Full wwPDB NMR Structure Validation Report

Mar 8, 2026 – 04:16 PM UTC

PDB ID	:	6QK5 / pdb_00006qk5
BMRB ID	:	34355
Title	:	Solution Structure of the Zn-loaded form of a Metallothionein from Helix Pomatia
Authors	:	Zerbe, O.; Jurt, S.; Beil, A.
Deposited on	:	2019-01-28

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:

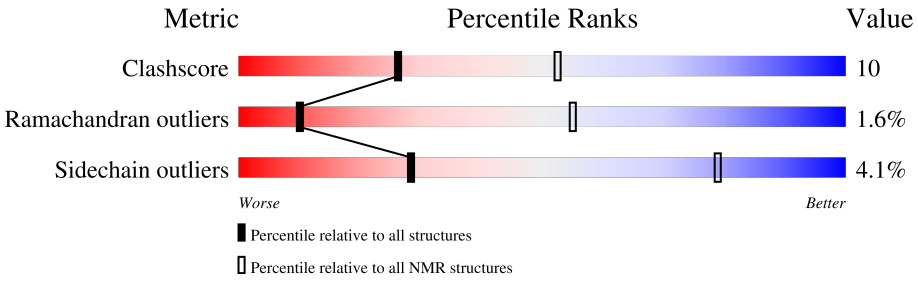
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	67	69% 19% 12%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:9-A:67 (59)	1.08	13

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 843 atoms, of which 397 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cadmium-metallothionein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	837	244	397	82	96	18	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P33187

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	6	6	6

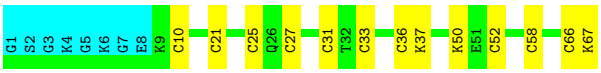
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Cadmium-metallothionein

Chain A:



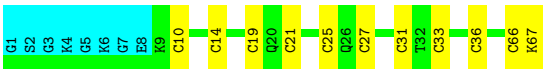
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Cadmium-metallothionein

Chain A:



4.2.2 Score per residue for model 2

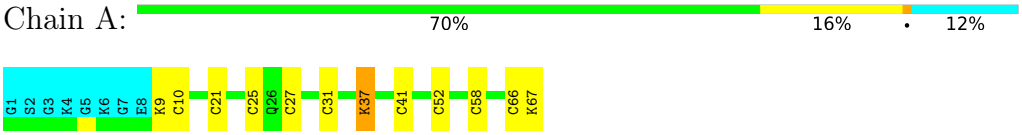
• Molecule 1: Cadmium-metallothionein

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Cadmium-metallothionein

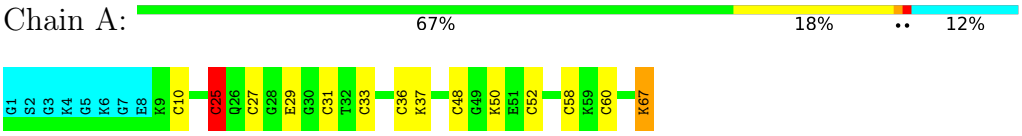
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Cadmium-metallothionein

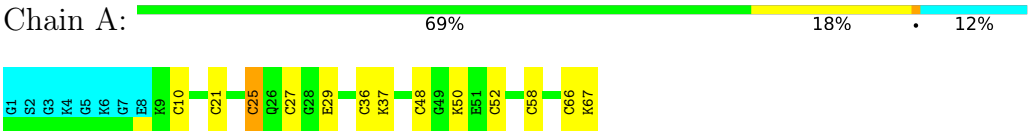
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Cadmium-metallothionein

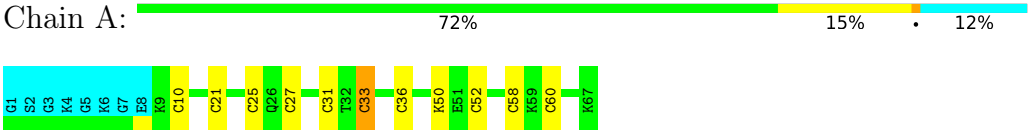
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Cadmium-metallothionein

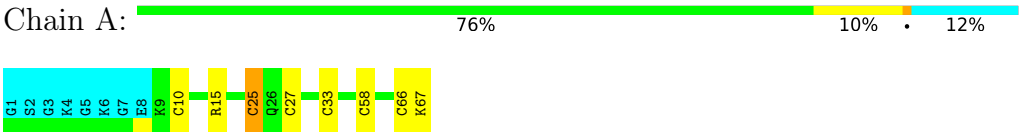
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Cadmium-metallothionein

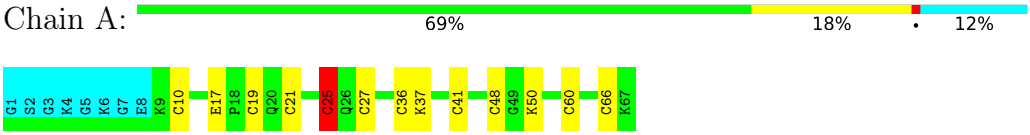
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Cadmium-metallothionein

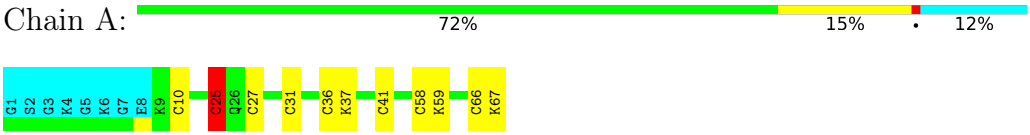
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Cadmium-metallothionein

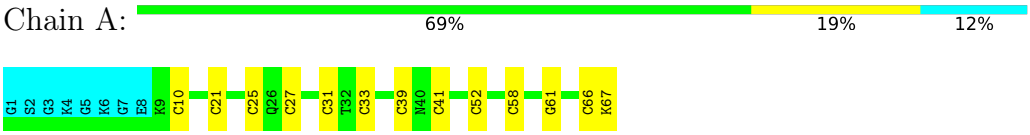
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Cadmium-metallothionein

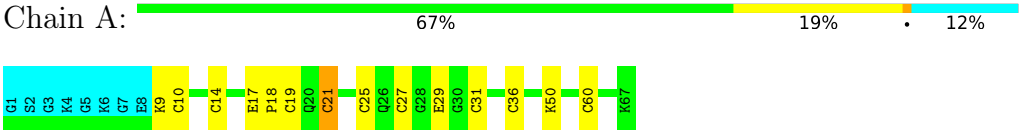
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Cadmium-metallothionein

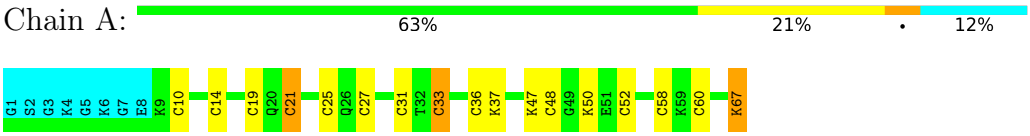
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Cadmium-metallothionein

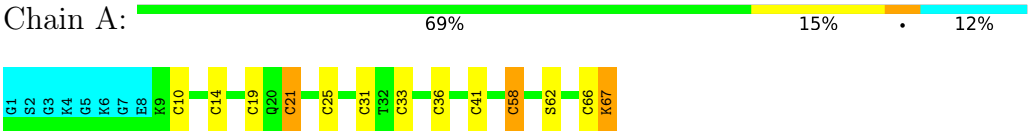
Chain A:



4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Cadmium-metallothionein

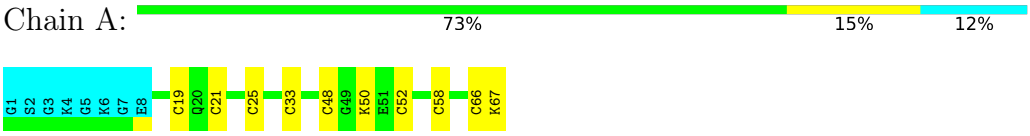
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Cadmium-metallothionein

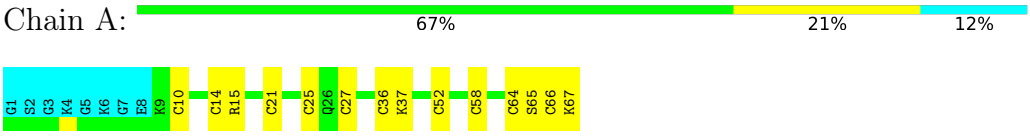
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Cadmium-metallothionein

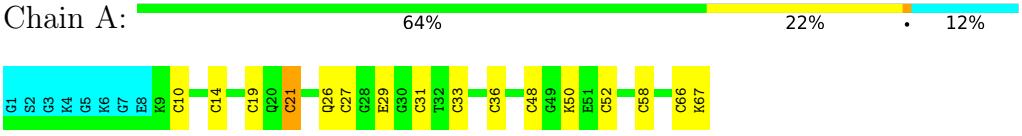
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Cadmium-metallothionein

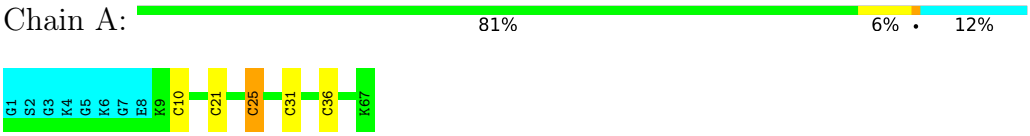
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Cadmium-metallothionein

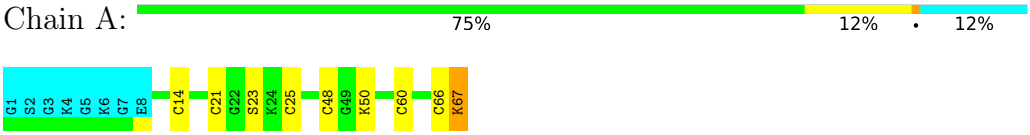
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Cadmium-metallothionein

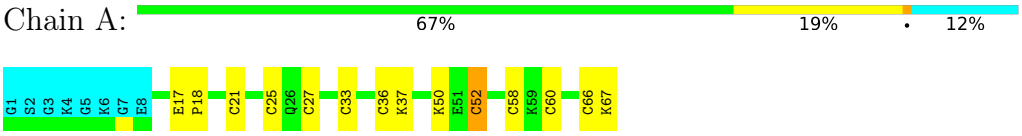
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Cadmium-metallothionein

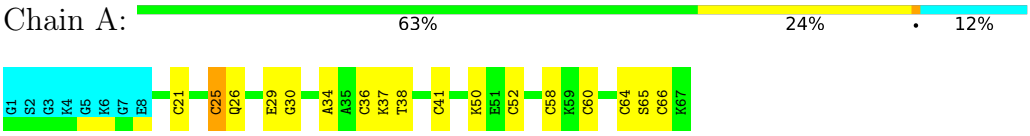
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Cadmium-metallothionein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CNS	refinement	
CYANA	structure calculation	
X-PLOR	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	577
Number of shifts mapped to atoms	577
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	391	349	349	8±3
All	All	7940	6980	6980	150

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:CYS:SG	1:A:33:CYS:HB2	0.75	2.22	16	7
1:A:21:CYS:SG	1:A:25:CYS:HA	0.75	2.21	6	8
1:A:10:CYS:SG	1:A:31:CYS:HB3	0.74	2.22	3	7
1:A:50:LYS:HG3	1:A:60:CYS:SG	0.70	2.27	4	8
1:A:14:CYS:HB2	1:A:21:CYS:SG	0.65	2.31	11	6
1:A:19:CYS:SG	1:A:21:CYS:HB2	0.64	2.33	12	5
1:A:25:CYS:SG	1:A:36:CYS:HB2	0.57	2.39	5	6
1:A:10:CYS:HA	1:A:27:CYS:HB2	0.57	1.76	5	6
1:A:15:ARG:HA	1:A:15:ARG:NE	0.56	2.15	15	2
1:A:14:CYS:HA	1:A:19:CYS:SG	0.55	2.41	13	4
1:A:66:CYS:SG	1:A:67:LYS:HE3	0.55	2.41	19	4
1:A:27:CYS:SG	1:A:37:LYS:NZ	0.54	2.77	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:CYS:SG	1:A:66:CYS:HB3	0.54	2.43	10	7
1:A:10:CYS:HA	1:A:27:CYS:CB	0.53	2.33	9	6
1:A:17:GLU:HA	1:A:18:PRO:C	0.53	2.29	11	2
1:A:21:CYS:HB3	1:A:36:CYS:HB3	0.53	1.81	8	9
1:A:33:CYS:O	1:A:37:LYS:HB2	0.53	2.04	4	2
1:A:66:CYS:SG	1:A:67:LYS:NZ	0.50	2.85	7	4
1:A:34:ALA:C	1:A:38:THR:HB	0.49	2.32	20	1
1:A:64:CYS:SG	1:A:65:SER:N	0.49	2.86	15	2
1:A:10:CYS:SG	1:A:27:CYS:HB2	0.48	2.49	11	5
1:A:21:CYS:HB3	1:A:36:CYS:CB	0.48	2.38	6	5
1:A:31:CYS:SG	1:A:37:LYS:HE2	0.47	2.50	4	2
1:A:52:CYS:CB	1:A:58:CYS:HA	0.47	2.39	16	7
1:A:36:CYS:SG	1:A:37:LYS:HG3	0.47	2.50	12	1
1:A:48:CYS:SG	1:A:50:LYS:HG2	0.47	2.49	18	7
1:A:37:LYS:NZ	1:A:37:LYS:HB2	0.46	2.25	3	1
1:A:21:CYS:HB2	1:A:36:CYS:HB3	0.46	1.88	5	1
1:A:52:CYS:HB2	1:A:58:CYS:HA	0.45	1.87	6	6
1:A:61:GLY:O	1:A:67:LYS:HG3	0.45	2.12	10	1
1:A:33:CYS:HB3	1:A:36:CYS:SG	0.45	2.50	12	2
1:A:58:CYS:SG	1:A:67:LYS:NZ	0.45	2.90	4	4
1:A:31:CYS:SG	1:A:33:CYS:CB	0.44	3.03	16	1
1:A:66:CYS:SG	1:A:67:LYS:HE2	0.42	2.54	5	2
1:A:9:LYS:N	1:A:9:LYS:HD2	0.42	2.30	3	1
1:A:21:CYS:SG	1:A:26:GLN:N	0.41	2.93	20	1
1:A:21:CYS:HB3	1:A:25:CYS:HA	0.41	1.90	15	1
1:A:39:CYS:SG	1:A:66:CYS:HB2	0.40	2.56	10	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/67 (87%)	52±2 (90±3%)	5±2 (9±3%)	1±1 (2±1%)	10	55
All	All	1160/1340 (87%)	1042 (90%)	100 (9%)	18 (2%)	10	55

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	25	CYS	13
1	A	9	LYS	1
1	A	62	SER	1
1	A	23	SER	1
1	A	29	GLU	1
1	A	30	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	49/53 (92%)	47±1 (96±2%)	2±1 (4±2%)	28	79
All	All	980/1060 (92%)	940 (96%)	40 (4%)	28	79

All 14 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	21	CYS	7
1	A	33	CYS	6
1	A	37	LYS	5
1	A	25	CYS	4
1	A	67	LYS	4
1	A	29	GLU	3
1	A	58	CYS	3
1	A	52	CYS	2
1	A	17	GLU	1
1	A	59	LYS	1
1	A	47	LYS	1
1	A	19	CYS	1
1	A	26	GLN	1
1	A	60	CYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shiftFile_1*

7.1.1 Bookkeeping

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

Total number of shifts	577
Number of shifts mapped to atoms	577
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	67	-0.15 ± 0.29	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	56	0.55 ± 0.24	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	60	-1.01 ± 0.47	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 86%, i.e. 514 atoms were assigned a chemical shift out of a possible 601. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	235/298 (79%)	121/123 (98%)	59/118 (50%)	55/57 (96%)
Sidechain	279/303 (92%)	187/192 (97%)	89/98 (91%)	3/13 (23%)

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	Total	^{1}H	^{13}C	^{15}N
Overall	514/601 (86%)	308/315 (98%)	148/216 (69%)	58/70 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 577 atoms were assigned a chemical shift out of a possible 681. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	265/342 (77%)	138/143 (97%)	67/134 (50%)	60/65 (92%)
Sidechain	312/339 (92%)	209/214 (98%)	100/110 (91%)	3/15 (20%)
Overall	577/681 (85%)	347/357 (97%)	167/244 (68%)	63/80 (79%)

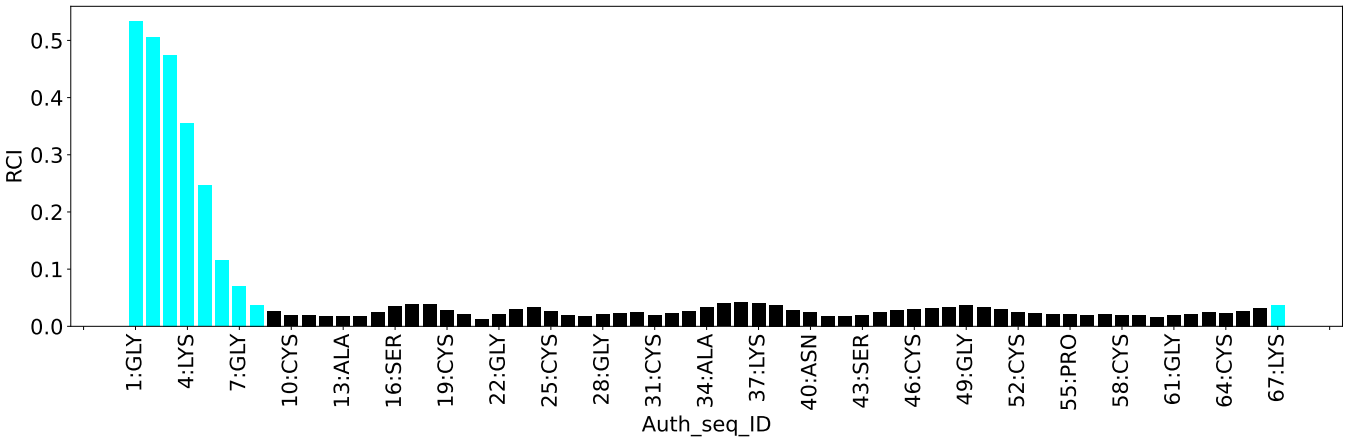
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2144
Intra-residue (|i-j|=0)	411
Sequential (|i-j|=1)	659
Medium range (|i-j|>1 and |i-j|<5)	499
Long range (|i-j|≥5)	575
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	29.4
Number of long range restraints per residue[1]	7.9

[1]Long 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)	32.2	0.2
0.2-0.5 (Medium)	38.0	0.5
>0.5 (Large)	305.3	18.02

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 (i)

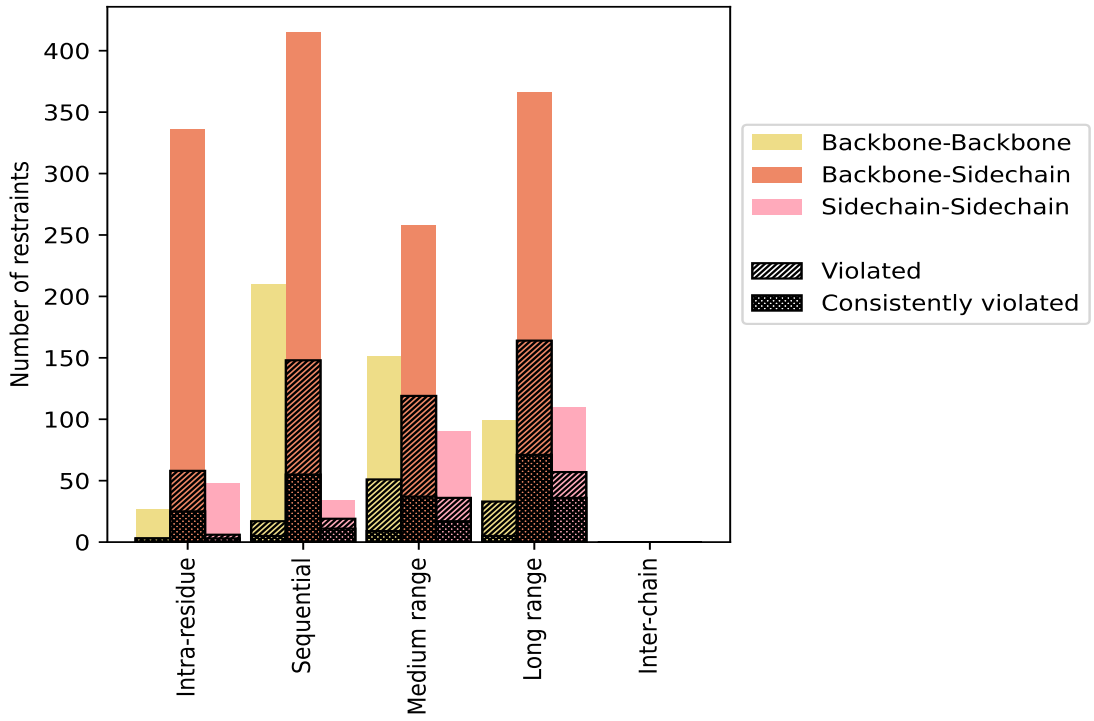
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	411	19.2	67	16.3	3.1	31	7.5	1.4
Backbone-Backbone	27	1.3	3	11.1	0.1	3	11.1	0.1
Backbone-Sidechain	336	15.7	58	17.3	2.7	25	7.4	1.2
Sidechain-Sidechain	48	2.2	6	12.5	0.3	3	6.2	0.1
Sequential (|i-j|=1)	659	30.7	184	27.9	8.6	71	10.8	3.3
Backbone-Backbone	210	9.8	17	8.1	0.8	5	2.4	0.2
Backbone-Sidechain	415	19.4	148	35.7	6.9	55	13.3	2.6
Sidechain-Sidechain	34	1.6	19	55.9	0.9	11	32.4	0.5
Medium range (|i-j|>1 & |i-j|<5)	499	23.3	206	41.3	9.6	63	12.6	2.9
Backbone-Backbone	151	7.0	51	33.8	2.4	9	6.0	0.4
Backbone-Sidechain	258	12.0	119	46.1	5.6	37	14.3	1.7
Sidechain-Sidechain	90	4.2	36	40.0	1.7	17	18.9	0.8
Long range (|i-j|≥5)	575	26.8	254	44.2	11.8	112	19.5	5.2
Backbone-Backbone	99	4.6	33	33.3	1.5	5	5.1	0.2
Backbone-Sidechain	366	17.1	164	44.8	7.6	71	19.4	3.3
Sidechain-Sidechain	110	5.1	57	51.8	2.7	36	32.7	1.7
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	2144	100.0	711	33.2	33.2	277	12.9	12.9
Backbone-Backbone	487	22.7	104	21.4	4.9	22	4.5	1.0
Backbone-Sidechain	1375	64.1	489	35.6	22.8	188	13.7	8.8
Sidechain-Sidechain	282	13.2	118	41.8	5.5	67	23.8	3.1

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

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	34	93	95	148	0	370	3.8	16.28	2.66	4.12
2	36	100	79	146	0	361	3.75	14.98	2.44	4.03
3	36	92	83	138	0	349	4.01	15.48	2.59	4.2
4	42	106	91	144	0	383	3.67	16.25	2.72	3.96
5	38	99	94	144	0	375	3.78	14.83	2.67	4.07
6	32	101	88	144	0	365	3.87	15.85	2.76	4.13
7	39	99	91	137	0	366	3.58	12.0	2.31	3.93
8	38	106	102	150	0	396	3.47	15.75	2.52	3.72
9	37	101	90	152	0	380	3.5	14.01	2.37	3.91
10	36	100	104	142	0	382	3.59	15.56	2.5	3.96

