0.18
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	2	0.18
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	5	0.18
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	10	0.18
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	1	0.18
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	6	0.18
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	6	0.18
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	6	0.18
(1,187)	1:17:A:MET:H	1:16:A:LYS:HD2	7	0.18
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	4	0.18
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	8	0.18
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	9	0.18
(1,100)	1:13:A:THR:H	1:11:A:LYS:HB2	2	0.18
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	1	0.18
(1,76)	1:9:A:CYS:H	1:11:A:LYS:HA	5	0.18
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	4	0.18
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	6	0.18
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	7	0.18
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	8	0.18
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	2	0.17
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	1	0.17
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	6	0.17
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	9	0.17
(1,1382)	1:116:A:ALA:H	1:113:A:LEU:HA	1	0.17
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	6	0.17
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	2	0.17
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	6	0.17
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	10	0.17
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	5	0.17
(1,1325)	1:111:A:THR:H	1:109:A:ARG:HA	1	0.17
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	1	0.17
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	6	0.17
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	2	0.17
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	7	0.17
(1,1241)	1:104:A:VAL:HG11	1:103:A:MET:H	7	0.17
(1,1241)	1:104:A:VAL:HG12	1:103:A:MET:H	7	0.17
(1,1241)	1:104:A:VAL:HG13	1:103:A:MET:H	7	0.17
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	4	0.17
(1,1179)	1:100:A:THR:HG21	1:113:A:LEU:H	9	0.17
(1,1179)	1:100:A:THR:HG22	1:113:A:LEU:H	9	0.17
(1,1179)	1:100:A:THR:HG23	1:113:A:LEU:H	9	0.17
(1,1158)	1:99:A:THR:H	1:110:A:CYS:HB3	4	0.17
(1,1089)	1:93:A:ILE:HG13	1:92:A:ASP:H	2	0.17
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	4	0.17
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	8	0.17
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	4	0.17
(1,1051)	1:88:A:PRO:HG2	1:89:A:THR:H	6	0.17
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	10	0.17
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	8	0.17
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	4	0.17
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	10	0.17
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	8	0.17
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	8	0.17
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	8	0.17
(1,812)	1:72:A:THR:H	1:86:A:ASN:HB2	4	0.17
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	2	0.17
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	3	0.17
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	3	0.17
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	3	0.17
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	3	0.17
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	5	0.17
(1,612)	1:51:A:CYS:HB3	1:36:A:CYS:H	9	0.17
(1,591)	1:48:A:TRP:HE1	1:49:A:PRO:HG2	10	0.17
(1,587)	1:48:A:TRP:HE1	1:48:A:TRP:HB3	9	0.17
(1,586)	1:48:A:TRP:HE1	1:48:A:TRP:HB2	7	0.17
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	9	0.17
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	2	0.17
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	2	0.17
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	2	0.17
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	8	0.17
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	8	0.17
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	8	0.17
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	7	0.17
(1,346)	1:28:A:GLN:HE22	1:12:A:GLY:H	4	0.17
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	5	0.17
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	7	0.17
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	4	0.17
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	4	0.17
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	4	0.17
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	8	0.17
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	10	0.17
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	2	0.17