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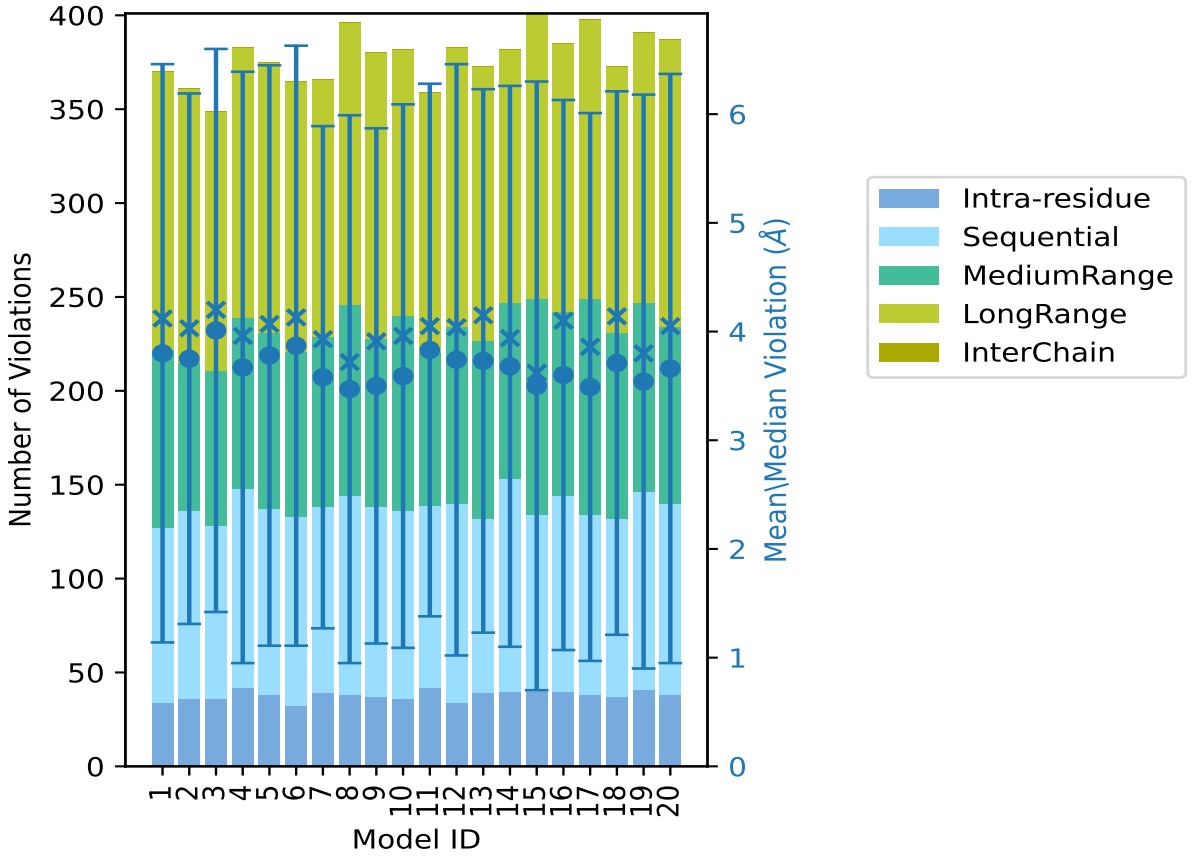
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	42	97	81	139	0	359	3.83	15.43	2.45	4.05
12	34	106	94	149	0	383	3.74	15.07	2.72	4.04
13	39	93	95	146	0	373	3.73	15.02	2.5	4.15
14	40	113	94	135	0	382	3.68	12.97	2.58	3.94
15	40	94	115	152	0	401	3.5	15.21	2.8	3.62
16	40	104	98	143	0	385	3.6	15.15	2.53	4.1
17	38	96	115	149	0	398	3.49	15.67	2.52	3.86
18	37	95	99	142	0	373	3.71	15.46	2.5	4.14
19	41	105	101	144	0	391	3.54	15.59	2.64	3.8
20	38	102	94	153	0	387	3.66	18.02	2.71	4.05

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

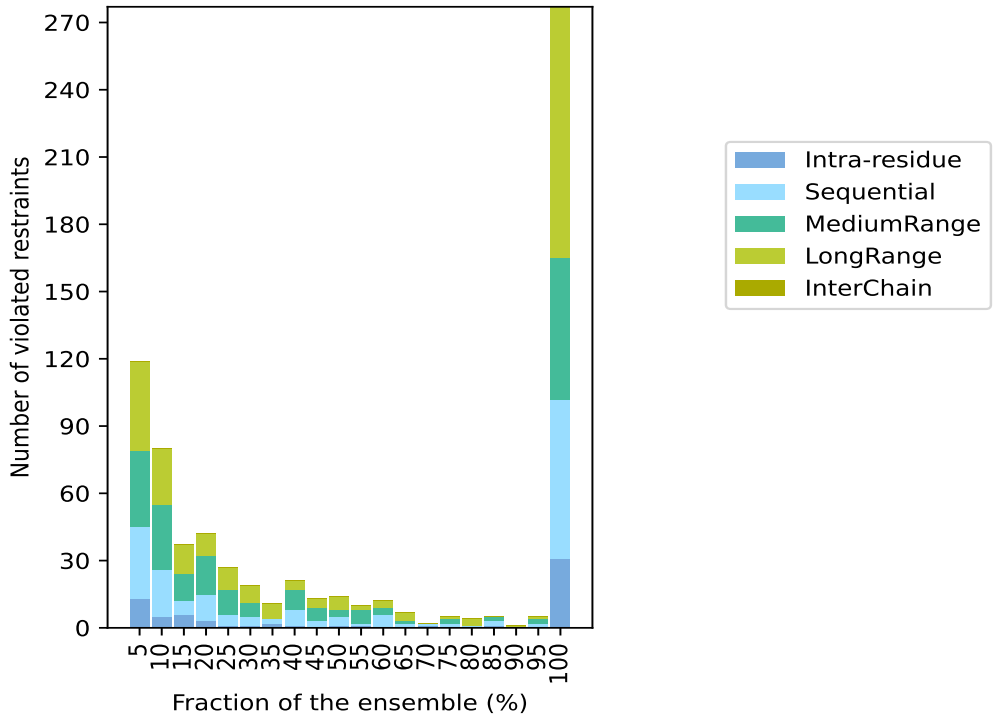
9.3 Distance violation statistics for the ensemble (i)

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, 1433(IR:344, SQ:475, MR:293, LR:321, 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]	%
13	32	34	40	0	119	1	5.0
5	21	29	25	0	80	2	10.0
6	6	12	13	0	37	3	15.0
3	12	17	10	0	42	4	20.0
1	5	11	10	0	27	5	25.0
1	4	6	8	0	19	6	30.0
2	2	0	7	0	11	7	35.0
1	7	9	4	0	21	8	40.0
0	3	6	4	0	13	9	45.0
1	4	3	6	0	14	10	50.0
1	1	6	2	0	10	11	55.0
0	6	3	3	0	12	12	60.0
0	2	1	4	0	7	13	65.0
1	1	0	0	0	2	14	70.0
0	2	2	1	0	5	15	75.0
0	1	0	3	0	4	16	80.0
1	2	2	0	0	5	17	85.0
0	0	0	1	0	1	18	90.0
0	2	2	1	0	5	19	95.0
31	71	63	112	0	277	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

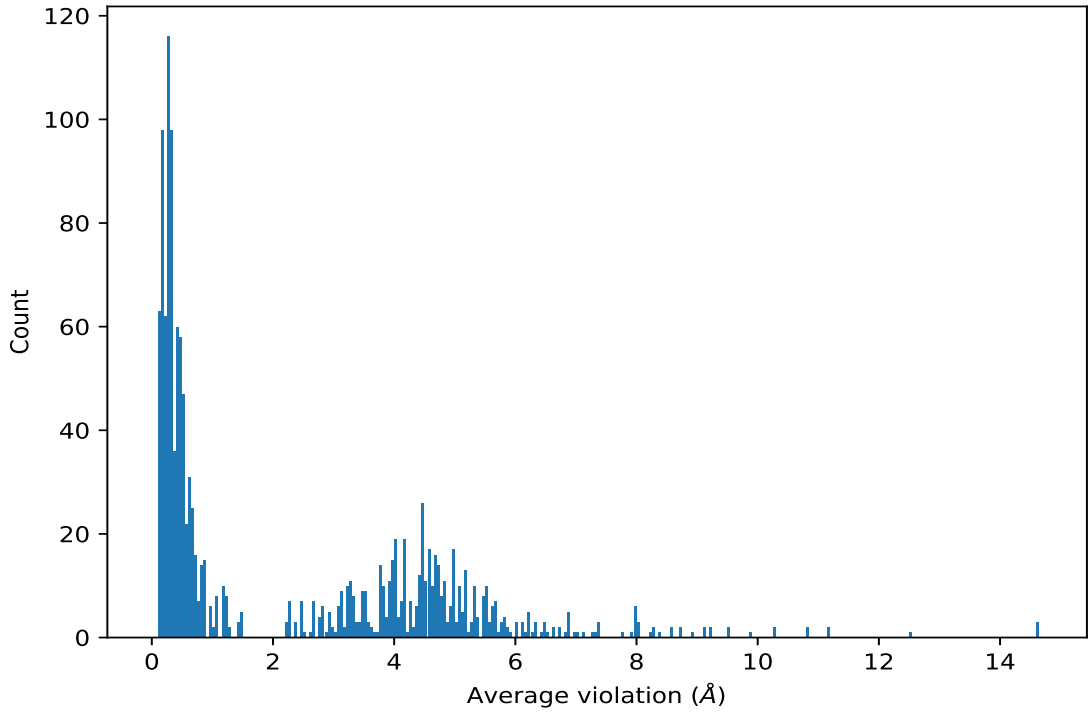
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 theviolation 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)
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	20	14.62	1.06	15.0
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	20	14.62	1.06	15.0
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	20	14.62	1.06	15.0
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	20	12.54	3.1	12.63
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	20	11.16	2.07	11.46
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	20	11.16	2.07	11.46
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	20	10.84	2.15	11.0
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	20	10.84	2.15	11.0
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	20	10.27	0.98	10.34
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	20	10.27	0.98	10.34
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	20	9.87	2.26	10.18
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	20	9.51	2.27	10.12
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	20	9.51	2.27	10.12
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	20	9.21	0.97	9.26
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	20	9.21	0.97	9.26
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	20	9.13	1.84	9.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	20	9.13	1.84	9.25
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	20	8.94	1.77	8.86
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	20	8.71	2.0	9.1
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	20	8.71	2.0	9.1
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	20	8.59	2.42	9.22
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	20	8.59	2.42	9.22
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	20	8.39	2.2	9.46
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	20	8.23	1.32	8.14
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	20	8.03	1.57	7.99
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	20	8.03	1.57	7.99
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	20	8.03	1.57	7.99
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	20	7.99	2.01	8.46
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	20	7.99	2.01	8.46
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	20	7.99	2.01	8.46
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	20	7.98	2.01	8.47
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	20	7.98	2.01	8.47
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	20	7.98	2.01	8.47
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	20	7.94	0.64	7.78
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	20	7.76	1.35	7.74
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	20	7.36	1.53	7.66
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	20	7.36	1.53	7.66
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	20	7.36	1.53	7.66
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	20	7.33	1.34	7.78
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	20	7.26	0.42	7.28
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	20	7.14	0.78	7.03
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	20	7.01	0.86	7.29
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	20	6.98	0.23	6.95
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	20	6.87	2.28	7.28
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	20	6.87	2.28	7.28
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	20	6.87	2.28	7.28
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	20	6.87	2.28	7.28
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	20	6.86	0.43	6.86
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	20	6.8	0.65	6.8
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	20	6.73	0.96	6.8
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	20	6.73	0.96	6.8
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	20	6.63	0.77	6.93
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	20	6.63	0.77	6.93
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	20	6.5	0.41	6.4
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	20	6.47	0.4	6.35
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	20	6.46	0.88	6.7
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	20	6.45	0.16	6.46
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	20	6.42	0.35	6.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	20	6.34	0.2	6.32
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	20	6.3	0.81	6.4
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	20	6.3	0.81	6.4
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	20	6.29	0.08	6.28
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	20	6.22	0.93	6.64
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	20	6.22	0.93	6.64
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	20	6.22	0.93	6.64
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	20	6.22	1.04	6.26
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	20	6.22	1.04	6.26
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	20	6.16	0.35	6.16
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	20	6.14	0.41	6.23
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	20	6.14	0.41	6.23
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	20	6.14	0.41	6.23
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	20	6.04	0.3	6.14
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	20	6.03	0.2	6.01
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	20	6.01	0.89	6.02
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	20	5.91	0.63	5.9
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	20	5.88	1.06	6.12
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	20	5.87	0.39	5.82
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	20	5.83	1.12	6.04
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	20	5.83	1.12	6.04
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	20	5.83	0.7	6.2
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	20	5.83	0.7	6.2
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	20	5.79	1.29	5.52
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	20	5.76	0.91	5.87
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	20	5.76	0.44	5.72
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	20	5.72	1.2	6.22
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	20	5.68	0.92	5.94
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	20	5.68	0.6	5.58
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	20	5.68	0.6	5.58
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	20	5.68	1.39	5.54
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	20	5.67	0.39	5.56
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	20	5.67	0.23	5.64
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	20	5.66	1.06	5.72
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	20	5.6	0.24	5.64
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	20	5.6	0.24	5.64
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	20	5.6	0.58	5.59
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	20	5.6	0.17	5.59
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	20	5.6	0.17	5.59
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	20	5.6	0.17	5.59
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	20	5.57	0.99	5.7
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	20	5.56	0.95	6.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	20	5.56	0.95	6.12
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	20	5.54	0.33	5.49
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	20	5.52	1.13	5.3
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	20	5.52	1.13	5.3
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	20	5.52	0.82	5.81
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	20	5.52	0.82	5.81
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	20	5.52	0.82	5.81
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	20	5.51	0.73	5.8
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	20	5.51	0.73	5.8
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	20	5.51	0.73	5.8
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	20	5.5	0.26	5.5
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	20	5.49	0.08	5.49
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	20	5.49	0.49	5.6
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	20	5.48	0.67	5.46
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	20	5.47	0.99	4.96
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	20	5.47	0.99	4.96
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	20	5.47	0.99	4.96
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	20	5.46	0.14	5.46
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	20	5.46	0.24	5.46
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	20	5.39	0.44	5.42
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	20	5.39	0.44	5.42
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	20	5.37	0.81	5.8
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	20	5.37	0.81	5.8
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	20	5.34	0.5	5.22
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	20	5.34	0.52	5.2
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	20	5.33	0.13	5.28
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	20	5.33	0.8	5.56
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	20	5.33	0.8	5.56
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	20	5.32	0.33	5.24
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	20	5.32	0.46	5.26
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	20	5.31	0.24	5.3
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	20	5.31	0.24	5.3
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	20	5.3	0.53	5.38
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	20	5.28	0.9	4.84
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	20	5.28	0.9	4.84
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	20	5.28	0.9	4.84
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	20	5.24	0.19	5.3
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	20	5.19	0.71	5.3
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	20	5.19	0.72	4.94
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	20	5.19	0.22	5.32
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	20	5.19	0.22	5.32
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	20	5.19	0.22	5.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	20	5.18	0.79	5.04
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	20	5.17	1.19	4.82
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	20	5.17	0.21	5.18
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	5.15	0.85	5.32
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	5.15	0.85	5.32
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	20	5.15	0.49	5.34
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	20	5.15	0.99	5.12
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	20	5.15	0.99	5.12
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	20	5.13	0.92	5.34
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	20	5.13	0.92	5.34
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	20	5.11	0.38	5.11
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	20	5.1	0.21	5.09
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	20	5.1	0.32	5.22
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	20	5.09	0.3	5.16
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	20	5.08	0.29	5.14
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	20	5.08	0.29	5.14
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	20	5.08	0.29	5.14
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	20	5.08	0.29	5.14
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	20	5.08	0.29	5.14
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	20	5.08	0.29	5.14
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	20	5.06	0.26	5.08
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	20	5.06	0.26	5.08
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	20	5.06	0.26	5.08
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	20	5.01	0.43	5.08
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	20	5.01	0.43	5.08
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	20	5.01	0.43	5.08
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	20	4.99	1.64	4.74
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	20	4.99	1.64	4.74
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	20	4.99	1.64	4.74
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	20	4.99	0.38	4.95
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	20	4.99	0.38	4.95
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	20	4.98	0.7	4.94
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	20	4.98	0.7	4.94
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	20	4.98	0.7	4.94
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	20	4.97	0.11	4.96
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	20	4.97	0.11	4.96
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	20	4.97	0.11	4.96
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	20	4.96	0.51	4.94
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	20	4.96	0.51	4.94
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	20	4.96	0.16	4.88
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	20	4.96	0.16	4.88
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	20	4.95	0.8	4.99

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	20	4.95	0.8	4.99
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	20	4.93	0.37	4.97
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	20	4.92	0.08	4.92
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	20	4.9	0.62	4.8
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	20	4.9	0.67	5.16
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	20	4.9	0.67	5.16
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	20	4.9	0.67	5.16
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	20	4.89	0.77	4.66
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	20	4.89	0.77	4.66
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	20	4.87	0.35	4.87
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	20	4.84	1.19	4.9
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	20	4.84	1.19	4.9
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	20	4.84	1.19	4.9
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	4.84	1.19	4.9
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	20	4.84	1.19	4.9
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	4.84	1.19	4.9
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	20	4.83	0.88	4.76
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	20	4.83	0.88	4.76
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	20	4.83	0.88	4.76
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	20	4.83	0.88	4.76
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	20	4.82	0.1	4.84
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	4.76	0.33	4.78
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	20	4.76	0.33	4.78
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	20	4.75	0.52	4.7
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	20	4.75	0.52	4.7
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	20	4.75	0.52	4.7
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	20	4.75	0.52	4.7
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	20	4.75	0.52	4.7
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	20	4.75	0.52	4.7
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	20	4.74	0.4	4.73
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	20	4.74	0.4	4.73
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	20	4.74	0.4	4.73
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	20	4.73	0.69	4.82
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	20	4.73	0.69	4.82
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	20	4.73	0.93	4.99
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	20	4.73	0.93	4.99
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	20	4.72	0.32	4.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	20	4.72	0.32	4.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	20	4.72	0.32	4.66
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	4.71	0.11	4.71
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	20	4.7	0.85	4.55
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	20	4.7	0.85	4.55

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	20	4.7	0.24	4.71
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	20	4.69	0.69	4.82
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	20	4.69	0.69	4.82
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	20	4.69	0.77	4.84
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	4.68	0.28	4.71
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	4.68	0.28	4.71
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	20	4.68	0.28	4.71
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	20	4.68	0.39	4.66
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	20	4.68	0.39	4.66
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	20	4.67	0.53	4.66
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	20	4.67	0.07	4.69
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	20	4.67	0.44	4.61
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	20	4.67	0.44	4.61
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	20	4.66	0.39	4.56
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	4.66	1.07	4.69
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	20	4.65	0.16	4.7
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	20	4.65	0.22	4.68
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	20	4.63	0.17	4.64
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	20	4.63	0.68	4.53
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	20	4.63	0.43	4.56
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	20	4.62	0.19	4.64
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	20	4.61	0.34	4.5
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	20	4.61	0.34	4.5
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	20	4.61	0.34	4.5
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	20	4.61	0.34	4.5
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	20	4.6	0.48	4.5
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	20	4.6	0.48	4.5
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	20	4.59	0.56	4.63
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	20	4.59	0.56	4.63
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	20	4.59	0.56	4.63
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	4.58	0.11	4.58
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	20	4.58	0.11	4.58
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	20	4.58	0.19	4.58
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	20	4.57	0.65	4.54
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	20	4.57	0.65	4.54
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	20	4.57	0.65	4.54
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	20	4.57	0.65	4.54
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	20	4.57	0.65	4.54
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	20	4.57	0.65	4.54
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	20	4.55	0.09	4.54
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	20	4.55	0.09	4.54
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	20	4.55	0.09	4.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	20	4.55	0.16	4.54
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	4.55	0.16	4.54
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	20	4.53	0.13	4.53
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	20	4.53	0.13	4.53
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	20	4.53	0.13	4.53
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	20	4.52	0.21	4.51
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	20	4.52	0.21	4.51
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	20	4.52	0.21	4.51
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	20	4.52	0.21	4.51
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	20	4.5	1.23	4.97
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	20	4.5	1.23	4.97
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	20	4.5	1.23	4.97
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	20	4.5	1.23	4.97
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	20	4.48	0.33	4.51
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	20	4.48	0.33	4.51
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	20	4.48	0.33	4.51
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	20	4.48	0.33	4.51
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	20	4.48	0.33	4.51
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	20	4.48	0.33	4.51
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	20	4.47	0.99	4.28
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	20	4.47	0.99	4.28
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	20	4.47	0.99	4.28
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	20	4.47	0.99	4.28
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	20	4.46	0.23	4.46
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	20	4.46	0.23	4.46
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	20	4.46	0.62	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	20	4.46	0.62	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	20	4.46	0.62	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	20	4.46	0.62	4.61
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	20	4.46	1.36	4.26
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	20	4.46	1.36	4.26
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	20	4.46	1.36	4.26
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	20	4.46	1.36	4.26
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	20	4.46	1.36	4.26
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	20	4.46	1.36	4.26
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	20	4.45	1.06	4.61
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	20	4.45	1.06	4.61
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	20	4.45	0.16	4.42
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	20	4.45	0.16	4.42
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	20	4.44	0.05	4.42
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	20	4.44	0.05	4.42
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	20	4.42	0.28	4.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	20	4.42	0.28	4.36
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	20	4.41	0.21	4.38
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	20	4.41	0.21	4.38
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	4.41	0.58	4.52
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	20	4.41	0.58	4.52
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	20	4.41	0.58	4.52
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	20	4.41	0.58	4.52
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	4.41	0.58	4.52
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	20	4.4	0.04	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	20	4.38	0.06	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	20	4.38	0.06	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	20	4.38	0.06	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	20	4.38	0.06	4.38
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	20	4.38	1.29	3.68
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	20	4.38	1.29	3.68
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	20	4.32	0.17	4.3
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	4.32	0.59	4.44
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	20	4.28	0.73	3.93
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	20	4.28	0.73	3.93
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	20	4.27	0.37	4.37
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	20	4.27	0.14	4.26
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	20	4.27	0.14	4.26
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	20	4.25	0.1	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	20	4.25	0.1	4.27
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	20	4.23	0.15	4.27
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	20	4.19	1.25	4.01
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	20	4.19	1.25	4.01
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	20	4.19	0.8	4.44
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	20	4.19	0.8	4.44
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	20	4.19	0.8	4.44
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	20	4.19	0.97	4.62
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	20	4.19	0.97	4.62
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	20	4.19	0.97	4.62
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	20	4.17	0.75	3.99
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	20	4.17	0.75	3.99

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	20	4.17	0.75	3.99
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	20	4.17	0.75	3.99
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	4.14	0.2	4.14
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	4.14	0.2	4.14
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	4.14	0.2	4.14
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	4.14	0.2	4.14
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	20	4.1	0.72	4.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	20	4.1	0.72	4.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	20	4.1	0.72	4.04
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	20	4.08	0.44	4.02
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	20	4.08	0.44	4.02
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	20	4.06	1.3	4.36
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	20	4.05	0.23	4.04
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	20	4.04	0.96	3.54
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	20	4.04	0.96	3.54
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	20	4.03	0.78	4.01
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	20	4.03	0.78	4.01
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	20	4.03	0.2	4.07
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	20	4.03	0.2	4.07
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	20	4.03	0.2	4.07
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	20	4.02	0.34	4.12
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	20	4.02	0.34	4.12
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	20	4.02	0.34	4.12
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	20	4.02	0.26	4.04
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	20	4.02	0.26	4.04
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	20	4.02	0.24	4.05
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	4.01	0.23	3.98
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	20	4.01	0.23	3.98
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	20	4.01	0.29	3.96
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	20	4.01	0.29	3.96
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	20	4.01	0.29	3.96
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	20	4.01	0.29	3.96
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	20	3.99	0.63	4.26
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	20	3.99	0.63	4.26
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	20	3.99	0.63	4.26
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	20	3.98	0.09	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	20	3.98	0.09	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	20	3.98	0.09	4.0
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	20	3.97	0.87	3.72

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	20	3.97	0.87	3.72
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	20	3.97	0.87	3.72
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	3.94	0.82	4.01
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	3.94	0.82	4.01
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	20	3.94	0.3	4.08
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	20	3.94	0.3	4.08
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	20	3.94	0.3	4.08
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	20	3.94	0.42	3.92
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	20	3.94	0.42	3.92
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	20	3.94	0.42	3.92
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	20	3.94	0.42	3.92
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	20	3.94	0.42	3.92
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	20	3.94	0.42	3.92
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	20	3.89	0.56	4.05
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	20	3.86	0.07	3.86
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	20	3.86	0.07	3.86
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	20	3.86	0.07	3.86
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	20	3.83	0.25	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	20	3.83	0.25	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	20	3.83	0.25	3.87
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	20	3.83	0.05	3.84
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	20	3.83	0.05	3.84
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	20	3.83	0.05	3.84
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	20	3.83	0.47	3.86
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	20	3.83	0.47	3.86
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	20	3.83	0.47	3.86
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	20	3.83	0.16	3.86
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	20	3.79	0.74	3.6
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	20	3.79	0.74	3.6
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	20	3.79	0.74	3.6
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	20	3.78	0.73	3.96
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	20	3.77	0.08	3.79
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	20	3.76	0.85	3.88
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	20	3.76	0.85	3.88
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	20	3.76	0.17	3.68
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	20	3.76	0.17	3.68
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	3.76	0.74	3.86
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	3.76	0.74	3.86
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	3.76	0.74	3.86

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	3.76	0.74	3.86
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	3.76	0.74	3.86
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	20	3.72	0.58	3.55
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	20	3.67	0.38	3.54
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	20	3.63	0.42	3.62
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	20	3.63	0.42	3.62
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	20	3.59	0.2	3.64
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	20	3.58	0.02	3.58
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	20	3.55	0.62	3.85
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	20	3.52	0.27	3.6
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	20	3.52	0.27	3.6
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	20	3.51	0.34	3.38
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	20	3.51	0.12	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	3.51	0.12	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	20	3.51	0.12	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	20	3.51	0.12	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	3.51	0.12	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	20	3.51	0.12	3.53
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	20	3.49	0.43	3.6
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	20	3.49	0.43	3.6
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	20	3.49	0.43	3.6
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	20	3.48	0.05	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	20	3.48	0.05	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	20	3.48	0.05	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	20	3.48	0.05	3.48
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	20	3.45	0.9	3.96
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	20	3.45	0.9	3.96
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	20	3.44	0.09	3.44
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	20	3.42	0.53	3.44
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	20	3.4	0.05	3.42
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	20	3.36	0.79	3.68
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	20	3.36	0.79	3.68
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	20	3.35	0.77	3.32
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	20	3.32	0.62	3.2
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	20	3.32	0.3	3.24
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	20	3.32	0.3	3.24
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	20	3.31	0.64	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	20	3.31	0.64	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	20	3.31	0.64	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	20	3.31	0.64	3.54
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	20	3.31	0.7	3.16
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	20	3.27	0.38	3.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	20	3.27	0.38	3.1
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	20	3.27	0.38	3.1
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	20	3.27	0.38	3.1
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	20	3.27	0.38	3.1
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	20	3.27	0.38	3.1
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	20	3.27	0.14	3.24
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	20	3.27	0.14	3.24
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	3.25	0.79	3.73
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	3.25	0.79	3.73
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	20	3.25	0.79	3.73
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	20	3.22	0.01	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	20	3.22	0.01	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	20	3.22	0.01	3.22
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	20	3.21	0.72	3.16
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	20	3.21	0.72	3.16
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	20	3.21	0.72	3.16
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	20	3.2	0.37	3.08
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	20	3.2	0.37	3.08
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	20	3.2	0.37	3.08
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	20	3.2	0.34	3.26
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	20	3.16	0.74	3.54
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	20	3.16	0.74	3.54
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	20	3.14	0.2	3.11
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	20	3.14	0.25	3.12
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	20	3.12	0.63	3.39
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	20	3.12	0.63	3.39
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	3.11	0.16	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	20	3.11	0.16	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	3.11	0.16	3.12
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	20	3.11	0.16	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	20	3.11	0.16	3.12
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	20	3.08	0.17	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	20	3.08	0.17	2.99
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	20	3.07	0.38	3.06
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	20	3.07	0.38	3.06
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	20	3.0	1.0	2.61
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	20	2.95	0.55	3.08
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	20	2.95	0.55	3.08
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	20	2.94	0.65	2.94
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	20	2.94	0.65	2.94
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	20	2.94	0.65	2.94
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	20	2.91	0.37	2.85

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	20	2.9	0.35	3.0
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	20	2.86	0.02	2.86
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	20	2.84	0.66	2.62
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	20	2.83	0.4	2.56
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	20	2.83	0.4	2.56
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	20	2.81	0.16	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	20	2.81	0.16	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	20	2.81	0.16	2.73
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	20	2.79	0.24	2.78
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	20	2.78	0.22	2.86
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	20	2.78	0.22	2.86
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	20	2.77	0.08	2.78
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.69	0.26	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.69	0.26	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	20	2.69	0.26	2.65
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	20	2.69	0.26	2.65
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	20	2.69	0.26	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.69	0.26	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	20	2.69	0.26	2.65
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	20	2.64	0.32	2.86
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	20	2.5	0.08	2.51
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	20	2.49	0.41	2.56
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	2.49	0.41	2.56
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	20	2.49	0.41	2.56
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	2.45	0.81	2.04
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	2.45	0.81	2.04
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	2.45	0.81	2.04
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	2.45	0.81	2.04
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	20	2.39	0.2	2.36
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	20	2.39	0.2	2.36
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	20	2.39	0.2	2.36
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	20	2.28	0.05	2.27
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	20	2.28	0.05	2.27
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	20	2.26	0.37	2.16
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	20	2.25	0.41	2.18
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	20	2.25	0.41	2.18
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	20	2.25	0.41	2.18
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	20	2.25	0.41	2.18
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.22	0.19	2.25
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.22	0.19	2.25
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	20	2.22	0.19	2.25
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	20	0.99	0.59	1.0

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	20	0.97	0.25	0.96
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	20	0.64	0.26	0.67
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	20	0.64	0.26	0.67
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HB3	20	0.64	0.26	0.67
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	20	0.55	0.2	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	20	0.55	0.2	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	20	0.55	0.2	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	20	0.55	0.2	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	20	0.55	0.2	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	20	0.55	0.2	0.56
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	20	0.22	0.04	0.22
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	20	0.22	0.04	0.22
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	19	8.26	2.78	8.2
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	19	8.26	2.78	8.2
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	19	3.06	1.52	3.15
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	19	3.06	1.52	3.15
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	19	0.71	0.18	0.69
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	19	0.71	0.18	0.69
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	19	0.7	0.33	0.59
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	19	0.55	0.17	0.53
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	19	0.55	0.17	0.53
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	18	0.32	0.11	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	18	0.32	0.11	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	18	0.32	0.11	0.32
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	17	1.23	0.38	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	17	1.23	0.38	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	17	1.23	0.38	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	17	1.23	0.38	1.22
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	17	0.47	0.01	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	17	0.47	0.01	0.47
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	17	0.31	0.21	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	17	0.31	0.21	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	17	0.31	0.21	0.26
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	17	0.16	0.04	0.17
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	17	0.16	0.04	0.17
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	16	1.07	0.53	0.84
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	16	1.07	0.53	0.84
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	16	1.07	0.53	0.84
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	16	1.07	0.53	0.84
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	16	0.49	0.2	0.48
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	16	0.49	0.2	0.48
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	16	0.15	0.04	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	16	0.15	0.04	0.15
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	15	1.49	0.47	1.43
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	15	0.79	0.43	0.8
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	15	0.79	0.43	0.8
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	15	0.73	0.09	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	15	0.73	0.09	0.74
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	15	0.52	0.24	0.52
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	15	0.26	0.08	0.26
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	15	0.26	0.08	0.26
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	14	0.65	0.22	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	14	0.65	0.22	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	14	0.65	0.22	0.65
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	14	0.34	0.21	0.29
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	14	0.34	0.21	0.29
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	13	0.76	0.27	0.8
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	13	0.76	0.27	0.8
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	13	0.76	0.27	0.8
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	13	0.6	0.44	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	13	0.6	0.44	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	13	0.6	0.44	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	13	0.6	0.44	0.41
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	13	0.45	0.22	0.49
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	13	0.45	0.22	0.49
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	13	0.45	0.22	0.49
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	13	0.35	0.05	0.36
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	13	0.35	0.05	0.36
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	13	0.35	0.05	0.36
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	13	0.25	0.23	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	13	0.25	0.23	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	13	0.25	0.23	0.18
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	13	0.19	0.07	0.17
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	13	0.19	0.07	0.17
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	1.19	0.52	1.05
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	1.19	0.52	1.05
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	12	1.19	0.52	1.05

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	1.19	0.52	1.05
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	12	1.19	0.52	1.05
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	1.19	0.52	1.05
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	1.19	0.52	1.05
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	1.19	0.52	1.05
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	12	1.16	0.5	1.25
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	12	1.16	0.5	1.25
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	12	0.71	0.35	0.78
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	12	0.71	0.35	0.78
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	12	0.71	0.35	0.78
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	12	0.54	0.29	0.51
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	12	0.52	0.18	0.55
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	12	0.52	0.18	0.55
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	12	0.52	0.18	0.55
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	12	0.52	0.18	0.55
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	12	0.52	0.17	0.57
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	12	0.52	0.17	0.57
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	12	0.48	0.28	0.53
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	12	0.46	0.21	0.5
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	12	0.46	0.21	0.5
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	12	0.46	0.21	0.5
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	12	0.46	0.21	0.5
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	12	0.46	0.21	0.5
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	12	0.46	0.21	0.5
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	12	0.34	0.24	0.24
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	12	0.34	0.24	0.24
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	12	0.34	0.24	0.24
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	12	0.19	0.07	0.18
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	12	0.19	0.07	0.18
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	11	1.48	0.88	1.09
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	11	1.48	0.88	1.09
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	11	1.48	0.88	1.09
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	11	1.48	0.88	1.09
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	11	0.66	0.14	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	11	0.66	0.14	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	11	0.66	0.14	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	11	0.66	0.14	0.69
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	11	0.66	0.14	0.69
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	11	0.66	0.14	0.69
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	11	0.62	0.27	0.62
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	11	0.62	0.27	0.62
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	11	0.57	0.22	0.68

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	11	0.57	0.22	0.68
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	11	0.57	0.22	0.68
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	11	0.57	0.22	0.68
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	11	0.57	0.22	0.68
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	11	0.57	0.22	0.68
(4,807)	1:15:A:ARG:HD2	1:16:A:SER:H	11	0.52	0.24	0.51
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	11	0.52	0.24	0.51
(4,807)	1:11:A:THR:H	1:15:A:ARG:HD2	11	0.52	0.24	0.51
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	11	0.26	0.12	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	11	0.26	0.12	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	11	0.26	0.12	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	11	0.26	0.12	0.23
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	11	0.23	0.07	0.24
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	11	0.23	0.07	0.24
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	11	0.23	0.07	0.24
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	11	0.23	0.07	0.24
(4,907)	1:9:A:LYS:HE2	1:29:A:GLU:H	10	0.98	0.34	1.08
(4,907)	1:9:A:LYS:HE3	1:29:A:GLU:H	10	0.98	0.34	1.08
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG2	10	0.86	0.27	0.79
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	10	0.86	0.27	0.79
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	10	0.49	0.19	0.56
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	10	0.49	0.19	0.56
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	10	0.49	0.19	0.56
(4,805)	1:9:A:LYS:HG2	1:29:A:GLU:H	10	0.48	0.34	0.31
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	10	0.48	0.34	0.31
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	10	0.45	0.29	0.42
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	10	0.45	0.29	0.42
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	10	0.45	0.31	0.34
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	10	0.45	0.31	0.34
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	10	0.45	0.31	0.34
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	10	0.43	0.13	0.4
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	10	0.43	0.13	0.4
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	10	0.43	0.13	0.4
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.42	0.17	0.44
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.42	0.17	0.44
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.42	0.17	0.44
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.42	0.17	0.44
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.42	0.17	0.44
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.42	0.17	0.44
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	10	0.33	0.15	0.3
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	10	0.28	0.11	0.28
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	10	0.28	0.11	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	10	0.22	0.08	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	10	0.22	0.08	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	10	0.22	0.08	0.21
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	10	0.14	0.05	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	10	0.14	0.05	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	10	0.14	0.05	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	10	0.14	0.05	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	10	0.14	0.05	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	10	0.14	0.05	0.14
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	9	1.2	0.47	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	9	1.2	0.47	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	9	1.2	0.47	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	9	1.2	0.47	0.99
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	9	0.8	0.22	0.87
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	9	0.8	0.22	0.87
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	9	0.8	0.22	0.87
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG3	9	0.65	0.41	0.56
(4,941)	1:6:A:LYS:HG3	1:9:A:LYS:H	9	0.65	0.41	0.56
(4,941)	1:6:A:LYS:HG2	1:9:A:LYS:H	9	0.65	0.41	0.56
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG2	9	0.65	0.41	0.56
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	9	0.65	0.26	0.7
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	9	0.65	0.26	0.7
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	9	0.65	0.26	0.7
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	9	0.58	0.54	0.32
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	9	0.51	0.21	0.55
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	9	0.51	0.21	0.55
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	9	0.51	0.21	0.55
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	9	0.43	0.17	0.41
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	9	0.43	0.17	0.41
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	9	0.42	0.15	0.41
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	9	0.42	0.15	0.41
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	9	0.42	0.15	0.41
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	9	0.42	0.15	0.41
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	9	0.41	0.09	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	9	0.41	0.09	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	9	0.41	0.09	0.4
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	9	0.36	0.15	0.37
(4,277)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	9	0.27	0.16	0.19
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	9	0.27	0.16	0.19
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	9	0.17	0.05	0.17
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	9	0.17	0.05	0.17
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	8	1.27	0.3	1.35
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD3	8	1.27	0.3	1.35
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	8	1.08	0.37	1.11
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	8	1.08	0.37	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	8	1.08	0.37	1.11
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	8	0.89	0.26	0.8
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	8	0.89	0.26	0.8
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	8	0.89	0.26	0.8
(4,787)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	8	0.88	0.32	0.82
(4,787)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	8	0.88	0.32	0.82
(4,787)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	8	0.88	0.32	0.82
(4,787)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	8	0.88	0.32	0.82
(4,787)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	8	0.88	0.32	0.82
(4,787)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	8	0.88	0.32	0.82
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	8	0.7	0.37	0.68
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	8	0.48	0.24	0.46
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	8	0.39	0.12	0.4
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	8	0.38	0.08	0.39
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	8	0.38	0.08	0.39
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	8	0.36	0.15	0.39
(4,298)	1:62:A:SER:H	1:67:A:LYS:HE3	8	0.36	0.15	0.39
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	8	0.31	0.05	0.32
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	8	0.31	0.05	0.32
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	8	0.31	0.05	0.32
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	8	0.31	0.05	0.32
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	8	0.31	0.05	0.32
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	8	0.29	0.11	0.3
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	8	0.29	0.11	0.3
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	8	0.26	0.11	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	8	0.26	0.11	0.22
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	8	0.26	0.13	0.22
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	8	0.26	0.13	0.22
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	8	0.24	0.07	0.23
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	8	0.24	0.07	0.23
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	8	0.23	0.13	0.18
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	8	0.23	0.13	0.18
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	8	0.23	0.13	0.18
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	8	0.23	0.13	0.18
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	8	0.23	0.13	0.18
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	8	0.23	0.13	0.18
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	8	0.17	0.05	0.16
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	8	0.17	0.04	0.16
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	8	0.17	0.04	0.16
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	8	0.17	0.04	0.16
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	8	0.17	0.05	0.16
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	8	0.16	0.03	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	8	0.16	0.03	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	8	0.16	0.03	0.15
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	7	1.06	0.51	1.09
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	7	0.96	0.28	1.06
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE3	7	0.96	0.28	1.06
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	7	0.66	0.28	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	7	0.66	0.28	0.59