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	3	0.17
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	8	0.17
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	3	0.17
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	3	0.17
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	3	0.17
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	1	0.17
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	2	0.17
(1,77)	1:9:A:CYS:H	1:13:A:THR:H	8	0.17
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	2	0.17
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	9	0.17
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	7	0.17
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	7	0.17
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	7	0.17
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	7	0.17
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	4	0.17
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	10	0.17
(1,5)	1:3:A:GLY:H	1:4:A:CYS:HB2	6	0.17
(1,1448)	1:62:A:SER:H	1:65:A:ASP:HB2	10	0.16
(1,1447)	1:62:A:SER:H	1:64:A:SER:H	9	0.16
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	6	0.16
(1,1430)	1:89:A:THR:H	1:90:A:CYS:HB2	4	0.16
(1,1276)	1:107:A:TRP:H	1:103:A:MET:HG3	1	0.16
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	1	0.16
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	3	0.16
(1,1239)	1:104:A:VAL:H	1:103:A:MET:HG3	4	0.16
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	6	0.16
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	4	0.16
(1,1215)	1:102:A:GLN:HG2	1:104:A:VAL:H	9	0.16
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	2	0.16
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	3	0.16
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	4	0.16
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	7	0.16
(1,1088)	1:93:A:ILE:H	1:92:A:ASP:H	5	0.16
(1,1065)	1:90:A:CYS:H	1:92:A:ASP:HB2	7	0.16
(1,1051)	1:88:A:PRO:HG2	1:89:A:THR:H	7	0.16
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	5	0.16
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	8	0.16
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	10	0.16
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	7	0.16
(1,884)	1:77:A:ILE:H	1:75:A:LYS:H	9	0.16
(1,837)	1:74:A:CYS:HA	1:68:A:CYS:H	4	0.16
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	7	0.16
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	7	0.16
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	7	0.16
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	4	0.16
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	7	0.16
(1,726)	1:60:A:ARG:H	1:62:A:SER:HA	3	0.16
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	5	0.16
(1,675)	1:55:A:LYS:H	1:53:A:GLN:HB2	8	0.16
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	6	0.16
(1,656)	1:53:A:GLN:HG3	1:55:A:LYS:H	8	0.16
(1,646)	1:52:A:ILE:HG12	1:53:A:GLN:H	9	0.16
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	1	0.16
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	10	0.16
(1,587)	1:48:A:TRP:HE1	1:48:A:TRP:HB3	6	0.16
(1,587)	1:48:A:TRP:HE1	1:48:A:TRP:HB3	8	0.16
(1,586)	1:48:A:TRP:HE1	1:48:A:TRP:HB2	2	0.16
(1,586)	1:48:A:TRP:HE1	1:48:A:TRP:HB2	3	0.16
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	10	0.16
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	3	0.16
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	10	0.16
(1,478)	1:41:A:THR:HG21	1:40:A:THR:H	8	0.16
(1,478)	1:41:A:THR:HG22	1:40:A:THR:H	8	0.16
(1,478)	1:41:A:THR:HG23	1:40:A:THR:H	8	0.16
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	2	0.16
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	7	0.16
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	10	0.16
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	9	0.16
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	1	0.16
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	2	0.16
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	6	0.16
(1,301)	1:25:A:VAL:HG11	1:28:A:GLN:H	2	0.16
(1,301)	1:25:A:VAL:HG12	1:28:A:GLN:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:25:A:VAL:HG13	1:28:A:GLN:H	2	0.16
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	10	0.16
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	1	0.16
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	5	0.16
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	1	0.16
(1,261)	1:23:A:GLN:H	1:17:A:MET:H	3	0.16
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	1	0.16
(1,260)	1:23:A:GLN:H	1:16:A:LYS:HB2	7	0.16
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG21	2	0.16
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG22	2	0.16
(1,259)	1:23:A:GLN:H	1:7:A:ILE:HG23	2	0.16
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	8	0.16
(1,66)	1:9:A:CYS:H	1:7:A:ILE:HA	3	0.16
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD11	8	0.16
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD12	8	0.16
(1,59)	1:8:A:TYR:H	1:7:A:ILE:HD13	8	0.16
(1,57)	1:8:A:TYR:H	1:7:A:ILE:HG13	5	0.16
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	2	0.16
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	6	0.16
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	4	0.15
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	9	0.15
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	5	0.15
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	10	0.15
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	1	0.15
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	5	0.15
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	2	0.15
(1,1276)	1:107:A:TRP:H	1:103:A:MET:HG3	7	0.15
(1,1241)	1:104:A:VAL:HG11	1:103:A:MET:H	2	0.15
(1,1241)	1:104:A:VAL:HG12	1:103:A:MET:H	2	0.15
(1,1241)	1:104:A:VAL:HG13	1:103:A:MET:H	2	0.15
(1,1241)	1:104:A:VAL:HG11	1:103:A:MET:H	3	0.15
(1,1241)	1:104:A:VAL:HG12	1:103:A:MET:H	3	0.15
(1,1241)	1:104:A:VAL:HG13	1:103:A:MET:H	3	0.15
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	1	0.15
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	2	0.15
(1,1055)	1:89:A:THR:HG21	1:87:A:GLN:H	7	0.15
(1,1055)	1:89:A:THR:HG22	1:87:A:GLN:H	7	0.15
(1,1055)	1:89:A:THR:HG23	1:87:A:GLN:H	7	0.15
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	8	0.15
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	10	0.15
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD11	1	0.15
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD12	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD13	1	0.15
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD11	6	0.15
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD12	6	0.15
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD13	6	0.15
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	4	0.15
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	7	0.15
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	10	0.15
(1,901)	1:77:A:ILE:H	1:81:A:PRO:HB2	5	0.15
(1,884)	1:77:A:ILE:H	1:75:A:LYS:H	4	0.15
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	6	0.15
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	6	0.15
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	6	0.15
(1,800)	1:72:A:THR:H	1:70:A:LYS:HD2	6	0.15
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	5	0.15
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	8	0.15
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	8	0.15
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	5	0.15
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	4	0.15
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	4	0.15
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	4	0.15
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	5	0.15
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	5	0.15
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	5	0.15
(1,688)	1:56:A:ALA:H	1:54:A:ILE:HD11	4	0.15
(1,688)	1:56:A:ALA:H	1:54:A:ILE:HD12	4	0.15
(1,688)	1:56:A:ALA:H	1:54:A:ILE:HD13	4	0.15
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	9	0.15
(1,677)	1:55:A:LYS:HB2	1:54:A:ILE:H	4	0.15
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	7	0.15
(1,662)	1:54:A:ILE:HD11	1:53:A:GLN:H	3	0.15
(1,662)	1:54:A:ILE:HD12	1:53:A:GLN:H	3	0.15
(1,662)	1:54:A:ILE:HD13	1:53:A:GLN:H	3	0.15
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	6	0.15
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	6	0.15
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	6	0.15
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	9	0.15
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG21	9	0.15
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG22	9	0.15
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG23	9	0.15
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	10	0.15
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	9	0.15
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	9	0.15
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	10	0.15
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	10	0.15
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	10	0.15
(1,523)	1:44:A:MET:H	1:43:A:GLN:HE22	1	0.15
(1,499)	1:43:A:GLN:HB2	1:41:A:THR:H	4	0.15
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	5	0.15
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	10	0.15
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	9	0.15
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	10	0.15
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	3	0.15