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	7	0.62	0.37	0.57
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	7	0.62	0.37	0.57
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	7	0.62	0.37	0.57
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	7	0.5	0.2	0.54
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	7	0.5	0.2	0.54
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	7	0.5	0.2	0.54
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	7	0.5	0.2	0.54
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	7	0.45	0.14	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	7	0.45	0.14	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	7	0.45	0.14	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	7	0.45	0.14	0.49
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	7	0.38	0.27	0.25
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	7	0.38	0.27	0.25
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	7	0.38	0.27	0.25
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	7	0.38	0.27	0.25
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	7	0.36	0.08	0.36
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	7	0.31	0.13	0.27
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	7	0.31	0.13	0.27
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	7	0.31	0.13	0.27
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	7	0.31	0.13	0.27
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD22	7	0.26	0.15	0.2
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	7	0.26	0.15	0.2
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	0.2	0.06	0.21
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	7	0.2	0.06	0.21
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	0.2	0.06	0.21
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	7	0.2	0.06	0.21
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	6	0.86	0.48	0.84
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	6	0.86	0.48	0.84
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	6	0.86	0.48	0.84
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	6	0.86	0.48	0.84
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	6	0.64	0.51	0.46
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	6	0.64	0.51	0.46
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	6	0.64	0.51	0.46
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	6	0.54	0.33	0.52
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	6	0.54	0.33	0.52
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	6	0.54	0.33	0.52
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	6	0.49	0.33	0.4
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	6	0.49	0.33	0.4
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.47	0.28	0.4
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.47	0.28	0.4
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	0.47	0.28	0.4
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.47	0.28	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	6	0.47	0.28	0.4
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.47	0.28	0.4
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.47	0.28	0.4
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.47	0.28	0.4
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	6	0.45	0.26	0.5
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	6	0.44	0.21	0.42
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	6	0.44	0.21	0.42
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	6	0.44	0.21	0.42
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	6	0.44	0.21	0.42
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	6	0.44	0.21	0.42
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	6	0.38	0.22	0.31
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	6	0.34	0.11	0.33
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	6	0.29	0.11	0.29
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	6	0.29	0.11	0.29
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	6	0.29	0.11	0.29
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG22	6	0.25	0.08	0.24
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG21	6	0.25	0.08	0.24
(4,702)	1:38:A:THR:HG21	1:40:A:ASN:HB3	6	0.25	0.08	0.24
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	6	0.19	0.05	0.2
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	6	0.19	0.05	0.2
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	6	0.19	0.05	0.2
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	6	0.18	0.04	0.18
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	6	0.18	0.04	0.18
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	6	0.17	0.04	0.16
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	6	0.17	0.04	0.16
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	6	0.12	0.01	0.12
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	6	0.12	0.01	0.12
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	5	0.82	0.27	0.87
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	5	0.82	0.27	0.87
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	5	0.82	0.27	0.87
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	5	0.82	0.27	0.87
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD3	5	0.72	0.23	0.73
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD2	5	0.72	0.23	0.73
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	5	0.63	0.24	0.64
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	5	0.63	0.24	0.64
(1,671)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	5	0.63	0.24	0.64
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	5	0.6	0.56	0.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	0.6	0.56	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	5	0.6	0.56	0.44
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	5	0.53	0.15	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	5	0.53	0.15	0.59
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	5	0.46	0.17	0.53
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	5	0.46	0.17	0.53
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD3	5	0.46	0.17	0.53
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	5	0.45	0.21	0.4
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	5	0.44	0.25	0.35
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD2	5	0.44	0.25	0.35
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	5	0.44	0.25	0.35
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	5	0.41	0.21	0.43
(1,892)	1:33:A:CYS:HB2	1:36:A:CYS:HA	5	0.41	0.21	0.43
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	5	0.41	0.21	0.43
(1,487)	1:11:A:THR:H	1:26:A:GLN:H	5	0.37	0.11	0.37
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	5	0.33	0.13	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	5	0.33	0.13	0.35
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	5	0.32	0.15	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	5	0.32	0.15	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB2	5	0.32	0.15	0.27
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	5	0.32	0.15	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB2	5	0.32	0.15	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	5	0.32	0.15	0.27
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	5	0.32	0.15	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	5	0.32	0.15	0.27
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	5	0.31	0.13	0.24
(1,747)	1:21:A:CYS:HB2	1:25:A:CYS:HA	5	0.31	0.13	0.24
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	5	0.31	0.13	0.24
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD2	5	0.31	0.04	0.3
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	0.31	0.04	0.3
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	0.31	0.04	0.3
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD2	5	0.31	0.04	0.3
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	0.31	0.04	0.3
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	5	0.3	0.13	0.26
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	5	0.3	0.13	0.26
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	5	0.3	0.13	0.26
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	5	0.3	0.13	0.26
(4,850)	1:37:A:LYS:HG2	1:38:A:THR:H	5	0.3	0.13	0.26
(4,850)	1:37:A:LYS:HG3	1:38:A:THR:H	5	0.3	0.13	0.26
(4,405)	1:11:A:THR:HG21	1:26:A:GLN:HE21	5	0.28	0.12	0.25
(4,405)	1:11:A:THR:HG21	1:26:A:GLN:HE22	5	0.28	0.12	0.25
(4,405)	1:11:A:THR:HG22	1:26:A:GLN:HE22	5	0.28	0.12	0.25
(1,858)	1:11:A:THR:HG21	1:14:A:CYS:HB2	5	0.26	0.14	0.23
(1,858)	1:11:A:THR:HG22	1:14:A:CYS:HB2	5	0.26	0.14	0.23
(1,858)	1:11:A:THR:HG23	1:14:A:CYS:HB2	5	0.26	0.14	0.23
(1,943)	1:8:A:GLU:HB2	1:10:A:CYS:HA	5	0.25	0.11	0.22
(1,943)	1:8:A:GLU:HB3	1:10:A:CYS:HA	5	0.25	0.11	0.22
(4,797)	1:8:A:GLU:HB2	1:10:A:CYS:HA	5	0.25	0.11	0.22
(4,797)	1:8:A:GLU:HB3	1:10:A:CYS:HA	5	0.25	0.11	0.22
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	5	0.18	0.06	0.15
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	5	0.18	0.06	0.15
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE3	5	0.18	0.06	0.15
(1,1125)	1:11:A:THR:HG21	1:28:A:GLY:H	5	0.15	0.03	0.16
(1,1125)	1:11:A:THR:HG22	1:28:A:GLY:H	5	0.15	0.03	0.16
(1,1125)	1:11:A:THR:HG23	1:28:A:GLY:H	5	0.15	0.03	0.16
(4,925)	1:11:A:THR:HG21	1:28:A:GLY:H	5	0.15	0.03	0.16
(4,925)	1:11:A:THR:HG22	1:28:A:GLY:H	5	0.15	0.03	0.16
(4,925)	1:11:A:THR:HG23	1:28:A:GLY:H	5	0.15	0.03	0.16
(1,332)	1:35:A:ALA:HA	1:37:A:LYS:H	5	0.13	0.03	0.14
(4,305)	1:35:A:ALA:HA	1:37:A:LYS:H	5	0.13	0.03	0.14
(4,782)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	4	1.4	0.32	1.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,782)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	4	1.4	0.32	1.4
(4,782)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	4	1.4	0.32	1.4
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG2	4	1.03	0.04	1.0
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG3	4	1.03	0.04	1.0
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	4	0.73	0.29	0.61
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	4	0.73	0.29	0.61
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	4	0.73	0.29	0.61
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	4	0.73	0.29	0.61
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	4	0.57	0.33	0.59
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	4	0.57	0.33	0.59
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	4	0.57	0.33	0.59
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	4	0.57	0.33	0.59
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.52	0.19	0.5
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.52	0.19	0.5
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG3	4	0.52	0.19	0.5
(1,956)	1:9:A:LYS:HG2	1:29:A:GLU:H	4	0.44	0.12	0.42
(1,956)	1:9:A:LYS:HG3	1:29:A:GLU:H	4	0.44	0.12	0.42
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	4	0.37	0.11	0.37
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	4	0.37	0.11	0.37
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	4	0.37	0.11	0.37
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	4	0.37	0.11	0.37
(1,651)	1:38:A:THR:HB	1:55:A:PRO:HB3	4	0.33	0.01	0.33
(4,585)	1:38:A:THR:HB	1:55:A:PRO:HB3	4	0.33	0.01	0.33
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	4	0.32	0.18	0.29
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	4	0.32	0.18	0.29
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	4	0.32	0.18	0.29
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	4	0.32	0.18	0.29
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	4	0.31	0.19	0.29
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	4	0.31	0.19	0.29
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG3	4	0.31	0.19	0.29
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	4	0.3	0.09	0.26
(1,275)	1:21:A:CYS:HB2	1:24:A:LYS:H	4	0.3	0.09	0.26
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	4	0.3	0.09	0.26
(1,1099)	1:28:A:GLY:HA2	1:29:A:GLU:H	4	0.29	0.09	0.26
(1,1099)	1:28:A:GLY:HA3	1:29:A:GLU:H	4	0.29	0.09	0.26
(4,206)	1:43:A:SER:H	1:54:A:GLY:HA3	4	0.27	0.03	0.27
(4,206)	1:43:A:SER:H	1:54:A:GLY:HA2	4	0.27	0.03	0.27
(4,646)	1:43:A:SER:H	1:54:A:GLY:HA3	4	0.27	0.03	0.27
(4,646)	1:43:A:SER:H	1:54:A:GLY:HA2	4	0.27	0.03	0.27
(1,144)	1:60:A:CYS:HB2	1:61:A:GLY:H	4	0.26	0.1	0.26
(1,409)	1:29:A:GLU:HA	1:30:A:GLY:H	4	0.26	0.08	0.22
(4,139)	1:60:A:CYS:HB2	1:61:A:GLY:H	4	0.26	0.1	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,377)	1:29:A:GLU:HA	1:30:A:GLY:H	4	0.26	0.08	0.22
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	4	0.25	0.11	0.21
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	4	0.25	0.11	0.21
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	4	0.25	0.11	0.21
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	4	0.25	0.11	0.21
(1,322)	1:62:A:SER:H	1:64:A:CYS:HB2	4	0.25	0.09	0.26
(4,297)	1:62:A:SER:H	1:64:A:CYS:HB2	4	0.25	0.09	0.26
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD2	4	0.25	0.13	0.22
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD3	4	0.25	0.13	0.22
(4,656)	1:21:A:CYS:HB2	1:25:A:CYS:HA	4	0.23	0.11	0.23
(4,656)	1:21:A:CYS:HB3	1:25:A:CYS:HA	4	0.23	0.11	0.23
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	4	0.22	0.05	0.22
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	4	0.22	0.05	0.22
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD3	4	0.22	0.05	0.22
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD2	4	0.21	0.06	0.22
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD3	4	0.21	0.06	0.22
(1,373)	1:63:A:SER:H	1:64:A:CYS:HB2	4	0.2	0.06	0.21
(4,343)	1:63:A:SER:H	1:64:A:CYS:HB2	4	0.2	0.06	0.21
(1,871)	1:50:A:LYS:HG3	1:52:A:CYS:H	4	0.19	0.07	0.16
(1,145)	1:61:A:GLY:H	1:64:A:CYS:H	4	0.17	0.08	0.14
(4,140)	1:61:A:GLY:H	1:64:A:CYS:H	4	0.17	0.08	0.14
(1,179)	1:37:A:LYS:HA	1:38:A:THR:H	4	0.16	0.02	0.16
(4,172)	1:37:A:LYS:HA	1:38:A:THR:H	4	0.16	0.02	0.16
(1,131)	1:13:A:ALA:H	1:21:A:CYS:HA	4	0.15	0.03	0.15
(4,128)	1:13:A:ALA:H	1:21:A:CYS:HA	4	0.15	0.03	0.15
(1,108)	1:29:A:GLU:H	1:31:A:CYS:H	4	0.14	0.04	0.14
(4,105)	1:29:A:GLU:H	1:31:A:CYS:H	4	0.14	0.04	0.14
(1,360)	1:33:A:CYS:H	1:36:A:CYS:H	4	0.14	0.04	0.12
(4,332)	1:33:A:CYS:H	1:36:A:CYS:H	4	0.14	0.04	0.12
(4,74)	1:14:A:CYS:HB2	1:15:A:ARG:H	4	0.11	0.01	0.12
(1,427)	1:22:A:GLY:H	1:24:A:LYS:H	4	0.11	0.01	0.11
(4,392)	1:22:A:GLY:H	1:24:A:LYS:H	4	0.11	0.01	0.11
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	3	0.84	0.87	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG2	3	0.84	0.87	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	3	0.84	0.87	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	3	0.84	0.87	0.28
(1,520)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	3	0.84	0.87	0.28
(1,262)	1:30:A:GLY:HA2	1:32:A:THR:H	3	0.74	0.27	0.56
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	3	0.59	0.42	0.31
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG2	3	0.59	0.42	0.31
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	3	0.59	0.42	0.31
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	3	0.54	0.3	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE2	3	0.54	0.3	0.69
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	3	0.54	0.3	0.69
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	3	0.52	0.15	0.49
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	3	0.52	0.15	0.49
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	3	0.52	0.15	0.49
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	3	0.52	0.15	0.49
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	3	0.52	0.15	0.49
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	3	0.52	0.15	0.49
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	3	0.52	0.15	0.49
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	3	0.52	0.15	0.49
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	3	0.52	0.15	0.49
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	3	0.52	0.15	0.49
(4,477)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	3	0.44	0.3	0.28
(4,477)	1:10:A:CYS:HB2	1:15:A:ARG:HG2	3	0.44	0.3	0.28
(1,304)	1:8:A:GLU:HA	1:10:A:CYS:H	3	0.41	0.14	0.5
(4,438)	1:39:A:CYS:H	1:40:A:ASN:HD22	3	0.35	0.2	0.3
(4,438)	1:39:A:CYS:H	1:40:A:ASN:HD21	3	0.35	0.2	0.3
(4,826)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	3	0.35	0.17	0.43
(4,826)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	3	0.35	0.17	0.43
(4,826)	1:24:A:LYS:HB2	1:26:A:GLN:HE21	3	0.35	0.17	0.43
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	3	0.32	0.26	0.17
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB2	3	0.32	0.26	0.17
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	3	0.32	0.26	0.17
(4,951)	1:38:A:THR:H	1:67:A:LYS:HB3	3	0.31	0.05	0.28
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB2	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB3	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	3	0.31	0.14	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	3	0.31	0.14	0.21
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB2	3	0.31	0.14	0.21
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB3	3	0.31	0.14	0.21
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB2	3	0.31	0.14	0.21
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB3	3	0.31	0.14	0.21
(1,643)	1:50:A:LYS:HB2	1:58:A:CYS:HA	3	0.3	0.18	0.24
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	3	0.28	0.14	0.26
(1,1116)	1:9:A:LYS:HG2	1:10:A:CYS:H	3	0.28	0.14	0.26
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	3	0.28	0.14	0.26
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	3	0.26	0.05	0.24
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	3	0.26	0.05	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	3	0.26	0.05	0.24
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	3	0.26	0.05	0.24
(1,927)	1:7:A:GLY:HA2	1:9:A:LYS:H	3	0.26	0.06	0.26
(1,927)	1:7:A:GLY:HA3	1:9:A:LYS:H	3	0.26	0.06	0.26
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	3	0.26	0.07	0.28
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	3	0.26	0.07	0.28
(4,789)	1:7:A:GLY:HA2	1:9:A:LYS:H	3	0.26	0.06	0.26
(4,789)	1:7:A:GLY:HA3	1:9:A:LYS:H	3	0.26	0.06	0.26
(1,117)	1:55:A:PRO:HB2	1:57:A:SER:H	3	0.25	0.1	0.2
(4,114)	1:55:A:PRO:HB2	1:57:A:SER:H	3	0.25	0.1	0.2
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	3	0.24	0.06	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	3	0.24	0.06	0.28
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	3	0.21	0.11	0.15
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	3	0.21	0.11	0.15
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB3	3	0.21	0.11	0.15
(1,180)	1:38:A:THR:H	1:67:A:LYS:HA	3	0.17	0.05	0.18
(4,445)	1:14:A:CYS:H	1:26:A:GLN:H	3	0.16	0.03	0.17
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD3	3	0.16	0.02	0.15
(1,800)	1:54:A:GLY:HA2	1:55:A:PRO:HD2	3	0.16	0.02	0.15
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD2	3	0.16	0.02	0.15
(1,91)	1:10:A:CYS:HA	1:14:A:CYS:H	3	0.15	0.04	0.13
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	3	0.15	0.03	0.13
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD3	3	0.15	0.03	0.13
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG21	3	0.15	0.04	0.14
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG22	3	0.15	0.04	0.14
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG23	3	0.15	0.04	0.14
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG21	3	0.15	0.04	0.14
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG22	3	0.15	0.04	0.14
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG23	3	0.15	0.04	0.14
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	3	0.13	0.03	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	3	0.13	0.03	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	3	0.13	0.03	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	3	0.13	0.03	0.11
(1,1139)	1:42:A:THR:HG21	1:47:A:LYS:H	3	0.13	0.01	0.13
(1,1139)	1:42:A:THR:HG22	1:47:A:LYS:H	3	0.13	0.01	0.13
(1,1139)	1:42:A:THR:HG23	1:47:A:LYS:H	3	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,932)	1:42:A:THR:HG21	1:47:A:LYS:H	3	0.13	0.01	0.13
(4,932)	1:42:A:THR:HG22	1:47:A:LYS:H	3	0.13	0.01	0.13
(4,932)	1:42:A:THR:HG23	1:47:A:LYS:H	3	0.13	0.01	0.13
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	3	0.12	0.0	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	3	0.12	0.0	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB3	3	0.12	0.0	0.12
(1,72)	1:13:A:ALA:HB1	1:21:A:CYS:H	3	0.11	0.0	0.11
(1,72)	1:13:A:ALA:HB2	1:21:A:CYS:H	3	0.11	0.0	0.11
(1,72)	1:13:A:ALA:HB3	1:21:A:CYS:H	3	0.11	0.0	0.11
(4,69)	1:13:A:ALA:HB1	1:21:A:CYS:H	3	0.11	0.0	0.11
(4,69)	1:13:A:ALA:HB2	1:21:A:CYS:H	3	0.11	0.0	0.11
(4,69)	1:13:A:ALA:HB3	1:21:A:CYS:H	3	0.11	0.0	0.11
(1,1152)	1:37:A:LYS:HG2	1:62:A:SER:HA	2	0.82	0.04	0.82
(1,1152)	1:37:A:LYS:HG3	1:62:A:SER:HA	2	0.82	0.04	0.82
(4,722)	1:32:A:THR:HA	1:37:A:LYS:HE3	2	0.78	0.13	0.78
(4,722)	1:32:A:THR:HA	1:37:A:LYS:HE2	2	0.78	0.13	0.78
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB2	2	0.6	0.34	0.6
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB2	2	0.6	0.34	0.6
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB3	2	0.6	0.34	0.6
(4,355)	1:11:A:THR:HG21	1:26:A:GLN:HE21	2	0.48	0.02	0.48
(4,355)	1:11:A:THR:HG22	1:26:A:GLN:HE21	2	0.48	0.02	0.48
(1,1136)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	2	0.46	0.33	0.46
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD2	2	0.46	0.01	0.46
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD2	2	0.46	0.01	0.46
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD3	2	0.46	0.01	0.46
(1,911)	1:15:A:ARG:HB3	1:15:A:ARG:HD2	2	0.46	0.01	0.46
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG21	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG22	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG23	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG21	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG22	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG23	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG21	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG22	2	0.44	0.25	0.44
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG23	2	0.44	0.25	0.44
(1,184)	1:38:A:THR:H	1:67:A:LYS:HD3	2	0.44	0.19	0.44
(1,485)	1:21:A:CYS:HB3	1:26:A:GLN:H	2	0.43	0.19	0.43
(1,485)	1:21:A:CYS:HB2	1:26:A:GLN:H	2	0.43	0.19	0.43
(1,485)	1:21:A:CYS:HB3	1:26:A:GLN:H	2	0.43	0.19	0.43
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB3	2	0.4	0.01	0.4
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB2	2	0.4	0.01	0.4
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB2	2	0.4	0.01	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB3	2	0.4	0.01	0.4
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD3	2	0.39	0.03	0.39
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD2	2	0.39	0.03	0.39
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD3	2	0.39	0.03	0.39
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG2	2	0.38	0.26	0.38
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG3	2	0.38	0.26	0.38
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG3	2	0.38	0.26	0.38
(4,830)	1:25:A:CYS:H	1:26:A:GLN:HG2	2	0.38	0.26	0.38
(4,830)	1:25:A:CYS:H	1:26:A:GLN:HG3	2	0.38	0.26	0.38
(4,303)	1:37:A:LYS:HG3	1:62:A:SER:H	2	0.36	0.12	0.36
(4,303)	1:62:A:SER:H	1:67:A:LYS:HG2	2	0.36	0.12	0.36
(4,282)	1:8:A:GLU:HA	1:10:A:CYS:H	2	0.36	0.15	0.36
(4,731)	1:32:A:THR:H	1:37:A:LYS:HE2	2	0.34	0.23	0.34
(4,731)	1:32:A:THR:H	1:37:A:LYS:HE3	2	0.34	0.23	0.34
(4,174)	1:38:A:THR:H	1:67:A:LYS:HE2	2	0.33	0.04	0.33
(4,174)	1:38:A:THR:H	1:67:A:LYS:HE3	2	0.33	0.04	0.33
(1,411)	1:29:A:GLU:HG2	1:30:A:GLY:H	2	0.31	0.04	0.31
(1,411)	1:29:A:GLU:HG3	1:30:A:GLY:H	2	0.31	0.04	0.31
(1,411)	1:29:A:GLU:HG2	1:30:A:GLY:H	2	0.31	0.04	0.31
(1,411)	1:29:A:GLU:HG3	1:30:A:GLY:H	2	0.31	0.04	0.31
(1,141)	1:60:A:CYS:HB3	1:61:A:GLY:H	2	0.3	0.11	0.3
(1,141)	1:60:A:CYS:HB2	1:61:A:GLY:H	2	0.3	0.11	0.3
(1,141)	1:60:A:CYS:HB3	1:61:A:GLY:H	2	0.3	0.11	0.3
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	2	0.3	0.04	0.3
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	2	0.3	0.04	0.3
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	2	0.3	0.04	0.3
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	2	0.3	0.04	0.3
(4,649)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	2	0.3	0.04	0.3
(4,649)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	2	0.3	0.04	0.3
(4,910)	1:9:A:LYS:H	1:27:A:CYS:HB2	2	0.29	0.1	0.29
(4,910)	1:9:A:LYS:H	1:9:A:LYS:HE3	2	0.29	0.1	0.29
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG2	2	0.29	0.02	0.29
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG3	2	0.29	0.02	0.29
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG2	2	0.29	0.02	0.29
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG3	2	0.29	0.02	0.29
(4,814)	1:16:A:SER:HA	1:17:A:GLU:HG2	2	0.29	0.02	0.29
(4,814)	1:16:A:SER:HA	1:17:A:GLU:HG3	2	0.29	0.02	0.29
(1,460)	1:60:A:CYS:HB2	1:64:A:CYS:H	2	0.28	0.08	0.28
(1,460)	1:60:A:CYS:HB2	1:64:A:CYS:H	2	0.28	0.08	0.28
(1,460)	1:60:A:CYS:HB3	1:64:A:CYS:H	2	0.28	0.08	0.28
(1,740)	1:38:A:THR:H	1:67:A:LYS:HD2	2	0.28	0.1	0.28
(4,650)	1:39:A:CYS:H	1:67:A:LYS:HD3	2	0.27	0.11	0.27

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,650)	1:38:A:THR:H	1:67:A:LYS:HD2	2	0.27	0.11	0.27
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE2	2	0.26	0.09	0.26
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE3	2	0.26	0.09	0.26
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE2	2	0.26	0.09	0.26
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE3	2	0.26	0.09	0.26
(4,844)	1:33:A:CYS:H	1:37:A:LYS:HE2	2	0.26	0.09	0.26
(4,844)	1:33:A:CYS:H	1:37:A:LYS:HE3	2	0.26	0.09	0.26
(1,142)	1:61:A:GLY:H	1:64:A:CYS:HB2	2	0.26	0.14	0.26
(1,142)	1:61:A:GLY:H	1:64:A:CYS:HB3	2	0.26	0.14	0.26
(4,138)	1:61:A:GLY:H	1:64:A:CYS:HB3	2	0.26	0.14	0.26
(1,26)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	2	0.24	0.01	0.24
(1,26)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	2	0.24	0.01	0.24
(4,944)	1:31:A:CYS:HA	1:37:A:LYS:HG3	2	0.24	0.03	0.24
(4,944)	1:37:A:LYS:HG3	1:62:A:SER:HA	2	0.24	0.03	0.24
(1,198)	1:20:A:GLN:H	1:20:A:GLN:HE22	2	0.24	0.02	0.24
(1,198)	1:20:A:GLN:H	1:20:A:GLN:HE21	2	0.24	0.02	0.24
(4,25)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	2	0.24	0.0	0.24
(4,25)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	2	0.24	0.0	0.24
(1,924)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	2	0.24	0.02	0.24
(1,924)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	2	0.24	0.02	0.24
(1,924)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	2	0.24	0.02	0.24
(1,924)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	2	0.24	0.02	0.24
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB2	2	0.21	0.04	0.21
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB2	2	0.21	0.04	0.21
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB3	2	0.21	0.04	0.21
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB3	2	0.21	0.04	0.21
(1,433)	1:18:A:PRO:HG2	1:19:A:CYS:H	2	0.2	0.03	0.2
(4,400)	1:18:A:PRO:HG2	1:19:A:CYS:H	2	0.2	0.03	0.2
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB2	2	0.2	0.02	0.2
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB2	2	0.2	0.02	0.2
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB3	2	0.2	0.02	0.2
(1,390)	1:64:A:CYS:HB2	1:67:A:LYS:H	2	0.19	0.04	0.19
(1,980)	1:24:A:LYS:HB2	1:26:A:GLN:HE21	2	0.19	0.01	0.19
(1,980)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	2	0.19	0.01	0.19
(1,326)	1:62:A:SER:H	1:67:A:LYS:HB3	2	0.18	0.03	0.18
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB1	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB2	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB3	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB1	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB2	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB3	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB1	2	0.18	0.06	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB2	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB3	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB1	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB2	2	0.18	0.06	0.18
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB3	2	0.18	0.06	0.18
(1,973)	1:17:A:GLU:HB2	1:18:A:PRO:HA	2	0.18	0.0	0.18
(1,973)	1:17:A:GLU:HB3	1:18:A:PRO:HA	2	0.18	0.0	0.18
(4,22)	1:17:A:GLU:H	1:20:A:GLN:HE21	2	0.18	0.06	0.18
(4,22)	1:17:A:GLU:H	1:20:A:GLN:HE22	2	0.18	0.06	0.18
(4,300)	1:62:A:SER:H	1:67:A:LYS:HB3	2	0.18	0.03	0.18
(4,818)	1:17:A:GLU:HB2	1:18:A:PRO:HA	2	0.18	0.0	0.18
(4,818)	1:17:A:GLU:HB3	1:18:A:PRO:HA	2	0.18	0.0	0.18
(4,547)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	2	0.16	0.01	0.16
(1,1094)	1:66:A:CYS:H	1:67:A:LYS:HE2	2	0.16	0.02	0.16
(1,1094)	1:66:A:CYS:H	1:67:A:LYS:HE3	2	0.16	0.02	0.16
(4,903)	1:66:A:CYS:H	1:67:A:LYS:HE2	2	0.16	0.02	0.16
(4,903)	1:66:A:CYS:H	1:67:A:LYS:HE3	2	0.16	0.02	0.16
(1,962)	1:11:A:THR:HB	1:12:A:SER:HB2	2	0.16	0.02	0.16
(1,962)	1:11:A:THR:HB	1:12:A:SER:HB3	2	0.16	0.02	0.16
(4,808)	1:11:A:THR:HB	1:12:A:SER:HB2	2	0.16	0.02	0.16
(4,808)	1:11:A:THR:HB	1:12:A:SER:HB3	2	0.16	0.02	0.16
(1,289)	1:40:A:ASN:H	1:67:A:LYS:HG2	2	0.15	0.02	0.15
(4,270)	1:40:A:ASN:H	1:67:A:LYS:HG2	2	0.15	0.02	0.15
(1,888)	1:33:A:CYS:HB3	1:34:A:ALA:H	2	0.15	0.03	0.15
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB1	2	0.15	0.0	0.15
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB2	2	0.15	0.0	0.15
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB3	2	0.15	0.0	0.15
(4,380)	1:6:A:LYS:HB2	1:7:A:GLY:H	2	0.15	0.0	0.15
(4,380)	1:6:A:LYS:HB3	1:7:A:GLY:H	2	0.15	0.0	0.15
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB1	2	0.15	0.0	0.15
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB2	2	0.15	0.0	0.15
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB3	2	0.15	0.0	0.15
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG21	2	0.13	0.03	0.13
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG22	2	0.13	0.03	0.13
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG23	2	0.13	0.03	0.13
(1,493)	1:47:A:LYS:H	1:49:A:GLY:HA2	2	0.13	0.01	0.13
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG21	2	0.13	0.03	0.13
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG22	2	0.13	0.03	0.13
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG23	2	0.13	0.03	0.13
(4,450)	1:47:A:LYS:H	1:49:A:GLY:HA2	2	0.13	0.01	0.13
(1,309)	1:9:A:LYS:HB2	1:10:A:CYS:H	2	0.12	0.01	0.12
(1,313)	1:10:A:CYS:H	1:28:A:GLY:H	2	0.12	0.02	0.12