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	5	0.15
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	2	0.15
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	5	0.15
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	8	0.15
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	9	0.15
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	9	0.15
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	3	0.15
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	9	0.15
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	2	0.15
(1,215)	1:19:A:ASP:H	1:18:A:MET:HG3	5	0.15
(1,176)	1:16:A:LYS:H	1:23:A:GLN:HB2	7	0.15
(1,175)	1:16:A:LYS:HG2	1:18:A:MET:H	10	0.15
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	2	0.15
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	5	0.15
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	3	0.14
(1,1356)	1:113:A:LEU:HA	1:112:A:GLN:H	9	0.14
(1,1336)	1:111:A:THR:H	1:112:A:GLN:HA	4	0.14
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	9	0.14
(1,1325)	1:111:A:THR:H	1:109:A:ARG:HA	2	0.14
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	8	0.14
(1,1314)	1:110:A:CYS:H	1:109:A:ARG:HD2	2	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	4	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	4	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	4	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	6	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	6	0.14
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	6	0.14
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	8	0.14
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	10	0.14
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	10	0.14
(1,1181)	1:101:A:CYS:HB2	1:90:A:CYS:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:100:A:THR:HG21	1:113:A:LEU:H	10	0.14
(1,1179)	1:100:A:THR:HG22	1:113:A:LEU:H	10	0.14
(1,1179)	1:100:A:THR:HG23	1:113:A:LEU:H	10	0.14
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG21	9	0.14
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG22	9	0.14
(1,1116)	1:95:A:CYS:H	1:93:A:ILE:HG23	9	0.14
(1,1084)	1:93:A:ILE:H	1:90:A:CYS:HB3	5	0.14
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	8	0.14
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	10	0.14
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	7	0.14
(1,983)	1:84:A:VAL:H	1:75:A:LYS:HG2	6	0.14
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	4	0.14
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	9	0.14
(1,931)	1:79:A:GLY:H	1:80:A:HIS:HE2	5	0.14
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	1	0.14
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	2	0.14
(1,904)	1:78:A:ASP:H	1:76:A:MET:HA	5	0.14
(1,884)	1:77:A:ILE:H	1:75:A:LYS:H	6	0.14
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD11	8	0.14
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD12	8	0.14
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD13	8	0.14
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	1	0.14
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	1	0.14
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	1	0.14
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	3	0.14
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	3	0.14
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	3	0.14
(1,828)	1:73:A:THR:HG21	1:85:A:GLN:H	5	0.14
(1,828)	1:73:A:THR:HG22	1:85:A:GLN:H	5	0.14
(1,828)	1:73:A:THR:HG23	1:85:A:GLN:H	5	0.14
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	2	0.14
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	5	0.14
(1,765)	1:65:A:ASP:H	1:67:A:HIS:HD2	6	0.14
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	6	0.14
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	1	0.14
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	1	0.14
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	1	0.14
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	3	0.14
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	3	0.14
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	3	0.14
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	10	0.14
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	10	0.14
(1,677)	1:55:A:LYS:HB2	1:54:A:ILE:H	3	0.14
(1,613)	1:51:A:CYS:HB3	1:40:A:THR:H	10	0.14
(1,586)	1:48:A:TRP:HE1	1:48:A:TRP:HB2	4	0.14
(1,586)	1:48:A:TRP:HE1	1:48:A:TRP:HB2	5	0.14
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	6	0.14
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	6	0.14
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	6	0.14
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	6	0.14
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	9	0.14
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	4	0.14
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	6	0.14
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	5	0.14
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	8	0.14
(1,424)	1:36:A:CYS:HB2	1:34:A:ILE:H	8	0.14
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	5	0.14
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	9	0.14
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	7	0.14
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	9	0.14
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	10	0.14
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG11	7	0.14
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG12	7	0.14
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG13	7	0.14
(1,305)	1:26:A:GLN:H	1:14:A:THR:HB	3	0.14
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	1	0.14
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	3	0.14
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	9	0.14
(1,185)	1:17:A:MET:H	1:1:A:SER:HA	4	0.14
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	1	0.13
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	10	0.13
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	1	0.13
(1,1325)	1:111:A:THR:H	1:109:A:ARG:HA	4	0.13
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	7	0.13
(1,1312)	1:110:A:CYS:H	1:109:A:ARG:HG2	3	0.13
(1,1312)	1:110:A:CYS:H	1:109:A:ARG:HG2	7	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	1	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	1	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	1	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	2	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	2	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	2	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	3	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	3	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	7	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	7	0.13
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	7	0.13
(1,1218)	1:102:A:GLN:HG2	1:109:A:ARG:H	8	0.13
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	3	0.13
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	6	0.13
(1,1199)	1:102:A:GLN:H	1:93:A:ILE:HG12	2	0.13
(1,1159)	1:100:A:THR:H	1:95:A:CYS:HB3	4	0.13
(1,1158)	1:99:A:THR:H	1:110:A:CYS:HB3	1	0.13
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	3	0.13
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	7	0.13
(1,1082)	1:92:A:ASP:H	1:93:A:ILE:HB	9	0.13
(1,1052)	1:89:A:THR:H	1:83:A:CYS:HB2	4	0.13
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	5	0.13
(1,952)	1:82:A:GLN:H	1:80:A:HIS:HE1	7	0.13
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD11	10	0.13
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD12	10	0.13
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD13	10	0.13
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	3	0.13
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD11	2	0.13
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD12	2	0.13
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD13	2	0.13
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	1	0.13
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	3	0.13
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	5	0.13
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	6	0.13
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	10	0.13
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	1	0.13
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	9	0.13
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	10	0.13
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	10	0.13
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	8	0.13
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	8	0.13
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	8	0.13
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	10	0.13
(1,686)	1:56:A:ALA:H	1:53:A:GLN:HG2	4	0.13
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	2	0.13
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	7	0.13
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	8	0.13
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	5	0.13
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	5	0.13
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	5	0.13
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	6	0.13
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	4	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	3	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	3	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	3	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	4	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	4	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	4	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	7	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	7	0.13