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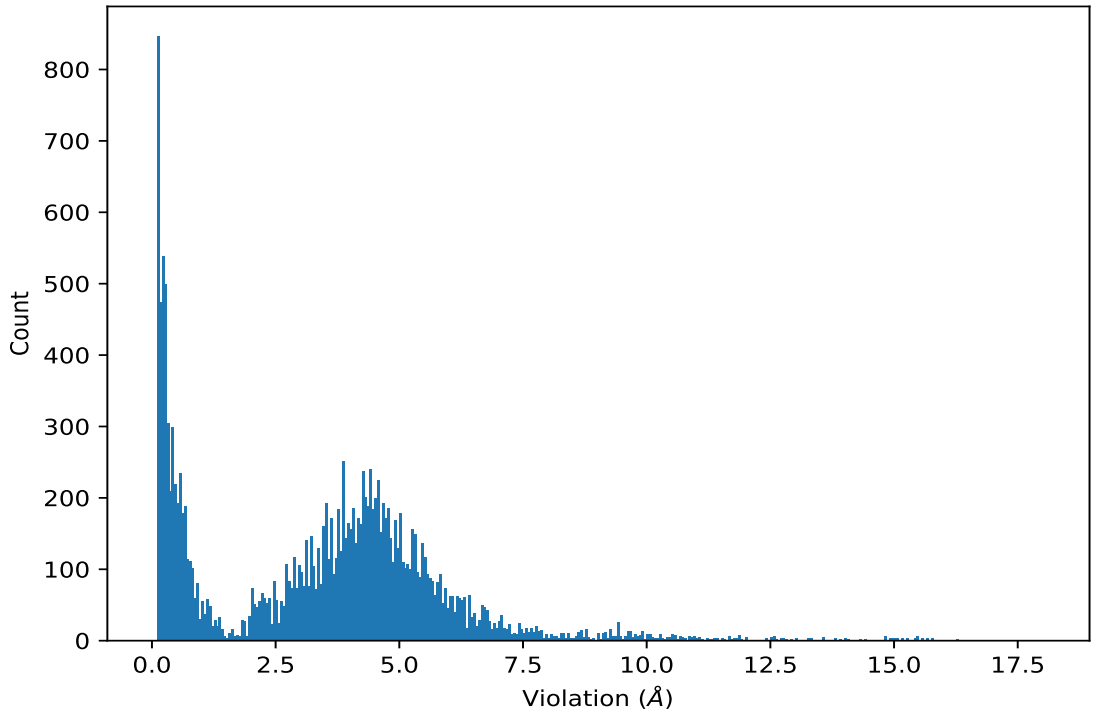
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(4,169)	1:46:A:CYS:H	1:47:A:LYS:HG2	2	0.12	0.02	0.12
(4,169)	1:46:A:CYS:H	1:47:A:LYS:HG3	2	0.12	0.02	0.12
(4,190)	1:45:A:GLY:H	1:47:A:LYS:HG2	2	0.12	0.02	0.12
(4,190)	1:45:A:GLY:H	1:47:A:LYS:HG3	2	0.12	0.02	0.12
(4,285)	1:9:A:LYS:HB2	1:10:A:CYS:H	2	0.12	0.01	0.12
(4,288)	1:10:A:CYS:H	1:28:A:GLY:H	2	0.12	0.02	0.12
(1,1111)	1:43:A:SER:HA	1:45:A:GLY:H	2	0.12	0.0	0.12
(4,914)	1:43:A:SER:HA	1:45:A:GLY:H	2	0.12	0.0	0.12
(1,833)	1:21:A:CYS:HB2	1:25:A:CYS:H	2	0.12	0.02	0.12
(4,720)	1:21:A:CYS:HB2	1:25:A:CYS:H	2	0.12	0.02	0.12
(1,558)	1:41:A:CYS:H	1:46:A:CYS:HA	2	0.12	0.0	0.12
(1,709)	1:55:A:PRO:HB3	1:58:A:CYS:H	2	0.12	0.0	0.12
(4,511)	1:41:A:CYS:H	1:46:A:CYS:HA	2	0.12	0.0	0.12
(4,628)	1:55:A:PRO:HB3	1:58:A:CYS:H	2	0.12	0.0	0.12
(4,420)	1:64:A:CYS:H	1:64:A:CYS:HB2	2	0.11	0.01	0.11
(1,93)	1:14:A:CYS:H	1:21:A:CYS:HA	2	0.11	0.0	0.11
(4,91)	1:14:A:CYS:H	1:21:A:CYS:HA	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	20	18.02
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	1	16.28
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	4	16.25
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	6	15.85
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	8	15.75
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	8	15.75
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	8	15.75
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	17	15.67
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	17	15.67
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	17	15.67
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	19	15.59
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	10	15.56
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	10	15.56
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	10	15.56
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	3	15.48
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	3	15.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	3	15.48
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	18	15.46
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	18	15.46
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	18	15.46
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	11	15.43
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	11	15.43
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	11	15.43
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	20	15.28
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	20	15.28
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	20	15.28
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	15	15.21
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	16	15.15
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	16	15.15
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	16	15.15
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	12	15.07
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	12	15.07
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	12	15.07
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	13	15.02
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	13	15.02
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	13	15.02
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	2	14.98
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	2	14.98
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	2	14.98
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	19	14.94
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	19	14.94
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	19	14.94
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	5	14.83
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	5	14.83
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	5	14.83
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	4	14.8
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	4	14.8
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	4	14.8
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	3	14.79
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	6	14.42
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	6	14.42
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	15	14.34
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	15	14.34
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	4	14.06
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	4	14.06
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	9	14.01
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	9	14.01
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	9	14.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	18	13.95
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	18	13.95
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	6	13.84
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	6	13.84
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	6	13.84
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	20	13.59
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	20	13.59
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	1	13.58
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	1	13.58
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	1	13.58
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	17	13.33
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	17	13.33
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	17	13.32
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	6	13.3
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	20	13.28
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	20	13.28
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	5	13.25
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	11	13.03
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	15	13.01
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	15	13.01
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	15	13.01
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	14	12.97
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	1	12.9
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	1	12.9
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	15	12.83
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	15	12.83
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	15	12.78
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	15	12.78
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	4	12.75
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	4	12.75
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	11	12.71
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	11	12.71
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	12	12.71
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	12	12.71
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	4	12.63
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	4	12.63
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	3	12.58
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	3	12.58
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	19	12.57
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	19	12.57
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	1	12.55
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	1	12.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	14	12.53
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	14	12.53
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	14	12.53
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	15	12.5
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	15	12.5
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	12	12.44
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	5	12.43
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	5	12.43
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	18	12.29
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	15	12.14
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	6	12.05
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	15	12.04
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	15	12.04
(1,809)	1:32:A:THR:HG21	1:40:A:ASN:HB3	7	12.0
(1,809)	1:32:A:THR:HG22	1:40:A:ASN:HB3	7	12.0
(1,809)	1:32:A:THR:HG23	1:40:A:ASN:HB3	7	12.0
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	14	11.93
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	14	11.93
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	1	11.89
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	1	11.89
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	15	11.88
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	15	11.88
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	19	11.88
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	19	11.88
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	6	11.86
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	6	11.86
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	15	11.83
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	6	11.82
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	6	11.82
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	20	11.77
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	20	11.77
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	19	11.75
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	19	11.75
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	12	11.72
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	12	11.72
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	7	11.68
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	7	11.68
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	5	11.67
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	5	11.67
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	6	11.66
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	6	11.66
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	4	11.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	4	11.59
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	5	11.51
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	5	11.51
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	14	11.5
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	14	11.5
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	10	11.48
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	7	11.45
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	7	11.45
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	3	11.4
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	20	11.37
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	20	11.37
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	11	11.37
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	11	11.37
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	5	11.34
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	5	11.34
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	6	11.29
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	6	11.29
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	3	11.24
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	3	11.24
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	9	11.24
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	9	11.24
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	12	11.11
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	13	11.11
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	12	11.06
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	12	11.06
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	12	11.06
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	12	11.06
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	13	11.05
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	12	11.02
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	12	11.02
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	12	11.01
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	12	11.01
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	7	10.99
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	6	10.98
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	6	10.98
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	6	10.98
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	13	10.98
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	13	10.98
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	15	10.92
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	15	10.92
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	15	10.92
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	14	10.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	14	10.92
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	3	10.89
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	3	10.89
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	13	10.87
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	13	10.87
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	6	10.87
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	6	10.87
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	6	10.87
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	5	10.79
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	5	10.79
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	4	10.78
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	15	10.72
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	15	10.72
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	15	10.72
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	6	10.72
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	6	10.72
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	16	10.7
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	16	10.7
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	1	10.68
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	14	10.67
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	19	10.66
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	19	10.66
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	10	10.64
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	10	10.64
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	19	10.6
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	19	10.6
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	19	10.6
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	15	10.57
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	15	10.57
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	16	10.56
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	16	10.56
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	5	10.56
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	6	10.53
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	6	10.53
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	2	10.52
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	2	10.5
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	2	10.5
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	2	10.5
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	2	10.5
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	1	10.5
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	1	10.5
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	10	10.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	10	10.48
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	2	10.47
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	19	10.46
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	19	10.46
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	5	10.45
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	14	10.41
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	14	10.41
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	2	10.41
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	2	10.41
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	8	10.37
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	8	10.37
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	17	10.32
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	17	10.32
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	14	10.31
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	14	10.31
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	8	10.29
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	15	10.28
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	15	10.28
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	6	10.26
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	6	10.26
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	4	10.26
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	4	10.26
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	11	10.26
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	11	10.26
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	20	10.24
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	7	10.23
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	7	10.23
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	7	10.23
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	10	10.2
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	2	10.19
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	12	10.17
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	12	10.16
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	17	10.14
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	17	10.14
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	8	10.13
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	14	10.12
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	14	10.12
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	6	10.1
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	6	10.1
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	6	10.1
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	4	10.09
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	13	10.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	14	10.07
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	14	10.07
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	3	10.06
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	5	10.05
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	5	10.03
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	5	10.03
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	5	10.03
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	5	10.03
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	2	10.02
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	3	10.01
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	3	10.01
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	18	10.01
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	18	10.01
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	12	9.96
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	12	9.96
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	12	9.95
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	9	9.95
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	4	9.94
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	5	9.94
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	5	9.94
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	9	9.93
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	9	9.93
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	9	9.93
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	4	9.93
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	4	9.93
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	9	9.93
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	9	9.93
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	10	9.9
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	3	9.89
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	15	9.88
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	15	9.88
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	15	9.88
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	3	9.86
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	3	9.86
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	3	9.86
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	3	9.86
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	4	9.85
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	4	9.85
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	20	9.83
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	3	9.81
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	3	9.81
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	10	9.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	10	9.81
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	20	9.77
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	20	9.77
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	19	9.76
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	19	9.76
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	4	9.75
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	1	9.75
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	1	9.75
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	3	9.75
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	3	9.75
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	14	9.72
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	20	9.71
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	20	9.71
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	20	9.71
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	12	9.71
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	18	9.7
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	18	9.7
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	1	9.69
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	1	9.69
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	12	9.69
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	12	9.69
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	12	9.69
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	16	9.66
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	3	9.66
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	3	9.66
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	3	9.66
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	6	9.66
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	6	9.66
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	16	9.65
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	19	9.64
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	19	9.64
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	19	9.64
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	14	9.64
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	14	9.64
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	11	9.64
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	11	9.64
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	18	9.63
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	3	9.62
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	3	9.62
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	3	9.62
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	15	9.61
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	15	9.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	18	9.6
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	20	9.59
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	20	9.59
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	6	9.57
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	12	9.56
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	12	9.56
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	12	9.56
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	19	9.53
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	19	9.53
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	14	9.49
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	14	9.49
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	14	9.49
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	14	9.48
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	14	9.48
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	13	9.48
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	13	9.48
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	5	9.45
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	5	9.45
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	5	9.45
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	14	9.45
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	14	9.45
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	14	9.45
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	11	9.45
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	11	9.45
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	11	9.45
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	5	9.44
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	5	9.44
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	5	9.44
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	20	9.44
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	20	9.44
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	20	9.44
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	16	9.43
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	16	9.43
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	8	9.43
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	8	9.43
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	13	9.41
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	13	9.41
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	2	9.4
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	2	9.4
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	19	9.4
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	19	9.4
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	19	9.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	1	9.37
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	1	9.37
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	1	9.36
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	1	9.35
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	1	9.35
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	1	9.35
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	14	9.34
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	14	9.34
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	14	9.34
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	1	9.33
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	1	9.33
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	1	9.33
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	5	9.32
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	20	9.29
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	20	9.29
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	18	9.28
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	18	9.28
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	1	9.28
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	2	9.27
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	2	9.27
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	1	9.27
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	1	9.27
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	5	9.26
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	5	9.26
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	1	9.26
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	1	9.26
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	1	9.26
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	10	9.25
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	10	9.25
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	5	9.23
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	19	9.21
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	19	9.21
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	15	9.19
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	15	9.19
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	15	9.19
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	16	9.18
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	16	9.18
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	8	9.17
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	8	9.17
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	19	9.16
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	20	9.16
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	20	9.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	7	9.15
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	7	9.15
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	19	9.14
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	3	9.14
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	3	9.14
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	3	9.14
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	4	9.12
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	4	9.12
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	4	9.12
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	4	9.1
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	4	9.1
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	4	9.1
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	11	9.09
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	11	9.09
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	4	9.04
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	4	9.04
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	4	9.04
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	12	9.03
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	12	9.03
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	12	9.03
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	12	9.03
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	18	9.03
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	20	9.01
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	8	9.0
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	19	8.96
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	17	8.93
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	17	8.93
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	1	8.9
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	17	8.85
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	17	8.85
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	4	8.83
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	4	8.83
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	1	8.81
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	9	8.81
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	9	8.81
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	4	8.79
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	4	8.79
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	17	8.78
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	8	8.76
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	8	8.76
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	8	8.76
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	8	8.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	10	8.76
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	10	8.76
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	10	8.76
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	10	8.76
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	18	8.76
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	18	8.76
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	18	8.75
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	18	8.75
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	7	8.75
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	18	8.73
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	14	8.72
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	20	8.71
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	20	8.71
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	20	8.71
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	8	8.7
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	8	8.7
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	19	8.7
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	8	8.69
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	3	8.68
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	3	8.68
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	3	8.68
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	3	8.68
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	20	8.67
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	20	8.67
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	20	8.67
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	3	8.67
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	3	8.67
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	10	8.67
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	18	8.65
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	16	8.64
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	16	8.64
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	13	8.63
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	5	8.63
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	5	8.63
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	5	8.63
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	2	8.62
(1,210)	1:37:A:LYS:HD2	1:58:A:CYS:H	13	8.62
(1,210)	1:37:A:LYS:HD3	1:58:A:CYS:H	13	8.62
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	2	8.6
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	2	8.6
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	2	8.6
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	16	8.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	16	8.58
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	16	8.58
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	16	8.58
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	6	8.56
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	2	8.56
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	3	8.52
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	9	8.51
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	11	8.5
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	11	8.5
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	8	8.48
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	8	8.48
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	20	8.48
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	20	8.48
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	16	8.45
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	16	8.45
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	16	8.44
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	6	8.44
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	6	8.43
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	6	8.43
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	6	8.43
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	9	8.42
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	9	8.42
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	8	8.41
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	19	8.38
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	19	8.38
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	4	8.38
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	4	8.34
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	3	8.34
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	12	8.34
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	12	8.34
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	12	8.34
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	15	8.33
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	7	8.32
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	7	8.32
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	18	8.32
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	8	8.31
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	2	8.28
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	2	8.28
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	12	8.28
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	11	8.26
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	20	8.26
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	20	8.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	20	8.26
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	20	8.26
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	12	8.26
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	12	8.26
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	12	8.26
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	16	8.24
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	16	8.24
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	12	8.23
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	13	8.2
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	13	8.2
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	10	8.18
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	10	8.18
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	19	8.15
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	17	8.15
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	8	8.14
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	8	8.14
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	13	8.11
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	13	8.11
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	8	8.11
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	8	8.11
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	8	8.11
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	11	8.09
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	11	8.09
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	17	8.09
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	17	8.09
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	9	8.07
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	18	8.07
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	17	8.05
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	17	8.05
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	5	8.05
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	9	8.03
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	2	8.03
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	10	8.01
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	1	8.01
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	5	7.99
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	14	7.98
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	9	7.98
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	3	7.98
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	3	7.98
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	3	7.98
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	3	7.96
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	10	7.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	10	7.95
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	18	7.94
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	15	7.93
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	1	7.92
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	17	7.88
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	1	7.88
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	1	7.88
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	1	7.88
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	8	7.87
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	8	7.87
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	8	7.87
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	4	7.87
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	4	7.87
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	4	7.87
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	7	7.86
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	7	7.86
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	14	7.86
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	14	7.86
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	14	7.86
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	12	7.85
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	2	7.84
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	2	7.84
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	2	7.84
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	10	7.84
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	11	7.83
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	13	7.82
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	13	7.82
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	13	7.82
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	13	7.82
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	8	7.81
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	8	7.81
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	13	7.81
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	10	7.8
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	10	7.8
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	17	7.8
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	17	7.8
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	17	7.8
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	8	7.8
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	10	7.8
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	13	7.79
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	13	7.79
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	6	7.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	13	7.78
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	9	7.78
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	11	7.77
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	11	7.77
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	16	7.77
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	16	7.77
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	15	7.77
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	18	7.76
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	16	7.76
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	1	7.76
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	14	7.75
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	13	7.74
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	16	7.72
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	19	7.72
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	19	7.72
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	19	7.72
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	5	7.71
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	3	7.71
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	1	7.71
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	1	7.71
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	1	7.71
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	8	7.7
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	11	7.7
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	2	7.69
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	2	7.68
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	2	7.68
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	2	7.68
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	16	7.66
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	16	7.66
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	2	7.66
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	2	7.66
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	2	7.66
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	2	7.66
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	20	7.66
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	3	7.65
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	3	7.65
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	4	7.65
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	4	7.65
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	6	7.65
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	8	7.65
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	16	7.64
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	16	7.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	7	7.64
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	12	7.63
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	1	7.62
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	1	7.62
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	20	7.62
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	17	7.62
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	12	7.61
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	18	7.61
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	18	7.61
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	18	7.61
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	9	7.6
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	16	7.6
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	16	7.6
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	16	7.6
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	17	7.6
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	18	7.59
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	7	7.59
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	14	7.58
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	10	7.57
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	10	7.57
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	12	7.57
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	12	7.57
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	12	7.57
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	13	7.57
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	8	7.57
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	20	7.57
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	14	7.56
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	13	7.55
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	13	7.55
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	13	7.55
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	2	7.55
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	3	7.53
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	9	7.53
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	9	7.53
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	16	7.53
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	16	7.53
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	5	7.53
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	8	7.53
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	12	7.49
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	12	7.49
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	12	7.49
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	12	7.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	12	7.49
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	12	7.49
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	15	7.48
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	14	7.48
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	14	7.48
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	17	7.48
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	8	7.46
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	8	7.46
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	8	7.46
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	1	7.45
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	20	7.45
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	20	7.45
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	10	7.44
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	14	7.44
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	14	7.44
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	6	7.44
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	6	7.44
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	6	7.44
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	6	7.44
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	6	7.43
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	6	7.43
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	16	7.42
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	3	7.42
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	3	7.42
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	17	7.42
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	17	7.42
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	1	7.42
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	19	7.41
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	19	7.41
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	5	7.41
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	15	7.4
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	15	7.4
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	17	7.4
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	11	7.4
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	17	7.4
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	17	7.4
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	17	7.4
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	11	7.39
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	11	7.39
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	19	7.39
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	19	7.39
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	19	7.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	5	7.38
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	11	7.36
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	11	7.36
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	11	7.36
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	20	7.35
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	15	7.35
(1,521)	1:37:A:LYS:HD2	1:58:A:CYS:HB2	13	7.34
(1,521)	1:37:A:LYS:HD3	1:58:A:CYS:HB2	13	7.34
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	6	7.33
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	11	7.31
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	11	7.31
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	2	7.31
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	2	7.31
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	2	7.31
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	16	7.3
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	15	7.29
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	11	7.29
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	15	7.28
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	10	7.27
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	12	7.27
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	8	7.26
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	19	7.25
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	19	7.25
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	6	7.24
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	6	7.24
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	13	7.24
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	13	7.24
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	13	7.24
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	3	7.24
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	3	7.24
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	11	7.23
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	11	7.23
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	11	7.23
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	11	7.23
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	5	7.23
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	16	7.22
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	16	7.22
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	16	7.22
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	4	7.22
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	17	7.21
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	7	7.21
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	10	7.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	20	7.21
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	13	7.2
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	9	7.2
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	9	7.2
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	13	7.18
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	3	7.18
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	16	7.18
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	9	7.17
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	9	7.17
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	8	7.17
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	4	7.17
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	13	7.16
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	15	7.15
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	8	7.15
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	13	7.15
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	18	7.15
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	18	7.15
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	7.15
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	7.15
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	5	7.15
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	11	7.14
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	4	7.14
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	17	7.14
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	1	7.13
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	1	7.13
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	1	7.13
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	1	7.13
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	6	7.13
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	4	7.13
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	12	7.12
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	12	7.12
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	12	7.12
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	5	7.12
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	13	7.11
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	5	7.11
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	5	7.11
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	16	7.11
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	15	7.1
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	15	7.1
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	18	7.1
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	16	7.1
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	14	7.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	11	7.09
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	9	7.09
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	4	7.09
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	14	7.09
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	15	7.09
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	7	7.08
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	7	7.08
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	16	7.08
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	16	7.08
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	16	7.08
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	4	7.08
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	4	7.08
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	10	7.08
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	10	7.08
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	10	7.08
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	2	7.08
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	11	7.08
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	12	7.08
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	10	7.08
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	12	7.08
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	2	7.07
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	7	7.07
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	7	7.07
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	12	7.07
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	15	7.06
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	5	7.06
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	5	7.06
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	14	7.06
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	20	7.06
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	20	7.06
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	20	7.06
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	20	7.05
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	18	7.05
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	12	7.05
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	12	7.05
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	12	7.05
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	12	7.05
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	12	7.05
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	12	7.05
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	12	7.05
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	12	7.05
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	12	7.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	18	7.04
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	2	7.04
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	18	7.04
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	8	7.04
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	7	7.03
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	5	7.03
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	5	7.03
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	16	7.02
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	9	7.01
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	9	7.01
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	19	7.01
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	12	7.0
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	13	7.0
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	13	7.0
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	1	7.0
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	7	7.0
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	20	7.0
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	12	6.99
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	10	6.99
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	3	6.99
(1,999)	1:6:A:LYS:HG2	1:31:A:CYS:H	8	6.98
(1,999)	1:6:A:LYS:HG3	1:31:A:CYS:H	8	6.98
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	16	6.98
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	16	6.98
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	16	6.98
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	4	6.98
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	17	6.96
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	17	6.96
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	6	6.96
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	5	6.96
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	10	6.95
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	5	6.95
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	5	6.95
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	5	6.95
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	11	6.94
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	16	6.94
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	14	6.94
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	14	6.94
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	8	6.94
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	12	6.94
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	8	6.94
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	3	6.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	3	6.93
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	19	6.93
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	19	6.93
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	15	6.93
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	15	6.93
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	3	6.93
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	2	6.92
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	9	6.92
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	8	6.91
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	8	6.91
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	16	6.9
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	4	6.9
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	4	6.9
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	4	6.9
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	3	6.9
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	18	6.9
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	8	6.89
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	8	6.89
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	12	6.89
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	9	6.88
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	10	6.88
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	10	6.88
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	10	6.88
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	18	6.87
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	18	6.87
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	1	6.87
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	7	6.87
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	10	6.87
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	16	6.87
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	20	6.86
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	9	6.86
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	6	6.86
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	17	6.85
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	17	6.85
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	3	6.85
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	3	6.85
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	9	6.84
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	11	6.83
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	7	6.83
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	7	6.83
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	10	6.83
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	11	6.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	19	6.83
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	13	6.83
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	6	6.82
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	6	6.82
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	11	6.82
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	16	6.82
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	2	6.82
(1,476)	1:36:A:CYS:HA	1:40:A:ASN:HD21	4	6.82
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	16	6.82
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	16	6.82
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	13	6.81
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	18	6.81
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	18	6.81
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	18	6.81
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	18	6.81
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	4	6.81
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	7	6.81
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	7	6.8
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	7	6.8
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	11	6.8
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	11	6.8
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	16	6.8
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	16	6.8
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	16	6.8
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	14	6.8
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	14	6.8
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	4	6.79
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	11	6.79
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	5	6.79
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	4	6.79
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	1	6.78
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	12	6.78
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	4	6.78
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	11	6.78
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	11	6.78
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	11	6.78
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	9	6.78
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	11	6.78
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	4	6.77
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	5	6.77
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	5	6.77
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	17	6.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	3	6.77
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	2	6.77
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	2	6.77
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	15	6.77
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	8	6.76
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	8	6.76
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	17	6.76
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	17	6.76
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	7	6.76
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	7	6.76
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	7	6.76
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	15	6.76
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	15	6.76
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	15	6.76
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	9	6.75
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	1	6.75
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	1	6.75
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	1	6.75
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	1	6.74
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	5	6.73
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	6	6.73
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	6	6.73
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	1	6.73
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	1	6.73
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	20	6.73
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	20	6.73
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	9	6.73
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	9	6.73
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	9	6.73
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	9	6.73
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	9	6.73
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	9	6.73
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	14	6.73
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	1	6.73
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	5	6.72
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	2	6.72
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	2	6.72
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	18	6.72
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	14	6.72
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	14	6.71
(1,953)	1:6:A:LYS:HG2	1:28:A:GLY:H	9	6.71
(1,953)	1:6:A:LYS:HG3	1:28:A:GLY:H	9	6.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	5	6.71
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	5	6.71
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	5	6.71
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	7	6.71
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	7	6.71
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	10	6.71
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	8	6.7
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	8	6.7
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	8	6.7
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	20	6.7
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	3	6.7
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	3	6.7
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	3	6.7
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	17	6.7
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	17	6.7
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	17	6.7
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	14	6.7
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	11	6.7
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	11	6.7
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	11	6.7
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	11	6.7
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	11	6.7
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	11	6.7
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	12	6.69
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	18	6.69
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	18	6.69
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	6	6.69
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	8	6.69
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	6	6.69
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	6	6.69
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	6	6.69
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	5	6.69
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	8	6.69
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	2	6.69
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	6	6.68
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	17	6.68
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	4	6.68
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	16	6.68
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	19	6.68
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	20	6.68
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	20	6.68
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	20	6.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	7	6.68
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	11	6.68
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	11	6.68
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	11	6.67
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	10	6.67
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	14	6.67
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	9	6.67
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	8	6.67
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	8	6.67
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	8	6.67
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	5	6.67
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	18	6.67
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	18	6.67
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	13	6.66
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	13	6.66
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	13	6.66
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	2	6.66
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	2	6.66
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	2	6.66
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	19	6.66
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	1	6.66
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	18	6.66
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	19	6.66
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	10	6.65
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	2	6.65
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	17	6.65
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	10	6.65
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	10	6.65
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	10	6.65
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	19	6.65
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	3	6.65
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	6	6.64
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	6	6.64
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	6	6.64
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	13	6.64
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	11	6.63
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	11	6.63
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	11	6.63
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	16	6.63
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	17	6.63
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	17	6.63
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	5	6.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	5	6.62
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	5	6.62
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	4	6.62
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	4	6.62
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	9	6.62
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	9	6.62
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	9	6.62
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	14	6.62
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	14	6.62
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	14	6.62
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	15	6.62
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	10	6.62