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	7	0.13
(1,494)	1:42:A:CYS:H	1:43:A:GLN:HB2	8	0.13
(1,466)	1:40:A:THR:H	1:37:A:SER:H	1	0.13
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	8	0.13
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	1	0.13
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	2	0.13
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	3	0.13
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	4	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG11	1	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG12	1	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG13	1	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG11	9	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG12	9	0.13
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG13	9	0.13
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	2	0.13
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	5	0.13
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	6	0.13
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	7	0.13
(1,241)	1:20:A:GLY:H	1:22:A:PRO:HA	7	0.13
(1,239)	1:20:A:GLY:H	1:21:A:HIS:HE2	5	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	7	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	7	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	7	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	9	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	9	0.13
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	9	0.13
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	2	0.13
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	3	0.13
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	10	0.13
(1,177)	1:16:A:LYS:H	1:23:A:GLN:HG2	1	0.13
(1,108)	1:13:A:THR:H	1:24:A:CYS:HB3	8	0.13
(1,108)	1:13:A:THR:H	1:24:A:CYS:HB3	9	0.13
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	1	0.13
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	8	0.13
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	8	0.12
(1,1428)	1:88:A:PRO:HG2	1:93:A:ILE:H	4	0.12
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD11	4	0.12
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD12	4	0.12
(1,1414)	1:30:A:SER:H	1:34:A:ILE:HD13	4	0.12
(1,1345)	1:112:A:GLN:HG2	1:114:A:LYS:H	7	0.12
(1,1325)	1:111:A:THR:H	1:109:A:ARG:HA	3	0.12
(1,1325)	1:111:A:THR:H	1:109:A:ARG:HA	6	0.12
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	4	0.12
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	5	0.12
(1,1294)	1:107:A:TRP:HE1	1:109:A:ARG:HG2	9	0.12
(1,1276)	1:107:A:TRP:H	1:103:A:MET:HG3	2	0.12
(1,1264)	1:106:A:GLY:HA2	1:105:A:ASP:H	5	0.12
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	5	0.12
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	9	0.12
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	10	0.12
(1,1158)	1:99:A:THR:H	1:110:A:CYS:HB3	2	0.12
(1,1052)	1:89:A:THR:H	1:83:A:CYS:HB2	2	0.12
(1,1022)	1:86:A:ASN:H	1:83:A:CYS:HB2	4	0.12
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD11	2	0.12
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD12	2	0.12
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD13	2	0.12
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD11	3	0.12
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD12	3	0.12
(1,948)	1:82:A:GLN:H	1:66:A:ILE:HD13	3	0.12
(1,916)	1:78:A:ASP:H	1:79:A:GLY:HA3	6	0.12
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	2	0.12
(1,798)	1:72:A:THR:H	1:70:A:LYS:HG2	4	0.12
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	6	0.12
(1,795)	1:71:A:GLY:H	1:87:A:GLN:HE21	1	0.12
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	7	0.12
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	8	0.12
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	6	0.12
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	9	0.12
(1,735)	1:62:A:SER:H	1:60:A:ARG:HD2	2	0.12
(1,730)	1:61:A:PRO:HG2	1:62:A:SER:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:60:A:ARG:H	1:61:A:PRO:HA	4	0.12
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	1	0.12
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	6	0.12
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	6	0.12
(1,684)	1:55:A:LYS:H	1:57:A:ALA:H	1	0.12
(1,677)	1:55:A:LYS:HB2	1:54:A:ILE:H	6	0.12
(1,660)	1:54:A:ILE:H	1:52:A:ILE:HA	1	0.12
(1,658)	1:54:A:ILE:H	1:40:A:THR:HA	4	0.12
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	3	0.12
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	4	0.12
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	6	0.12
(1,618)	1:51:A:CYS:H	1:50:A:ARG:HD3	8	0.12
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG21	8	0.12
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG22	8	0.12
(1,609)	1:50:A:ARG:H	1:52:A:ILE:HG23	8	0.12
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	4	0.12
(1,550)	1:45:A:VAL:H	1:48:A:TRP:HB2	5	0.12
(1,536)	1:44:A:MET:HB3	1:48:A:TRP:H	1	0.12
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG11	5	0.12
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG12	5	0.12
(1,532)	1:44:A:MET:H	1:45:A:VAL:HG13	5	0.12
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	3	0.12
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	5	0.12
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	3	0.12
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	4	0.12
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	6	0.12
(1,424)	1:36:A:CYS:HB2	1:34:A:ILE:H	6	0.12
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	5	0.12
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	1	0.12
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	6	0.12
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG11	5	0.12
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG12	5	0.12
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG13	5	0.12
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	8	0.12
(1,293)	1:25:A:VAL:H	1:16:A:LYS:HD2	8	0.12
(1,277)	1:23:A:GLN:HG2	1:26:A:GLN:H	4	0.12
(1,277)	1:23:A:GLN:HG2	1:26:A:GLN:H	8	0.12
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	8	0.12
(1,241)	1:20:A:GLY:H	1:22:A:PRO:HA	5	0.12
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	10	0.12
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	10	0.12
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	6	0.12
(1,221)	1:19:A:ASP:H	1:20:A:GLY:HA2	7	0.12
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	3	0.12
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	10	0.12
(1,161)	1:16:A:LYS:H	1:16:A:LYS:HE2	4	0.12
(1,108)	1:13:A:THR:H	1:24:A:CYS:HB3	5	0.12
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	5	0.12
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	7	0.12
(1,1434)	1:89:A:THR:HB	1:91:A:SER:H	7	0.11
(1,1404)	1:29:A:PRO:HB2	1:33:A:ASP:H	2	0.11
(1,1382)	1:116:A:ALA:H	1:113:A:LEU:HA	7	0.11
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG21	9	0.11
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG22	9	0.11
(1,1365)	1:114:A:LYS:H	1:111:A:THR:HG23	9	0.11
(1,1356)	1:113:A:LEU:HA	1:112:A:GLN:H	10	0.11
(1,1327)	1:111:A:THR:H	1:109:A:ARG:HG2	1	0.11
(1,1318)	1:110:A:CYS:H	1:111:A:THR:HA	9	0.11
(1,1312)	1:110:A:CYS:H	1:109:A:ARG:HG2	6	0.11
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG21	9	0.11
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG22	9	0.11
(1,1307)	1:110:A:CYS:H	1:100:A:THR:HG23	9	0.11
(1,1264)	1:106:A:GLY:HA2	1:105:A:ASP:H	4	0.11
(1,1264)	1:106:A:GLY:HA2	1:105:A:ASP:H	9	0.11
(1,1258)	1:106:A:GLY:H	1:103:A:MET:H	6	0.11
(1,1217)	1:102:A:GLN:H	1:109:A:ARG:HA	2	0.11
(1,1151)	1:99:A:THR:H	1:97:A:LYS:HB2	10	0.11
(1,1055)	1:89:A:THR:HG21	1:87:A:GLN:H	6	0.11
(1,1055)	1:89:A:THR:HG22	1:87:A:GLN:H	6	0.11
(1,1055)	1:89:A:THR:HG23	1:87:A:GLN:H	6	0.11
(1,1055)	1:89:A:THR:HG21	1:87:A:GLN:H	8	0.11
(1,1055)	1:89:A:THR:HG22	1:87:A:GLN:H	8	0.11
(1,1055)	1:89:A:THR:HG23	1:87:A:GLN:H	8	0.11
(1,908)	1:78:A:ASP:H	1:77:A:ILE:HG12	1	0.11
(1,884)	1:77:A:ILE:H	1:75:A:LYS:H	7	0.11
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD11	4	0.11
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD12	4	0.11
(1,879)	1:76:A:MET:H	1:77:A:ILE:HD13	4	0.11
(1,856)	1:75:A:LYS:H	1:76:A:MET:HG2	4	0.11
(1,835)	1:73:A:THR:H	1:86:A:ASN:HB2	5	0.11
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	2	0.11
(1,778)	1:70:A:LYS:H	1:69:A:PRO:HG2	4	0.11
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	2	0.11
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	4	0.11
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	5	0.11
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	7	0.11
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	8	0.11
(1,721)	1:60:A:ARG:H	1:60:A:ARG:HH11	3	0.11
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	2	0.11
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	3	0.11
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	4	0.11
(1,708)	1:57:A:ALA:HB1	1:59:A:SER:H	7	0.11
(1,708)	1:57:A:ALA:HB2	1:59:A:SER:H	7	0.11
(1,708)	1:57:A:ALA:HB3	1:59:A:SER:H	7	0.11
(1,677)	1:55:A:LYS:HB2	1:54:A:ILE:H	7	0.11
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	1	0.11
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD11	8	0.11
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD12	8	0.11
(1,661)	1:54:A:ILE:H	1:52:A:ILE:HD13	8	0.11