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	10	6.62
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	16	6.61
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	13	6.61
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	13	6.61
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	13	6.61
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	13	6.61
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	16	6.6
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	4	6.6
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	12	6.6
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	10	6.6
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	7	6.59
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	13	6.59
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	13	6.59
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	13	6.59
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	5	6.58
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	12	6.58
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	15	6.58
(1,826)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	2	6.58
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	7	6.58
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	10	6.57
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	1	6.57
(1,761)	1:38:A:THR:H	1:55:A:PRO:HG3	2	6.57
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	6	6.57
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	9	6.56
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	17	6.56
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	6	6.56
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	12	6.56
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	9	6.55
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	9	6.55
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	9	6.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	15	6.55
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	12	6.54
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	18	6.54
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	3	6.53
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	5	6.53
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	1	6.53
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	5	6.53
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	2	6.53
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	14	6.52
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	10	6.52
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	2	6.52
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	2	6.52
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	2	6.52
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	2	6.52
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	2	6.52
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	6.52
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	20	6.52
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	2	6.51
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	2	6.51
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	2	6.51
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	20	6.51
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	4	6.51
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	4	6.51
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	20	6.51
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	17	6.51
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	17	6.51
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	6	6.5
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	17	6.5
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	17	6.5
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	17	6.5
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	17	6.5
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	1	6.5
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	1	6.5
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	1	6.5
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	12	6.5
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	10	6.49
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	10	6.49
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	10	6.49
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	20	6.49
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	11	6.49
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	16	6.48
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	18	6.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	8	6.48
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	8	6.48
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	13	6.48
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	13	6.48
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	13	6.48
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	20	6.48
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	19	6.48
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	18	6.47
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	4	6.47
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	4	6.47
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	12	6.47
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	1	6.47
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	14	6.47
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	15	6.47
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	18	6.47
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	3	6.46
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	3	6.46
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	3	6.46
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	8	6.46
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	20	6.46
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	10	6.46
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	10	6.46
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	4	6.46
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	11	6.46
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	2	6.45
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	13	6.45
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	2	6.44
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	19	6.44
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	13	6.44
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	20	6.44
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	5	6.44
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	8	6.44
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	8	6.44
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	8	6.44
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	20	6.44
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	20	6.44
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	6	6.44
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	11	6.44
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	11	6.44
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	11	6.44
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	14	6.43
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	14	6.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	9	6.43
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	12	6.43
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	12	6.43
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	19	6.43
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	6	6.43
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	6	6.43
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	14	6.43
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	14	6.43
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	14	6.43
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	20	6.43
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	20	6.43
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	3	6.42
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	6	6.42
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	7	6.42
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	11	6.42
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	11	6.42
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	11	6.42
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	11	6.42
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	20	6.42
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	10	6.42
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	11	6.42
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	2	6.42
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	2	6.42
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	16	6.42
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	2	6.41
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	2	6.41
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	2	6.41
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	2	6.41
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	7	6.41
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	7	6.41
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	7	6.41
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	7	6.41
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	7	6.41
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	7	6.41
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	13	6.41
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	13	6.41
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	14	6.41
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	19	6.41
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	14	6.4
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	1	6.4
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	16	6.4
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	16	6.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	16	6.4
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	16	6.4
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	13	6.4
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	10	6.4
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	16	6.4
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	7	6.4
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	19	6.39
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	19	6.39
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	6	6.39
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	10	6.39
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	16	6.38
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	16	6.38
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	16	6.38
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	11	6.37
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	15	6.37
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	8	6.37
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	4	6.36
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	8	6.36
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	4	6.36
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	16	6.36
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	11	6.36
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	18	6.36
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	18	6.36
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	8	6.36
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	17	6.35
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	13	6.35
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	7	6.35
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	6	6.35
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	6	6.35
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	19	6.35
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	19	6.35
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	19	6.35
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	4	6.35
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	5	6.35
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	16	6.35
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	6	6.35
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	3	6.34
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	13	6.34
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	16	6.34
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	8	6.33
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	17	6.33
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	3	6.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	14	6.33
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	14	6.33
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	14	6.33
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	14	6.33
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	2	6.33
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	17	6.33
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	19	6.32
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	19	6.32
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	19	6.32
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	9	6.32
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	20	6.32
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	1	6.32
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	1	6.32
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	17	6.32
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	3	6.32
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	3	6.32
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	3	6.32
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	3	6.32
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	20	6.32
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	20	6.32
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	20	6.32
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	10	6.32
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	10	6.32
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	13	6.32
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	1	6.32
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	20	6.31
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	20	6.31
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	20	6.31
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	15	6.31
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	17	6.31
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	17	6.31
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	17	6.31
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	11	6.31
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	11	6.31
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	11	6.31
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	11	6.31
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	11	6.31
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	11	6.31
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	11	6.31
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	11	6.31
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	11	6.31
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	6	6.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	6	6.31
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	2	6.3
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	10	6.3
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	19	6.3
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	19	6.3
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	15	6.29
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	15	6.29
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	5	6.29
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	20	6.29
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	11	6.29
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	11	6.29
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	8	6.29
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	8	6.29
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	19	6.29
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	4	6.29
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	4	6.29
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	11	6.29
(1,1155)	1:37:A:LYS:HG2	1:55:A:PRO:HA	13	6.28
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	6	6.28
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	6	6.28
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	10	6.28
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	1	6.28
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	10	6.28
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	10	6.28
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	12	6.28
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	12	6.28
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	16	6.27
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	16	6.27
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	16	6.27
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	7	6.27
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	16	6.27
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	2	6.27
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	8	6.27
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	9	6.27
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	12	6.27
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	16	6.27
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	5	6.27
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	5	6.27
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	5	6.27
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	11	6.27
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	18	6.27
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	3	6.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	3	6.27
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	9	6.27
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	5	6.26
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	5	6.26
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	9	6.26
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	17	6.26
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	2	6.26
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	11	6.26
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	2	6.25
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	2	6.25
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	11	6.25
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	11	6.25
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	13	6.25
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	7	6.25
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	11	6.25
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	14	6.25
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	13	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	7	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	7	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	9	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	9	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	13	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	13	6.24
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	12	6.24
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	12	6.24
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	12	6.24
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	12	6.24
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	12	6.24
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	12	6.24
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	12	6.24
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	12	6.24
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	12	6.24
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	15	6.24
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	15	6.24
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	14	6.23
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	14	6.23
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	11	6.23
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	11	6.23
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	11	6.23
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	9	6.23
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	13	6.23
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	13	6.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	7	6.22
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	14	6.22
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	18	6.22
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	18	6.22
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	3	6.22
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	19	6.22
(1,1165)	1:14:A:CYS:H	1:20:A:GLN:HB3	11	6.21
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	19	6.21
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	15	6.21
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	11	6.21
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	11	6.21
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	11	6.21
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	11	6.21
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	11	6.21
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	11	6.21
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	2	6.21
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	2	6.21
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	19	6.21
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	17	6.21
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	13	6.21
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	13	6.21
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	13	6.21
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	17	6.21
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	17	6.21
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	17	6.21
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	1	6.2
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	6	6.2
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	3	6.2
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	9	6.2
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	7	6.2
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	3	6.2
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	12	6.2
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	3	6.2
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	3	6.2
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	6	6.19
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	15	6.19
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	15	6.19
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	15	6.19
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	17	6.19
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	17	6.19
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	14	6.19
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	4	6.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	15	6.19
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	5	6.19
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	5	6.19
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	12	6.19
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	12	6.19
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	5	6.19
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	5	6.19
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	8	6.18
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	9	6.18
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	5	6.18
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	6	6.18
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	20	6.18
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	6	6.18
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	17	6.18
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	1	6.18
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	1	6.18
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	6	6.18
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	6	6.18
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	7	6.17
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	1	6.17
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	11	6.17
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	8	6.17
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	8	6.17
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	6	6.17
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	2	6.17
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	12	6.17
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	12	6.17
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	6.17
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	9	6.16
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	9	6.16
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	1	6.16
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	7	6.16
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	6	6.16
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	7	6.16
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	7	6.16
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	20	6.16
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	19	6.16
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	19	6.16
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	12	6.16
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	16	6.16
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	16	6.16
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	16	6.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	1	6.16
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	1	6.16
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	1	6.16
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	1	6.16
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	1	6.16
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	1	6.16
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	4	6.16
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	4	6.16
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	19	6.16
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	5	6.15
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	5	6.15
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	4	6.15
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	17	6.14
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	17	6.14
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	17	6.14
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	11	6.14
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	16	6.14
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	1	6.14
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	7	6.14
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	7	6.14
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	12	6.14
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	16	6.13
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	16	6.13
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	20	6.13
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	6.13
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	6.13
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	9	6.13
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	9	6.13
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	10	6.12
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	10	6.12
(1,1053)	1:49:A:GLY:HA3	1:50:A:LYS:HG3	4	6.12
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	14	6.12
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	15	6.12
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	15	6.12
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	15	6.12
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	15	6.12
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	15	6.12
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	15	6.12
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	18	6.12
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	18	6.12
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	18	6.12
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	9	6.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	8	6.12
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	7	6.12
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	7	6.12
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	18	6.11
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	17	6.11
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	19	6.11
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	5	6.11
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	18	6.11
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	1	6.11
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	12	6.11
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	17	6.1
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	17	6.1
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	17	6.1
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	1	6.1
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	8	6.1
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	8	6.1
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	8	6.1
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	17	6.1
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	9	6.1
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	9	6.1
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	3	6.1
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	3	6.1
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	1	6.1
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	1	6.1
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	18	6.09
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	18	6.09
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	18	6.09
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	11	6.09
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	11	6.09
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	12	6.09
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	16	6.09
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	12	6.09
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	12	6.09
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	13	6.09
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	13	6.09
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	10	6.09
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	10	6.09
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	10	6.09
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	19	6.09
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	2	6.09
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	5	6.09
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	11	6.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	11	6.08
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	12	6.08
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	12	6.08
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	12	6.08
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	13	6.08
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	13	6.08
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	13	6.08
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	18	6.08
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	18	6.08
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	13	6.07
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	15	6.07
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	15	6.07
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	3	6.07
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	14	6.07
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	1	6.07
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	8	6.07
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	8	6.07
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	8	6.07
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	7	6.07
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	8	6.07
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	8	6.07
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	3	6.07
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	1	6.07
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	1	6.06
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	1	6.06
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	1	6.06
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	13	6.06
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	18	6.06
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	18	6.06
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	18	6.06
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	15	6.06
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	19	6.05
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	15	6.05
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	13	6.05
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	7	6.05
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	7	6.05
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	10	6.05
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	17	6.05
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	15	6.05
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	15	6.05
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	13	6.05
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	11	6.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	8	6.04
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	3	6.04
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	7	6.04
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	15	6.04
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	8	6.04
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	8	6.04
(1,1166)	1:14:A:CYS:H	1:20:A:GLN:HG2	19	6.03
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	2	6.03
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	2	6.03
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	13	6.03
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	10	6.03
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	10	6.03
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	10	6.03
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	10	6.03
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	10	6.03
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	10	6.03
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	16	6.03
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	4	6.02
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	20	6.02
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	20	6.02
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	10	6.01
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	10	6.01
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	4	6.01
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	4	6.01
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	1	6.01
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	2	6.01
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	9	6.01
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	9	6.01
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	9	6.01
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	15	6.01
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	15	6.01
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	19	6.01
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	19	6.01
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	19	6.01
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	3	6.01
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	3	6.01
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	3	6.01
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	3	6.01
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	20	6.0
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	20	6.0
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	3	6.0
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	6	6.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	6.0
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	18	6.0
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	12	6.0
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	3	6.0
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	3	6.0
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	3	6.0
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	10	6.0
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	10	6.0
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	10	6.0
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	14	6.0
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	11	5.99
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	20	5.99
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	8	5.99
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	16	5.99
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	16	5.99
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	20	5.99
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	20	5.99
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	20	5.99
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	18	5.99
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	9	5.99
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	8	5.99
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	8	5.99
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	17	5.99
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	17	5.99
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	18	5.98
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	17	5.98
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	3	5.98
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	19	5.98
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	19	5.98
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	19	5.98
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	5	5.98
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	5	5.98
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	19	5.97
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	19	5.97
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	15	5.97
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	9	5.97
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	5	5.96
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	8	5.96
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	7	5.96
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	14	5.96
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	18	5.96
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	19	5.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	19	5.96
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	19	5.96
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	19	5.96
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	19	5.96
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	19	5.96
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	14	5.95
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	17	5.95
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	6	5.95
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	6	5.95
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	12	5.95
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	12	5.95
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	15	5.95
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	15	5.95
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	11	5.95
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	10	5.94
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	5.94
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	5.94
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	13	5.94
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	16	5.94
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	10	5.94
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	12	5.94
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	9	5.94
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	10	5.94
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	10	5.94
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	9	5.94
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	9	5.94
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	9	5.94
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	9	5.93
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	19	5.93
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	3	5.93
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	12	5.93
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	20	5.93
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	1	5.93
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	1	5.93
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	11	5.93
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	13	5.93
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	10	5.92
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	7	5.92
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	1	5.92
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	1	5.92
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	8	5.92
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	20	5.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	16	5.92
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	9	5.92
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	3	5.92
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	3	5.92
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	4	5.92
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	4	5.92
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	19	5.92
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	19	5.92
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	17	5.92
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	17	5.92
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	14	5.92
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	14	5.92
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	14	5.92
(1,647)	1:50:A:LYS:HG3	1:58:A:CYS:HA	20	5.91
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	8	5.91
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	16	5.91
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	16	5.91
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	14	5.91
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	14	5.9
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	18	5.9
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	2	5.9
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	14	5.9
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	14	5.9
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	14	5.9
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	14	5.9
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	15	5.9
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	18	5.9
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	14	5.9
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	14	5.9
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	10	5.9
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	13	5.9
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	13	5.9
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	18	5.9
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	18	5.9
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	11	5.9
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	11	5.9
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	15	5.9
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	15	5.9
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	15	5.9
(1,472)	1:38:A:THR:HB	1:40:A:ASN:HD21	17	5.9
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	1	5.9
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	1	5.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	1	5.9
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	6	5.9
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	6	5.9
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	6	5.9
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	11	5.89
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	10	5.89
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	10	5.89
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	10	5.89
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	14	5.89
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	14	5.89
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	14	5.89
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	14	5.89
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	17	5.89
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	17	5.89
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	15	5.89
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	7	5.89
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	10	5.89
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	5	5.89
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	5	5.89
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	5	5.89
(1,1035)	1:37:A:LYS:HG2	1:39:A:CYS:HB2	13	5.88
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	12	5.88
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	12	5.88
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	15	5.88
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	20	5.88
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	20	5.88
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	2	5.88
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	16	5.88
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	5.88
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	5.88
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	6	5.88
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	14	5.88
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	12	5.88
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	12	5.88
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	17	5.87
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	2	5.87
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	17	5.87
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	17	5.87
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	17	5.87
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	11	5.87
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	14	5.86
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	4	5.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	4	5.86
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	4	5.86
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	4	5.86
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	10	5.86
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	16	5.86
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	8	5.86
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	8	5.86
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	1	5.86
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	1	5.86
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	7	5.86
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	7	5.86
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	5	5.86
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	10	5.86
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	5	5.86
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	7	5.85
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	7	5.85
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	3	5.85
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	3	5.85
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	20	5.85
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	20	5.85
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	10	5.85
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	10	5.85
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	10	5.85
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	10	5.85
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	10	5.85
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	10	5.85
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	15	5.85
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	11	5.85
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	17	5.85
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	2	5.84
(1,716)	1:38:A:THR:HB	1:67:A:LYS:HD3	10	5.84
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	14	5.84
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	20	5.84
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	6	5.84
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	6	5.84
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	6	5.84
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	20	5.84
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	15	5.84
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	2	5.84
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	2	5.84
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	2	5.84
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	11	5.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	11	5.84
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	11	5.84
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	17	5.83
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	20	5.83
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	14	5.83
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	14	5.83
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	9	5.83
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	18	5.83
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	18	5.83
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	18	5.83
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	14	5.83
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	14	5.83
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	18	5.83
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	18	5.83
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	18	5.83
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	10	5.83
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	16	5.83
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	16	5.83
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	13	5.83
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	13	5.83
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	3	5.83
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	18	5.82
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	17	5.82
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	3	5.82
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	19	5.82
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	19	5.82
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	19	5.82
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	19	5.82
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	19	5.82
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	19	5.82
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	8	5.82
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	8	5.82
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	18	5.82
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	18	5.82
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	10	5.82
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	10	5.82
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	15	5.82
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	15	5.82
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	9	5.82
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	11	5.81
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	11	5.81
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	11	5.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	11	5.81
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	6	5.81
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	6	5.81
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	13	5.81
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	13	5.81
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	15	5.81
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	1	5.81
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	1	5.81
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	1	5.81
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	1	5.81
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	1	5.81
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	1	5.81
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	1	5.81
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	1	5.81
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	1	5.81
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	4	5.81
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	17	5.81
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	12	5.81
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	12	5.81
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	1	5.81
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	16	5.81
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	16	5.81
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	16	5.81
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	7	5.8
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	7	5.8
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	7	5.8
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	2	5.8
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	12	5.8
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	2	5.8
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	3	5.8
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	5	5.8
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	9	5.79
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	9	5.79
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	17	5.79
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	17	5.79
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	17	5.79
(1,737)	1:38:A:THR:HB	1:67:A:LYS:HD2	20	5.79
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	15	5.79
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	7	5.79
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	18	5.79
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	18	5.79
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	15	5.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	15	5.79
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	15	5.79
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	11	5.78
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	11	5.78
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	14	5.78
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	14	5.78
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	14	5.78
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	13	5.78
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	13	5.78
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	3	5.78
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	10	5.77
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	10	5.77
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	10	5.77
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	7	5.77
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	20	5.77
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	20	5.77
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	20	5.77
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	5	5.77
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	5	5.77
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	5	5.77
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	5	5.77
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	8	5.77
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	8	5.77
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	8	5.77
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	9	5.77
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	9	5.77
(1,297)	1:38:A:THR:HB	1:40:A:ASN:HD22	20	5.77
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	4	5.77
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	4	5.77
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	13	5.77
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	5	5.76
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	5	5.76
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	2	5.76
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	2	5.76
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	1	5.76
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	1	5.76
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	9	5.76
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	9	5.76
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	18	5.76
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	18	5.76
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	3	5.75
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	18	5.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	9	5.75
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	4	5.75
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	4	5.75
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	4	5.75
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	4	5.75
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	4	5.75
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	4	5.75
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	5	5.75
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	5	5.75
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	5	5.75
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	18	5.75
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	2	5.75
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	2	5.75
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	1	5.75
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	9	5.75
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	12	5.75
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	12	5.75
(1,301)	1:36:A:CYS:HA	1:40:A:ASN:HD22	18	5.75
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	13	5.75
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	13	5.75
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	13	5.75
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	15	5.74
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	15	5.74
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	16	5.74
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	3	5.74
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	4	5.74
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	8	5.74
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	8	5.74
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	8	5.74
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	4	5.73
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	4	5.73
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	4	5.73
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	12	5.73
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	12	5.73
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	12	5.73
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	11	5.73
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	5	5.73
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	5	5.73
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	8	5.73
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	14	5.73
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	5	5.73
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	18	5.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	14	5.73
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	14	5.73
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	7	5.73
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	7	5.73
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	7	5.73
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	10	5.72
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	10	5.72
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	10	5.72
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	10	5.72
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	12	5.72
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	8	5.72
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	8	5.72
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	14	5.72
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	7	5.72
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	17	5.72
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	17	5.72
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	18	5.72
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	12	5.72
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	12	5.72
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	16	5.72
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	7	5.72
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	7	5.72
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	7	5.72
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	16	5.72
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	16	5.72
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	16	5.72
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	15	5.71
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	13	5.71
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	13	5.71
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	19	5.71
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	19	5.71
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	19	5.71
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	16	5.71
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	5	5.7
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	18	5.7
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	18	5.7
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	8	5.7
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	8	5.7
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	6	5.7
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	17	5.7
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	13	5.7
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	10	5.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	16	5.7
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	12	5.69
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	12	5.69
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	12	5.69
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	12	5.69
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	7	5.69
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	13	5.69
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	5	5.69
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	5	5.69
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	19	5.69
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	19	5.69
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	19	5.69
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	13	5.69
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	13	5.69
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	4	5.69
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	4	5.69
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	4	5.69
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	9	5.68
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	9	5.68
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	15	5.68
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	15	5.68
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	15	5.68
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	15	5.68
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	17	5.68
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	10	5.68
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	1	5.68
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	1	5.68
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	1	5.68
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	6	5.68
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	6	5.68
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	6	5.68
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	18	5.67
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	18	5.67
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	20	5.67
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	5	5.67
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	13	5.67
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	13	5.67
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	13	5.67
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	4	5.67
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	4	5.67
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	4	5.67
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	11	5.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	1	5.67
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	20	5.67
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	6	5.67
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	6	5.67
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	14	5.67
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	6	5.67
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	6	5.67
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	16	5.67
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	1	5.66
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	1	5.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	5	5.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	5	5.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	5	5.66
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	1	5.66
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	6	5.66
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	7	5.66
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	7	5.66
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	7	5.66
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	14	5.66
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	14	5.66
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	15	5.65
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	15	5.65
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	13	5.65
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	13	5.65
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	13	5.65
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	13	5.65
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	19	5.65
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	3	5.65
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	17	5.65
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	17	5.65
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	1	5.65
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	5	5.65
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	5	5.65
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	4	5.65
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	4	5.65
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	4	5.65
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	19	5.65
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	19	5.65
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	19	5.65
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	8	5.65
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	5.65
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	5.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	8	5.65
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	13	5.64
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	13	5.64
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	13	5.64
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	13	5.64
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	13	5.64
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	13	5.64
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	20	5.64
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	6	5.64
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	6	5.64
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	10	5.64
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	10	5.64
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	12	5.64
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	12	5.64
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	15	5.64
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	15	5.64
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	18	5.64
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	18	5.64
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	18	5.64
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	14	5.64
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	14	5.64
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	15	5.64
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	20	5.64
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	16	5.63
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	16	5.63
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	16	5.63
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	16	5.63
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	8	5.63
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	16	5.63
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	16	5.63
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	18	5.63
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	18	5.63
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	18	5.63
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	11	5.63
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	11	5.63
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	16	5.63
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	13	5.63
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	13	5.63
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	5.63
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	5.63
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	9	5.63
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	4	5.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	2	5.63
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	8	5.63
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	20	5.62
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	20	5.62
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	20	5.62
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	1	5.62
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	1	5.62
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	5	5.62
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	5	5.62
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	5	5.62
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	5	5.62
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	2	5.62
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	10	5.62
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	10	5.62
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	6	5.62
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	6	5.62
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	6	5.62
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	17	5.62
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	17	5.62
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	5	5.62
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	18	5.62
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	18	5.62
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	18	5.62
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	18	5.61
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	17	5.61
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	18	5.61
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	18	5.61
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	18	5.61
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	18	5.61
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	12	5.61
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	2	5.61
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	2	5.61
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	9	5.61
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	15	5.61
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	3	5.61
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	3	5.61
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	3	5.61
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	6	5.61
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	4	5.61
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	4	5.61
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	20	5.61
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	20	5.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	20	5.61
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	20	5.61
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	20	5.61
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	20	5.61
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	14	5.61
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	14	5.6
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	14	5.6
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	14	5.6
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	19	5.6
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	16	5.6
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	16	5.6
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	16	5.6
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	16	5.6
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	16	5.6
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	11	5.6
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	11	5.6
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	1	5.6
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	13	5.6
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	13	5.6