(1,656)	1:53:A:GLN:HG3	1:55:A:LYS:H	7	0.11
(1,647)	1:52:A:ILE:HD11	1:53:A:GLN:H	3	0.11
(1,647)	1:52:A:ILE:HD12	1:53:A:GLN:H	3	0.11
(1,647)	1:52:A:ILE:HD13	1:53:A:GLN:H	3	0.11
(1,646)	1:52:A:ILE:HG12	1:53:A:GLN:H	5	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	3	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	3	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	3	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	4	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	4	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	4	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD11	6	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD12	6	0.11
(1,610)	1:50:A:ARG:H	1:52:A:ILE:HD13	6	0.11
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	3	0.11
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	5	0.11
(1,500)	1:43:A:GLN:H	1:41:A:THR:HA	4	0.11
(1,498)	1:43:A:GLN:HG2	1:41:A:THR:H	8	0.11
(1,489)	1:42:A:CYS:HA	1:41:A:THR:H	1	0.11
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	7	0.11
(1,412)	1:34:A:ILE:HG13	1:35:A:GLN:H	2	0.11
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	10	0.11
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	4	0.11
(1,347)	1:28:A:GLN:HG2	1:13:A:THR:H	10	0.11
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG11	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG12	8	0.11
(1,329)	1:27:A:ASN:H	1:25:A:VAL:HG13	8	0.11
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	4	0.11
(1,294)	1:25:A:VAL:H	1:23:A:GLN:HA	7	0.11
(1,293)	1:25:A:VAL:H	1:16:A:LYS:HD2	4	0.11
(1,293)	1:25:A:VAL:H	1:16:A:LYS:HD2	6	0.11
(1,276)	1:23:A:GLN:H	1:25:A:VAL:H	2	0.11
(1,243)	1:21:A:HIS:HA	1:3:A:GLY:H	9	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	2	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	2	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	2	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	3	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	3	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	3	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE1	8	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE2	8	0.11
(1,227)	1:20:A:GLY:H	1:18:A:MET:HE3	8	0.11
(1,206)	1:18:A:MET:H	1:21:A:HIS:HB2	5	0.11
(1,185)	1:17:A:MET:H	1:1:A:SER:HA	3	0.11
(1,184)	1:16:A:LYS:HB3	1:25:A:VAL:H	8	0.11
(1,177)	1:16:A:LYS:H	1:23:A:GLN:HG2	3	0.11
(1,177)	1:16:A:LYS:H	1:23:A:GLN:HG2	8	0.11
(1,161)	1:16:A:LYS:H	1:16:A:LYS:HE2	8	0.11
(1,161)	1:16:A:LYS:H	1:16:A:LYS:HE2	10	0.11
(1,108)	1:13:A:THR:H	1:24:A:CYS:HB3	1	0.11
(1,108)	1:13:A:THR:H	1:24:A:CYS:HB3	10	0.11
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	7	0.11
(1,37)	1:7:A:ILE:HG12	1:6:A:ASP:H	8	0.11
(1,35)	1:7:A:ILE:H	1:4:A:CYS:HB3	4	0.11
(1,23)	1:6:A:ASP:HB2	1:3:A:GLY:H	10	0.11
(1,10)	1:3:A:GLY:H	1:6:A:ASP:H	3	0.11
(1,1264)	1:106:A:GLY:HA2	1:105:A:ASP:H	6	0.1
(1,1264)	1:106:A:GLY:HA2	1:105:A:ASP:H	10	0.1
(1,1248)	1:105:A:ASP:H	1:103:A:MET:H	6	0.1
(1,1158)	1:99:A:THR:H	1:110:A:CYS:HB3	7	0.1
(1,884)	1:77:A:ILE:H	1:75:A:LYS:H	8	0.1
(1,835)	1:73:A:THR:H	1:86:A:ASN:HB2	3	0.1
(1,835)	1:73:A:THR:H	1:86:A:ASN:HB2	9	0.1
(1,800)	1:72:A:THR:H	1:70:A:LYS:HD2	9	0.1
(1,797)	1:72:A:THR:H	1:70:A:LYS:HB2	7	0.1
(1,759)	1:65:A:ASP:H	1:66:A:ILE:H	3	0.1
(1,721)	1:60:A:ARG:H	1:60:A:ARG:HH11	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:60:A:ARG:H	1:60:A:ARG:HH11	6	0.1
(1,711)	1:58:A:PRO:HG2	1:59:A:SER:H	5	0.1
(1,687)	1:56:A:ALA:H	1:54:A:ILE:HA	3	0.1
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	3	0.1
(1,676)	1:55:A:LYS:H	1:54:A:ILE:H	6	0.1
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD11	5	0.1
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD12	5	0.1
(1,627)	1:51:A:CYS:H	1:52:A:ILE:HD13	5	0.1
(1,623)	1:51:A:CYS:H	1:52:A:ILE:HA	8	0.1
(1,559)	1:47:A:GLY:H	1:44:A:MET:H	7	0.1
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	1	0.1
(1,451)	1:37:A:SER:HG	1:40:A:THR:H	2	0.1
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG21	6	0.1
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG22	6	0.1
(1,426)	1:36:A:CYS:H	1:34:A:ILE:HG23	6	0.1
(1,424)	1:36:A:CYS:HB2	1:34:A:ILE:H	10	0.1
(1,385)	1:32:A:SER:H	1:34:A:ILE:H	4	0.1
(1,376)	1:31:A:CYS:H	1:33:A:ASP:H	8	0.1
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	3	0.1
(1,362)	1:30:A:SER:H	1:28:A:GLN:H	6	0.1
(1,193)	1:17:A:MET:HE1	1:21:A:HIS:H	7	0.1
(1,193)	1:17:A:MET:HE2	1:21:A:HIS:H	7	0.1
(1,193)	1:17:A:MET:HE3	1:21:A:HIS:H	7	0.1
(1,169)	1:16:A:LYS:HE2	1:17:A:MET:H	9	0.1
(1,144)	1:15:A:CYS:HB3	1:14:A:THR:H	4	0.1
(1,57)	1:8:A:TYR:H	1:7:A:ILE:HG13	2	0.1
(1,23)	1:6:A:ASP:HB2	1:3:A:GLY:H	1	0.1
(1,23)	1:6:A:ASP:HB2	1:3:A:GLY:H	2	0.1
(1,1)	1:3:A:GLY:H	1:1:A:SER:HG	2	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found