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	18	5.6
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	18	5.6
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	5	5.6
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	5	5.6
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	8	5.6
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	8	5.6
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	8	5.6
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	20	5.6
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	20	5.6
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	20	5.6
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	17	5.6
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	17	5.6
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	20	5.59
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	9	5.59
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	19	5.59
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	16	5.59
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	9	5.59
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	5	5.59
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	13	5.59
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	10	5.59
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	10	5.59
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	19	5.59
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	7	5.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	7	5.58
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	7	5.58
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	19	5.58
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	1	5.58
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	6	5.58
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	6	5.58
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	6	5.58
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	6	5.58
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	6	5.58
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	4	5.58
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	4	5.58
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	4	5.58
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	14	5.58
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	12	5.58
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	12	5.58
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	9	5.58
(1,480)	1:39:A:CYS:H	1:40:A:ASN:HD22	17	5.58
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	2	5.58
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	18	5.57
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	18	5.57
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	18	5.57
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	15	5.57
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	12	5.57
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	2	5.57
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	15	5.57
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	13	5.57
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	13	5.57
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	7	5.57
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	7	5.57
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	2	5.57
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	2	5.57
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	2	5.57
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	6	5.57
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	3	5.57
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	5	5.57
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	5	5.57
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	1	5.57
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	1	5.57
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	12	5.56
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	6	5.56
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	6	5.56
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	12	5.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	12	5.56
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	18	5.56
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	9	5.56
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	9	5.56
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	9	5.56
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	9	5.56
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	10	5.56
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	3	5.56
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	4	5.56
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	4	5.56
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	17	5.56
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	1	5.56
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	10	5.56
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	15	5.56
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	16	5.55
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	16	5.55
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	11	5.55
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	19	5.55
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	11	5.55
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	14	5.55
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	14	5.55
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	14	5.55
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	14	5.55
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	14	5.55
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	14	5.55
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	15	5.55
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	20	5.55
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	20	5.55
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	20	5.55
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	20	5.55
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	20	5.55
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	20	5.55
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	15	5.55
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	4	5.54
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	3	5.54
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	19	5.54
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	1	5.54
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	7	5.54
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	7	5.54
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	7	5.54
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	7	5.54
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	8	5.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	8	5.54
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	12	5.54
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	15	5.54
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	2	5.54
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	15	5.54
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	3	5.54
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	3	5.54
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	12	5.54
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	12	5.54
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	12	5.54
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	12	5.54
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	12	5.54
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	12	5.54
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	16	5.54
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	16	5.54
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	12	5.54
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	12	5.54
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	12	5.54
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	14	5.53
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	14	5.53
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	14	5.53
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	6	5.53
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	6	5.53
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	6	5.53
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	10	5.53
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	10	5.53
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	7	5.53
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	7	5.53
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	1	5.53
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	3	5.53
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	1	5.53
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	17	5.53
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	16	5.53
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	16	5.53
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	16	5.53
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	18	5.53
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	18	5.53
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	18	5.53
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	11	5.53
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	19	5.53
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	5	5.53
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	10	5.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	10	5.53
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	2	5.52
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	5	5.52
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	11	5.52
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	3	5.52
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	13	5.52
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	13	5.52
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	5.52
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	4	5.52
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	9	5.51
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	16	5.51
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	13	5.51
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	15	5.51
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	9	5.51
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	13	5.51
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	5.51
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	3	5.51
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	3	5.51
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	5.51
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	5.51
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	5.51
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	5.51
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	5.51
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	12	5.51
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	15	5.51
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	19	5.51
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	18	5.51
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	18	5.51
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	10	5.51
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	12	5.51
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	16	5.5
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	16	5.5
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	14	5.5
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	18	5.5
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	18	5.5
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	7	5.5
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	7	5.5
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	7	5.5
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	7	5.5
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	20	5.5
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	12	5.5
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	12	5.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	12	5.5
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	17	5.5
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	4	5.5
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	7	5.5
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	12	5.5
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE2	12	5.49
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	12	5.49
(1,1175)	1:38:A:THR:HB	1:67:A:LYS:HE3	12	5.49
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	4	5.49
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	5	5.49
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	8	5.49
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	2	5.49
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	2	5.49
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	2	5.49
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	4	5.49
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	16	5.49
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	10	5.49
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	13	5.49
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	7	5.49
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	8	5.49
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	14	5.49
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	18	5.49
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	18	5.49
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	18	5.49
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	3	5.49
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	17	5.49
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	17	5.49
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	13	5.49
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	18	5.49
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	15	5.49
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	15	5.49
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	15	5.49
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	15	5.49
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	15	5.49
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	15	5.49
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	8	5.49
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	8	5.49
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	6	5.48
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	2	5.48
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	19	5.48
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	7	5.48
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	4	5.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	4	5.48
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	4	5.48
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	13	5.48
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	13	5.48
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	8	5.48
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	8	5.48
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	8	5.48
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	20	5.48
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	20	5.48
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	1	5.48
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	1	5.48
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	1	5.48
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	12	5.48
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	12	5.48
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	12	5.48
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	5	5.48
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	9	5.48
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	9	5.48
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	15	5.48
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	15	5.48
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	15	5.48
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	7	5.48
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	7	5.48
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	7	5.48
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	12	5.47
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	15	5.47
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	18	5.47
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	6	5.47
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	6	5.47
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	19	5.47
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	19	5.47
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	1	5.47
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	1	5.47
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	1	5.47
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	1	5.47
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	1	5.47
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	1	5.47
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	1	5.47
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	1	5.47
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	16	5.47
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	5	5.47
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	11	5.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	6	5.46
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	11	5.46
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	18	5.46
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	11	5.46
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	11	5.46
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	11	5.46
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	12	5.46
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	12	5.46
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	12	5.46
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	4	5.46
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	4	5.46
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	17	5.46
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	17	5.46
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	17	5.46
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	10	5.46
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	5	5.46
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	5	5.46
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	8	5.46
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	8	5.46
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	8	5.46
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	2	5.45
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	2	5.45
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	5	5.45
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	13	5.45
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	13	5.45
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	17	5.45
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	17	5.45
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	17	5.45
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	16	5.45
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	16	5.45
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	16	5.45
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	16	5.45
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	16	5.45
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	16	5.45
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	16	5.45
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	16	5.45
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	16	5.45
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	19	5.45
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	19	5.45
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	19	5.45
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	16	5.45
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	16	5.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	3	5.45
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	14	5.45
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	14	5.45
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	11	5.45
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	20	5.45
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	12	5.45
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	12	5.45
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	16	5.45
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	16	5.45
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	16	5.45
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	16	5.45
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	16	5.45
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	16	5.45
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	14	5.45
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	1	5.45
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	11	5.44
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	11	5.44
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	11	5.44
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	11	5.44
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	20	5.44
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	6	5.44
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	7	5.44
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	7	5.44
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	4	5.44
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	6	5.44
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	12	5.44
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	14	5.44
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	1	5.44
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	1	5.44
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	1	5.44
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	19	5.44
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	19	5.44
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	19	5.44
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	19	5.44
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	19	5.44
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	19	5.44
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	19	5.44
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	19	5.44
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	19	5.44
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	8	5.44
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	16	5.44
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	16	5.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	19	5.43
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	10	5.43
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	4	5.43
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	11	5.43
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	3	5.43
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	3	5.43
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	3	5.43
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	3	5.43
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	18	5.43
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	17	5.43
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	14	5.43
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	16	5.43
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	2	5.42
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	17	5.42
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	15	5.42
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	15	5.42
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	13	5.42
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	13	5.42
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	13	5.42
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	9	5.42
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	9	5.42
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	10	5.42
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	10	5.42
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	6	5.42
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	17	5.42
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	20	5.42
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	20	5.42
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	6	5.42
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	15	5.42
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	10	5.42
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	18	5.42
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	1	5.41
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	17	5.41
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	19	5.41
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	15	5.41
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	15	5.41
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	15	5.41
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	18	5.41
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	18	5.41
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	4	5.41
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	4	5.41
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	13	5.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	5	5.41
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	16	5.4
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	16	5.4
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	2	5.4
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	2	5.4
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	2	5.4
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	3	5.4
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	15	5.4
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	11	5.4
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	11	5.4
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	11	5.4
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	20	5.4
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	19	5.4
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	6	5.4
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	6	5.4
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	4	5.4
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	13	5.4
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	18	5.4
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	18	5.4
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	12	5.4
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	17	5.39
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	17	5.39
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	5	5.39
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	19	5.39
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	9	5.39
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	9	5.39
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	10	5.39
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	8	5.39
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	8	5.39
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	4	5.39
(1,645)	1:50:A:LYS:HB3	1:58:A:CYS:HA	20	5.39
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	1	5.39
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	9	5.39
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	9	5.39
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	9	5.39
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	17	5.39
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	17	5.39
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	4	5.39
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	4	5.38
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	4	5.38
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	10	5.38
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	16	5.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	11	5.38
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	11	5.38
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	11	5.38
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	11	5.38
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	11	5.38
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	11	5.38
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	11	5.38
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	11	5.38
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	5	5.38
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	5	5.38
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	19	5.38
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	9	5.38
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	9	5.38
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	9	5.38
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	14	5.38
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	14	5.38
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	14	5.38
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	2	5.38
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	6	5.38
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	17	5.38
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	17	5.38
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	17	5.38
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	3	5.38
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	3	5.38
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	3	5.37
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	3	5.37
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	3	5.37
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	15	5.37
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	15	5.37
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	15	5.37
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	10	5.37
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	10	5.37
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	10	5.37
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	15	5.37
(1,872)	1:50:A:LYS:HG3	1:61:A:GLY:H	8	5.37
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	1	5.37
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	1	5.37
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	1	5.37
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	20	5.37
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	20	5.37
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	13	5.37
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	10	5.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	10	5.37
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	5	5.37
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	5	5.37
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	5	5.37
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	14	5.37
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	12	5.37
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	12	5.37
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	12	5.37
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	13	5.36
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	1	5.36
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	1	5.36
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	1	5.36
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	16	5.36
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	16	5.36
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	16	5.36
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	18	5.36
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	18	5.36
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	18	5.36
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	6	5.36
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	6	5.36
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	15	5.36
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	15	5.36
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	17	5.36
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	17	5.36
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	5	5.36
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	5	5.36
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	3	5.36
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	12	5.36
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	16	5.36
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	16	5.36
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	16	5.36
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	9	5.36
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	18	5.35
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	8	5.35
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	18	5.35
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	20	5.35
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	19	5.35
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	19	5.35
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	13	5.35
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	5	5.35
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	5	5.35
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	5	5.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	5	5.35
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	5	5.35
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	5	5.35
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	7	5.35
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	6	5.35
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	6	5.35
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	8	5.35
(1,873)	1:50:A:LYS:HG3	1:51:A:GLU:H	20	5.35
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	17	5.35
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	17	5.35
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	17	5.35
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	18	5.35
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	18	5.35
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	18	5.35
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	18	5.35
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	18	5.35
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	18	5.35
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	18	5.35
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	18	5.35
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	12	5.35
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	5.35
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	5.35
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	9	5.35
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	9	5.35
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	9	5.35
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	10	5.35
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	11	5.35
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	11	5.35
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	19	5.35
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	11	5.35
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	11	5.35
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	11	5.35
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	15	5.35
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	15	5.35
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	7	5.35
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	1	5.34
(1,1093)	1:62:A:SER:HA	1:67:A:LYS:H	9	5.34
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	12	5.34
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	14	5.34
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	14	5.34
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	3	5.34
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	3	5.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	3	5.34
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	2	5.34
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	14	5.34
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	17	5.34
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	19	5.34
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	17	5.33
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	14	5.33
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	7	5.33
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	3	5.33
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	3	5.33
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	3	5.33
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	3	5.33
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	3	5.33
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	3	5.33
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	19	5.33
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	19	5.33
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	19	5.33
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	11	5.33
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	11	5.33
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	11	5.33
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	11	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	5	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	5	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	5	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	10	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	10	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	10	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	15	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	15	5.33
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	15	5.33
(1,808)	1:38:A:THR:HG21	1:40:A:ASN:HB3	20	5.33
(1,808)	1:38:A:THR:HG22	1:40:A:ASN:HB3	20	5.33
(1,808)	1:38:A:THR:HG23	1:40:A:ASN:HB3	20	5.33
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	2	5.33
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	2	5.33
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	1	5.33
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	1	5.33
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	8	5.33
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	2	5.33
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	2	5.33
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	5	5.33
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	10	5.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	10	5.33
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	10	5.33
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	8	5.32
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	8	5.32
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	8	5.32
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	15	5.32
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	1	5.32
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	1	5.32
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	1	5.32
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	1	5.32
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	8	5.32
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	8	5.32
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	8	5.32
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	8	5.32
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	8	5.32
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	8	5.32
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	3	5.32
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	3	5.32
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	17	5.32
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	17	5.32
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	20	5.32
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	16	5.32
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	16	5.32
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	4	5.32
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	8	5.32
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	8	5.32
(1,62)	1:6:A:LYS:HG2	1:9:A:LYS:H	9	5.32
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	10	5.32
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	10	5.32
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	10	5.32
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	11	5.31
(1,1043)	1:40:A:ASN:HB2	1:48:A:CYS:H	12	5.31
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	4	5.31
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	5	5.31
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	6	5.31
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	6	5.31
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	6	5.31
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	12	5.31
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	9	5.31
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	9	5.31
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	9	5.31
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	9	5.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	16	5.31
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	16	5.31
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	16	5.31
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	3	5.31
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	17	5.31
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	5	5.31
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	4	5.31
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	4	5.31
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	4	5.31
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	4	5.31
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	4	5.31
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	4	5.31
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	17	5.31
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	13	5.3
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	13	5.3
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	13	5.3
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	1	5.3
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	18	5.3
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	3	5.3
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	3	5.3
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	3	5.3
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	3	5.3
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	7	5.3
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	8	5.3
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	18	5.3
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	18	5.3
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	7	5.3
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	7	5.3
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	7	5.3
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	13	5.3
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	13	5.3
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	13	5.3
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	13	5.3
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	4	5.3
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	4	5.3
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	4	5.3
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	4	5.3
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	7	5.3
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	7	5.3
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	13	5.3
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	13	5.3
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	9	5.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	9	5.3
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	16	5.3
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	10	5.29
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	15	5.29
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	18	5.29
(1,957)	1:6:A:LYS:HG3	1:29:A:GLU:H	2	5.29
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	13	5.29
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	13	5.29
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	16	5.29
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	16	5.29
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	12	5.29
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	12	5.29
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	12	5.29
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	16	5.29
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	16	5.29
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	13	5.29
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	11	5.29
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	11	5.29
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	13	5.29
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	13	5.29
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	13	5.29
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	13	5.29
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	13	5.29
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	13	5.29
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	14	5.29
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	19	5.29
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	6	5.29
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	11	5.29
(1,1178)	1:31:A:CYS:HB3	1:37:A:LYS:H	8	5.28
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	12	5.28
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	9	5.28
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	5	5.28
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	6	5.28
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	13	5.28
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	17	5.28
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	12	5.28
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	12	5.28
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	12	5.28
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	12	5.28
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	12	5.28
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	12	5.28
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	11	5.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	11	5.28
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	11	5.28
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	18	5.28
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	18	5.28
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	20	5.28
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	17	5.27
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	17	5.27
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	17	5.27
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	17	5.27
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	8	5.27
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	10	5.27
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	10	5.27
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	1	5.27
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	20	5.27
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	20	5.27
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	2	5.27
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	3	5.27
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	7	5.27
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	7	5.27
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	7	5.27
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	7	5.27
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	4	5.27
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	1	5.27
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	1	5.27
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	1	5.27
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	10	5.27
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	4	5.27
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	4	5.27
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	16	5.27
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	17	5.27
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	14	5.27
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	8	5.27
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	3	5.27
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	1	5.26
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	1	5.26
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	4	5.26
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	14	5.26
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	14	5.26
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	14	5.26
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	16	5.26
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	4	5.26
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	9	5.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	9	5.26
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	18	5.26
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	18	5.26
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	15	5.26
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	15	5.26
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	7	5.26
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	6	5.26
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	11	5.26
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	8	5.26
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	8	5.26
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	10	5.25
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	10	5.25
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	10	5.25
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	11	5.25
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	14	5.25
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	16	5.25
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	9	5.25
(1,1059)	1:50:A:LYS:H	1:52:A:CYS:HB3	5	5.25
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	2	5.25
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	19	5.25
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	2	5.25
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	2	5.25
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	2	5.25
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	2	5.25
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	2	5.25
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	2	5.25
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	12	5.25
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	5	5.25
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	3	5.25
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	3	5.25
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	16	5.25
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	8	5.25
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	8	5.25
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	8	5.25
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	8	5.25
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	8	5.25
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	8	5.25
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	3	5.25
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	16	5.25
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	2	5.25
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	2	5.25
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	2	5.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	2	5.25
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	8	5.24
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	7	5.24
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	5	5.24
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	5	5.24
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	14	5.24
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	6	5.24
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	10	5.24
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	10	5.24
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	12	5.24
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	12	5.24
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	16	5.24
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	16	5.24
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	16	5.24
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	6	5.24
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	4	5.24
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	18	5.24
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	2	5.23
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	5	5.23
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	3	5.23
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	3	5.23
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	14	5.23
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	20	5.23
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	20	5.23
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	12	5.23
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	12	5.23
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	12	5.23
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	19	5.23
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	19	5.23
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	19	5.23
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	19	5.23
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	11	5.23
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	9	5.23
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	1	5.23
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG2	4	5.22
(1,1156)	1:31:A:CYS:HA	1:37:A:LYS:HG3	4	5.22
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	14	5.22
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	19	5.22
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	19	5.22
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	14	5.22
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	17	5.22
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	10	5.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	10	5.22
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	10	5.22
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	10	5.22
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	10	5.22
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	10	5.22
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	5	5.22
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG3	5	5.22
(1,919)	1:6:A:LYS:H	1:9:A:LYS:HG2	5	5.22
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	11	5.22
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	11	5.22
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	10	5.22
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	10	5.22
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	18	5.22
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	14	5.22
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	5.22
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	20	5.22
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	9	5.22
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	9	5.22
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	9	5.22
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	5	5.22
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	13	5.21
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	20	5.21
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	20	5.21
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	20	5.21
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	20	5.21
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	20	5.21
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	20	5.21
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	3	5.21
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	3	5.21
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	3	5.21
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	18	5.21
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	1	5.21
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	1	5.21
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	20	5.21
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	20	5.21
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	6	5.21
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	16	5.21
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	16	5.21
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	16	5.21
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	12	5.21
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	12	5.21
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	5	5.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	5	5.21
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	5	5.21
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	5	5.21
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	1	5.21
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	1	5.21
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	1	5.21
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	7	5.21
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	14	5.21
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	14	5.21
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	1	5.2
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	1	5.2
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	1	5.2
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	1	5.2
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	7	5.2
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	10	5.2
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	10	5.2
(1,30)	1:19:A:CYS:H	1:20:A:GLN:HE22	17	5.2
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	16	5.19
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	15	5.19
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	6	5.19
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	6	5.19
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	6	5.19
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	12	5.19
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	12	5.19
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	12	5.19
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	3	5.19
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	3	5.19
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	3	5.19
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	4	5.19
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	9	5.19
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	9	5.19
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	9	5.19
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	9	5.19
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	9	5.19
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	9	5.19
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	9	5.19
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	15	5.19
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	9	5.19
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	4	5.19
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	4	5.19
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	4	5.19
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	5	5.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	10	5.19
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	9	5.18
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	15	5.18
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	8	5.18
(1,1061)	1:50:A:LYS:H	1:51:A:GLU:HB2	10	5.18
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	7	5.18
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	7	5.18
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	7	5.18
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	7	5.18
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	7	5.18
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	7	5.18
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	12	5.18
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	12	5.18
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	16	5.18
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	11	5.18
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	10	5.18
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	7	5.18
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	19	5.17
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	12	5.17
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	12	5.17
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	9	5.17
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	9	5.17
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	4	5.17
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	4	5.17
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	4	5.17
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	17	5.17
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	17	5.17
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	12	5.17
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	18	5.17
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	4	5.17
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	4	5.17
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	4	5.17
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	4	5.17
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	4	5.17
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	4	5.17
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	12	5.17
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	13	5.16
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	6	5.16
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	7	5.16
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	6	5.16
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	19	5.16
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	6	5.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	7	5.16
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	20	5.16
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	7	5.16
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	7	5.16
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	13	5.16
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	13	5.16
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	13	5.16
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	2	5.16
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	19	5.16
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	5.16
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	12	5.16
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	16	5.16
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	16	5.16
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	7	5.16
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	13	5.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	17	5.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	17	5.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	17	5.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	17	5.16
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	9	5.15
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	9	5.15
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	9	5.15
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	9	5.15
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	6	5.15
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	20	5.15
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	20	5.15
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	20	5.15
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	20	5.15
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	18	5.15
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	18	5.15
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	20	5.15
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	20	5.15
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	15	5.15
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	6	5.15
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	6	5.15
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	6	5.15
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	11	5.15
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	11	5.15
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	11	5.15
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	11	5.15
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	16	5.14
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	14	5.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	11	5.14
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	11	5.14
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	13	5.14
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	13	5.14
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	4	5.14
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	4	5.14
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	4	5.14
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	4	5.14
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	4	5.14
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	4	5.14
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	15	5.14
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	15	5.14
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	15	5.14
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	15	5.14
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	15	5.14
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	15	5.14
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	17	5.14
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	11	5.14
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	11	5.14
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	11	5.14
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	11	5.14
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	11	5.14
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	11	5.14
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	11	5.14
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	11	5.14
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	11	5.14
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	8	5.14
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	8	5.14
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	8	5.13
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	8	5.13
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	8	5.13
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	13	5.13
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	13	5.13
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	13	5.13
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	13	5.13
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	13	5.13
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	13	5.13
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	18	5.13
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	18	5.13
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	18	5.13
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	3	5.13
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	3	5.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	3	5.13
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	1	5.13
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	10	5.13
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	5	5.13
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	5	5.13
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	5	5.13
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	4	5.13
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	4	5.13
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	4	5.13
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	4	5.13
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	4	5.13
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	19	5.13
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	19	5.13
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	19	5.13
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	11	5.13
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	2	5.13
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	2	5.13
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	17	5.13
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	17	5.13
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	17	5.13
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	18	5.13
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	18	5.13
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	18	5.13
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	16	5.12
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	16	5.12
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	16	5.12
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	16	5.12
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	16	5.12
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	16	5.12
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	11	5.12
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	11	5.12
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	13	5.12
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	15	5.12
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	6	5.12
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	6	5.12
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	6	5.12
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	12	5.12
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	12	5.12
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	12	5.12
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	12	5.12
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	12	5.12
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	3	5.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	14	5.12
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	14	5.12
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	20	5.12
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	20	5.12
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	1	5.12
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	2	5.11
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	1	5.11
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	12	5.11
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	19	5.11
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	5	5.11
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	5	5.11
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	19	5.11
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	13	5.11
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	13	5.11
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	7	5.11
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	20	5.11
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	3	5.1
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	9	5.1
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	6	5.1
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	6	5.1
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	6	5.1
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	6	5.1
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	6	5.1
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	6	5.1
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	11	5.1
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	11	5.1
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	11	5.1
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	18	5.1
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	18	5.1
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	18	5.1
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	7	5.1
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	6	5.1
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	2	5.1
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	18	5.1
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	18	5.1
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	16	5.09
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	16	5.09
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	9	5.09
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	9	5.09
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	9	5.09
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	9	5.09
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	13	5.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	13	5.09
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	13	5.09
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	13	5.09
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	13	5.09
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	15	5.09
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	9	5.09
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	5	5.09
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	5	5.09
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	5	5.09
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	17	5.08
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	17	5.08
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	17	5.08
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	5	5.08
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	5	5.08
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	4	5.08
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	20	5.08
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	15	5.08
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	15	5.08
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	15	5.08
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	5	5.08
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	5	5.08
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	16	5.08
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	6	5.08
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	6	5.08
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	6	5.08
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	8	5.08
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	4	5.08
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	20	5.08
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	6	5.08
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	6	5.08
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	17	5.08
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	5.08
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	4	5.08
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	17	5.08
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	17	5.08
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	7	5.08
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	7	5.08
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	11	5.08
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	11	5.08
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	11	5.08
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	9	5.07
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	9	5.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	9	5.07
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	9	5.07
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	18	5.07
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	18	5.07
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	18	5.07
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	10	5.07
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	10	5.07
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	12	5.07
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	13	5.07
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	15	5.07
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	15	5.07
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	14	5.07
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	4	5.07
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	8	5.07
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	19	5.07
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	2	5.07
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	2	5.07
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	13	5.07
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	17	5.06
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	11	5.06
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	11	5.06
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	6	5.06
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	3	5.06
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	17	5.06
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	17	5.06
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	17	5.06
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	17	5.06
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	17	5.06
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	17	5.06
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	7	5.06
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	7	5.06
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	7	5.06
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	15	5.06
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	15	5.06
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	15	5.06
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	13	5.06
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	7	5.06
(1,575)	1:50:A:LYS:HD2	1:60:A:CYS:HA	19	5.06
(1,575)	1:50:A:LYS:HD3	1:60:A:CYS:HA	19	5.06
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	10	5.06
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	10	5.06
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	17	5.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	18	5.05
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	18	5.05
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	6	5.05
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	11	5.05
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	16	5.05
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	16	5.05
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	10	5.05
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	10	5.05
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	10	5.05
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	14	5.05
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	14	5.05
(1,630)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	2	5.05
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	16	5.05
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	20	5.05
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	20	5.05
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	20	5.05
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	20	5.05
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	20	5.05
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	20	5.05
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	20	5.05
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	20	5.05
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	20	5.05
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	1	5.05
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	1	5.05
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	3	5.05
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	13	5.05
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	13	5.05
(1,1138)	1:52:A:CYS:HB2	1:54:A:GLY:HA2	3	5.04
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	3	5.04
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	7	5.04
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	14	5.04
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	14	5.04
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	14	5.04
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	14	5.04
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	14	5.04
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	14	5.04
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	13	5.04
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	13	5.04
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	13	5.04
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	13	5.04
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	13	5.04
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	13	5.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	4	5.04
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	4	5.04
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	14	5.04
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	4	5.04
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	16	5.04
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	16	5.04
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	16	5.04
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	16	5.04
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	16	5.04
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	16	5.04
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	16	5.04
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	16	5.04
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	16	5.04
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	13	5.04
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	13	5.04
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	13	5.04
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	7	5.04
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	7	5.04
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	7	5.04
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	11	5.04
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	9	5.04
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	9	5.04
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	6	5.03
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	6	5.03
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	3	5.03
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	4	5.03
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	4	5.03
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	4	5.03
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	4	5.03
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	4	5.03
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	20	5.03
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	20	5.03
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	20	5.03
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	18	5.03
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	11	5.03
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	11	5.03
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	11	5.03
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	11	5.03
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	20	5.03
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	20	5.03
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	5	5.03
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	1	5.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	1	5.03
(1,488)	1:14:A:CYS:H	1:26:A:GLN:H	7	5.03
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	4	5.03
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	9	5.03
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	3	5.03
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	19	5.02
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	9	5.02
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	9	5.02
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	9	5.02
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	7	5.02
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	3	5.02
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	3	5.02
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	4	5.02
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	18	5.02
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	16	5.02
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	3	5.02
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	2	5.02
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	13	5.02
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	13	5.02
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	10	5.01
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	10	5.01
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	1	5.01
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	1	5.01
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	1	5.01
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	3	5.01
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	2	5.01
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	7	5.01
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	7	5.01
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	13	5.01
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	13	5.01
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	13	5.01
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	7	5.01
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	3	5.01
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	3	5.01
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	3	5.01
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	9	5.01
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	9	5.01
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	9	5.01
(1,672)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	11	5.01
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	20	5.01
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	11	5.01
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	2	5.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	9	5.01
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	8	5.01
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	8	5.01
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	12	5.0
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	18	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	11	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	11	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	11	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	18	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	18	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	18	5.0
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	4	5.0
(1,929)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	12	5.0
(1,929)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	12	5.0
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	19	5.0
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	19	5.0
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	19	5.0
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	19	5.0
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE2	9	5.0
(1,765)	1:37:A:LYS:HB3	1:67:A:LYS:HE3	9	5.0
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	1	5.0
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	1	5.0
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	1	5.0
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	16	5.0
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	16	5.0
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	16	5.0
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	5	5.0
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	5	5.0
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	8	5.0
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	20	5.0
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	1	5.0
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	1	5.0
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	1	5.0
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	1	5.0
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	1	5.0
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	1	5.0
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	19	5.0
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	19	5.0
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	19	5.0
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	19	5.0
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	19	5.0
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	19	5.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	14	5.0
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	14	5.0
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	17	5.0
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	17	5.0
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	17	5.0
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	14	5.0
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	3	5.0
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	3	5.0
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	3	5.0
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	9	5.0
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	15	4.99
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	15	4.99
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	15	4.99
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	19	4.99
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	19	4.99
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	19	4.99
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	20	4.99
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	13	4.99
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	3	4.99
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	10	4.99
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	10	4.99
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	10	4.99
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	10	4.99
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	10	4.99
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	10	4.99
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	1	4.99
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	1	4.99
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	1	4.99
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	1	4.99
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	12	4.99
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	12	4.99
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	18	4.99
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	18	4.99
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	9	4.99
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	9	4.99
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	9	4.99
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	20	4.99
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	20	4.99
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	20	4.98
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	20	4.98
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	20	4.98
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	5	4.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	5	4.98
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	5	4.98
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	5	4.98
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	13	4.98
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	13	4.98
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	17	4.98
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	12	4.98
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	12	4.98
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	12	4.98
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	16	4.98
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	16	4.98
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	16	4.98
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	16	4.98
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	16	4.98
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	16	4.98
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	11	4.98
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	11	4.98
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	17	4.98
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	20	4.98
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	20	4.98
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	4	4.98
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	1	4.97
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	4	4.97
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	9	4.97
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	9	4.97
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	9	4.97
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	9	4.97
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	9	4.97
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	9	4.97
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	7	4.97
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	7	4.97
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	7	4.97
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	3	4.97
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	3	4.97
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	3	4.97
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	3	4.97
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	3	4.97
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	3	4.97
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	12	4.97
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	4.97
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	16	4.97
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	17	4.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	3	4.97
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	13	4.97
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	11	4.96
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	5	4.96
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	11	4.96
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	14	4.96
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	14	4.96
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	6	4.96
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	6	4.96
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	6	4.96
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	8	4.96
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	4	4.96
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	15	4.96
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	1	4.96
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	1	4.96
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	5	4.96
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	5	4.96
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	5	4.96
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	5	4.96
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	5	4.95
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	4	4.95
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	10	4.95
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	10	4.95
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	10	4.95
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	6	4.95
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	6	4.95
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	6	4.95
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	6	4.95
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	6	4.95
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	6	4.95
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	11	4.95
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	11	4.95
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	12	4.95
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	12	4.95
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	12	4.95
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	12	4.95
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	12	4.95
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	12	4.95
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	9	4.95
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	9	4.95
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	9	4.95
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	10	4.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	10	4.95
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	10	4.95
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	5	4.95
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	5	4.95
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	9	4.95
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	9	4.95
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	1	4.95
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	15	4.95
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	19	4.95
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	18	4.95
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	1	4.95
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	1	4.95
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	1	4.95
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	10	4.95
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	4	4.94
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	4	4.94
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	16	4.94
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	16	4.94
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	17	4.94
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	17	4.94
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	17	4.94
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	17	4.94
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	8	4.94
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	8	4.94
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	8	4.94
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	14	4.94
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	8	4.94
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	8	4.94
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	8	4.94
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	5	4.94
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	14	4.94
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	14	4.94
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	2	4.94
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	2	4.94
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	7	4.94
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	7	4.94
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	2	4.94
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	15	4.94
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	20	4.94
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	20	4.94
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	20	4.94
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	18	4.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	18	4.94
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	18	4.93
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	18	4.93
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	2	4.93
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	2	4.93
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	2	4.93
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	19	4.93
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	19	4.93
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	19	4.93
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	13	4.93
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	17	4.93
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	12	4.93
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	1	4.93
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	10	4.93
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	19	4.92
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	13	4.92
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	13	4.92
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	18	4.92
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	18	4.92
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	7	4.92
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	7	4.92
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	7	4.92
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	8	4.92
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	16	4.92
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	16	4.92
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	16	4.92
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	16	4.92
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	16	4.92
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	16	4.92
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	17	4.92
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	11	4.92
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	11	4.92
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	9	4.92
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	9	4.92
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	9	4.92
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	11	4.92
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	9	4.92
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	9	4.92
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	9	4.92
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	15	4.92
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	14	4.92
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	11	4.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	11	4.92
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	11	4.92
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	11	4.92
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	11	4.92
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	11	4.92
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	8	4.92
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	8	4.92
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	8	4.92
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	3	4.92
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	5	4.92
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	19	4.92
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	19	4.92
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	20	4.92
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	20	4.92
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	20	4.92
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	20	4.92
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	11	4.91
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	11	4.91
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	11	4.91
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	17	4.91
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	17	4.91
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	15	4.91
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	15	4.91
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	3	4.91
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	5	4.91
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	5	4.91
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	11	4.91
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	11	4.91
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	13	4.91
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	13	4.91
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	13	4.91
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	10	4.91
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	9	4.91
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	17	4.91
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	17	4.91
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	17	4.91
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	17	4.91
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	17	4.91
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	17	4.91
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	17	4.91
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	17	4.91
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	17	4.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	17	4.91
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	17	4.91
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	17	4.91
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	13	4.91
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	13	4.91
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	13	4.91
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	7	4.91
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	7	4.91
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	12	4.91
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	18	4.91
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	13	4.91
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	13	4.91
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	13	4.91
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	7	4.91
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	11	4.9
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	11	4.9
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	11	4.9
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	4	4.9
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	4	4.9
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	17	4.9
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	17	4.9
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	4	4.9
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	4	4.9
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	4	4.9
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	20	4.9
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	20	4.9
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	10	4.9
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	2	4.9
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	2	4.9
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	2	4.9
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	5	4.9
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	5	4.9
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	5	4.9
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	5	4.9
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	17	4.9
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	17	4.9
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	17	4.9
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	17	4.9
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	14	4.9
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	14	4.9
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	14	4.9
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	16	4.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	16	4.9
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	9	4.9
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	9	4.9
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	4.9
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	19	4.9
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	8	4.9
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	7	4.9
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	10	4.9
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	3	4.9
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	3	4.9
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	16	4.9
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	16	4.9
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	6	4.9
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	13	4.9
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	15	4.9
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	3	4.89
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	3	4.89
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	3	4.89
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	3	4.89
(1,1096)	1:64:A:CYS:HB3	1:67:A:LYS:HA	13	4.89
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	6	4.89
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	15	4.89
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	15	4.89
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	14	4.89
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	1	4.89
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	1	4.89
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	1	4.89
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	1	4.89
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	1	4.89
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	1	4.89
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	2	4.89
(1,830)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	2	4.89
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	12	4.89
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	19	4.89
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	19	4.89
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	12	4.89
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	19	4.89
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	4	4.89
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	4	4.89
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	2	4.89
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	2	4.89
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	8	4.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	4	4.88
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	4	4.88
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	4	4.88
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	18	4.88
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	18	4.88
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	9	4.88
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	16	4.88
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	1	4.88
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	13	4.88
(1,478)	1:39:A:CYS:H	1:40:A:ASN:HD21	17	4.88
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	6	4.88
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	6	4.88
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	7	4.88
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	7	4.88
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	10	4.88
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	8	4.88
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	6	4.88
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	20	4.87
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	20	4.87
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	20	4.87
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	20	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	2	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	2	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	6	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	6	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	9	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	9	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	13	4.87
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	13	4.87
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	12	4.87
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	12	4.87
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	10	4.87
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	10	4.87
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	17	4.87
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	17	4.87
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	17	4.87
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	20	4.87
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	20	4.87
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	20	4.87
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	10	4.87
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	5	4.87
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	14	4.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	14	4.87
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	20	4.87
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	20	4.87
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	20	4.87
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	6	4.87
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	6	4.87
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	6	4.87
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	12	4.87
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	5	4.87
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	5	4.87
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	5	4.87
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	5	4.87
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	5	4.87
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	5	4.87
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	9	4.87
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	9	4.87
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	15	4.87
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	15	4.87
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	15	4.87
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	19	4.87
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	6	4.87
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	19	4.87
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	20	4.87
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	15	4.86
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	10	4.86
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	7	4.86
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	7	4.86
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	14	4.86
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	14	4.86
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	16	4.86
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	16	4.86
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	16	4.86
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	16	4.86
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	17	4.86
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	17	4.86
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	17	4.86
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	11	4.86
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	6	4.86
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	2	4.86
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	2	4.86
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	4	4.86
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	5	4.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	5	4.85
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	13	4.85
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	3	4.85
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	3	4.85
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	3	4.85
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	3	4.85
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	3	4.85
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	3	4.85
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	13	4.85
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	13	4.85
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	13	4.85
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	17	4.85
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	17	4.85
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	14	4.85
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	5	4.85
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	5	4.85
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	5	4.85
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	5	4.85
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	5	4.85
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	5	4.85
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	14	4.85
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	7	4.85
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	7	4.85
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	2	4.85
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	3	4.85
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	15	4.85
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	2	4.84
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	2	4.84
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	2	4.84
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	2	4.84
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	6	4.84
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	6	4.84
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	10	4.84
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	10	4.84
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	15	4.84
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	15	4.84
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	16	4.84
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	6	4.84
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	6	4.84
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	17	4.84
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	18	4.84
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	1	4.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:60:A:CYS:HB2	1:63:A:SER:H	11	4.84
(1,374)	1:60:A:CYS:HB3	1:63:A:SER:H	11	4.84
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	5	4.84
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	5	4.84
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	5	4.84
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	17	4.84
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	17	4.84
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	11	4.84
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	11	4.84
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	13	4.84
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	17	4.84
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	17	4.83
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	17	4.83
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	3	4.83
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	3	4.83
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	3	4.83
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	10	4.83
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	10	4.83
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	13	4.83
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	13	4.83
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	13	4.83
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	13	4.83
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	13	4.83
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	13	4.83
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	19	4.83
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	15	4.83
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	16	4.83
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	17	4.83
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	17	4.83
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	17	4.83
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	17	4.83
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	4.83
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	4.83
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE2	18	4.83
(1,315)	1:6:A:LYS:H	1:9:A:LYS:HE3	18	4.83
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	17	4.83
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	6	4.83
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	8	4.83
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	18	4.83
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	18	4.83
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	8	4.82
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	8	4.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	16	4.82
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	16	4.82
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	18	4.82
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	18	4.82
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	18	4.82
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	18	4.82
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	18	4.82
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	18	4.82
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	18	4.82
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	18	4.82
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	18	4.82
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	18	4.82
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	18	4.82
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	20	4.82
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	5	4.82
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	5	4.82
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	10	4.82
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	10	4.82
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	10	4.82
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	10	4.82
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	10	4.82
(1,517)	1:33:A:CYS:HA	1:37:A:LYS:HG2	2	4.82
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	20	4.82
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	19	4.82
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	13	4.82
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	5	4.82
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	5	4.82
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	5	4.82
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	7	4.82
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	12	4.81
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	12	4.81
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	12	4.81
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	15	4.81
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	15	4.81
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	14	4.81
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	14	4.81
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	6	4.81
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	6	4.81
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	6	4.81
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	13	4.81
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	20	4.81
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	4	4.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	18	4.81
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	15	4.81
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	15	4.81
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	15	4.81
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	15	4.81
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	15	4.81
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	15	4.81
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	10	4.81
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	6	4.81
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	6	4.81
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	6	4.81
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	6	4.81
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	20	4.81
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	20	4.81
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	18	4.81
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	12	4.81
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	12	4.81
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB2	10	4.8
(1,1063)	1:50:A:LYS:H	1:51:A:GLU:HB3	10	4.8
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	5	4.8
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB2	5	4.8
(1,1057)	1:50:A:LYS:H	1:52:A:CYS:HB3	5	4.8
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	2	4.8
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	2	4.8
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	2	4.8
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	8	4.8
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	8	4.8
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	8	4.8
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	8	4.8
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	17	4.8
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	13	4.8
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	13	4.8
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	13	4.8
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	18	4.8
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	12	4.8
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	14	4.8
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	4	4.8
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	10	4.8
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	10	4.8
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	10	4.8
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	5	4.8
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	5	4.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	16	4.8
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	18	4.8
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	6	4.79
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	7	4.79
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	7	4.79
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	20	4.79
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	20	4.79
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	3	4.79
(1,749)	1:65:A:SER:HA	1:67:A:LYS:HB2	18	4.79
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	19	4.79
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	19	4.79
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	14	4.79
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	14	4.79
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	14	4.79
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	14	4.79
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	2	4.79
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	2	4.79
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	2	4.79
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	7	4.79
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	11	4.79
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	5	4.79
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	19	4.79
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	19	4.79
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	9	4.79
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	9	4.79
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	9	4.79
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	18	4.79
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	1	4.78
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	1	4.78
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	1	4.78
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	1	4.78
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	11	4.78
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	16	4.78
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	11	4.78
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	11	4.78
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	11	4.78
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	8	4.78
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	8	4.78
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	8	4.78
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	11	4.78
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	11	4.78
(1,857)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	11	4.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	13	4.78
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	6	4.78
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	1	4.78
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	13	4.78
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	13	4.78
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	19	4.78
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	19	4.78
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	8	4.78
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	19	4.78
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	19	4.78
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	19	4.78
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	19	4.78
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	7	4.77
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	7	4.77
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	7	4.77
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	7	4.77
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	13	4.77
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	13	4.77
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	13	4.77
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	2	4.77
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	17	4.77
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	17	4.77
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	17	4.77
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	8	4.77
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	8	4.77
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	8	4.77
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	8	4.77
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	19	4.77
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	9	4.77
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	9	4.77
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	9	4.77
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	7	4.77
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	7	4.77
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	10	4.77
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	4.77
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	11	4.77
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	3	4.77
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	5	4.77
(1,445)	1:48:A:CYS:H	1:49:A:GLY:HA3	17	4.77
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	20	4.77
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	20	4.77
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	20	4.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	20	4.77
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	20	4.77
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	20	4.77
(1,116)	1:55:A:PRO:HG2	1:57:A:SER:H	1	4.77
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	6	4.77
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	6	4.77
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	20	4.76
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	20	4.76
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	20	4.76
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	7	4.76
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	7	4.76
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	9	4.76
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	9	4.76
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	2	4.76
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	7	4.76
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	8	4.76
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	4	4.76
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	4	4.76
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	5	4.76
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	15	4.76
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	15	4.76
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	15	4.76
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	16	4.76
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	16	4.76
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	6	4.76
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	6	4.76
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	6	4.76
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	6	4.76
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	17	4.76
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	17	4.76
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	17	4.76
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	17	4.76
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	17	4.76
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	9	4.76
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	8	4.76
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	8	4.76
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	8	4.76
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	14	4.76
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	6	4.76
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	6	4.76
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	6	4.76
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	6	4.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	4	4.75
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	4	4.75
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	3	4.75
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	12	4.75
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	10	4.75
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	12	4.75
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	9	4.75
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	9	4.75
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	10	4.75
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	10	4.75
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	10	4.75
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	10	4.75
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	2	4.75
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	15	4.75
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	15	4.75
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	15	4.75
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	4.75
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	20	4.75
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	20	4.75
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	20	4.75
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	10	4.75
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	8	4.75
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	8	4.75
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	7	4.75
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	2	4.75
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	2	4.75
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	9	4.75
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	4	4.75
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	4	4.75
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	4	4.75
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	14	4.75
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	14	4.75
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	20	4.75
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	14	4.75
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	14	4.75
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	18	4.74
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	18	4.74
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	18	4.74
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	18	4.74
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	16	4.74
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	16	4.74
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	12	4.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	11	4.74
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	11	4.74
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	10	4.74
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	10	4.74
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	10	4.74
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	10	4.74
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	10	4.74
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	10	4.74
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	6	4.74
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	7	4.74
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	11	4.74
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	7	4.74
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	7	4.74
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	18	4.74
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	15	4.74
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	15	4.74
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	12	4.74
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	4	4.74
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	4	4.74
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	4	4.74
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	20	4.74
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	3	4.74
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	3	4.74
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	3	4.74
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	1	4.74
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	2	4.74
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	15	4.73
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	15	4.73
(1,1107)	1:6:A:LYS:HE2	1:9:A:LYS:H	10	4.73
(1,1107)	1:6:A:LYS:HE3	1:9:A:LYS:H	10	4.73
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	12	4.73
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	12	4.73
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	4	4.73
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	19	4.73
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	8	4.73
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	8	4.73
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	1	4.73
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	3	4.73
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	16	4.73
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	12	4.73
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	12	4.73
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	15	4.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	15	4.73
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	15	4.73
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	1	4.73
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	20	4.73
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	13	4.73
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	14	4.73
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	12	4.73
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	12	4.73
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	12	4.73
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	18	4.73
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	18	4.73
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	18	4.73
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	18	4.73
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	13	4.72
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	13	4.72
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	3	4.72
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	6	4.72
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	13	4.72
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	19	4.72
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	19	4.72
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	19	4.72
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	19	4.72
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	19	4.72
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	19	4.72
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	16	4.72
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	5	4.72
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	5	4.72
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	4	4.72
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	19	4.72
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	19	4.72
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	16	4.72
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	16	4.72
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	16	4.72
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	19	4.72
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	19	4.72
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	19	4.72
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	3	4.71
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	10	4.71
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	19	4.71
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	5	4.71
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	18	4.71
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	18	4.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	18	4.71
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	18	4.71
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	18	4.71
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	18	4.71
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	14	4.71
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	14	4.71
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	10	4.71
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	13	4.71
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	19	4.71
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	19	4.71
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	2	4.71
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	2	4.71
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	12	4.71
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	14	4.71
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	14	4.71
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	14	4.71
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	2	4.71
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	9	4.71
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	9	4.71
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	9	4.71
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	11	4.71
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	13	4.71
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	7	4.71
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	7	4.71
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	15	4.71
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	15	4.71
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	9	4.7
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	14	4.7
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	14	4.7
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	17	4.7
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	17	4.7
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	17	4.7
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	17	4.7
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	17	4.7
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	17	4.7
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	15	4.7
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	8	4.7
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	18	4.7
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	18	4.7
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	18	4.7
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	18	4.7
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	6	4.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	8	4.7
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	9	4.7
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	20	4.7
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	14	4.7
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	14	4.7
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	20	4.7
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	20	4.7
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	10	4.7
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	4	4.7
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	16	4.7
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	16	4.7
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	17	4.7
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	17	4.7
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	13	4.7
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	4	4.7
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	20	4.7
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	13	4.7
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	13	4.7
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	13	4.7
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	13	4.7
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	13	4.7
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	13	4.7
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	7	4.7
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	7	4.7
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	7	4.7
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	10	4.7
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	10	4.7
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	10	4.7
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	16	4.7
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	16	4.7
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	16	4.7
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	12	4.7
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	9	4.7
(1,60)	1:6:A:LYS:HG2	1:9:A:LYS:H	9	4.7
(1,60)	1:6:A:LYS:HG3	1:9:A:LYS:H	9	4.7
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	7	4.7
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	7	4.7
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	3	4.7
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	2	4.69
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	17	4.69
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	11	4.69
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	11	4.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	3	4.69
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	4	4.69
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	4	4.69
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	14	4.69
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	18	4.69
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	2	4.69
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	2	4.69
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	2	4.69
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	15	4.69
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	8	4.69
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	8	4.69
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	8	4.69
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	15	4.69
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	15	4.69
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	8	4.69
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	11	4.69
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	19	4.69
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	19	4.69
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	19	4.69
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	18	4.69
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	18	4.69
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	18	4.69
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	14	4.69
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	14	4.69
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	14	4.69
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	5	4.69
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	5	4.69
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	16	4.68
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	16	4.68
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	16	4.68
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	1	4.68
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	15	4.68
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	16	4.68
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	10	4.68
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	7	4.68
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	7	4.68
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	10	4.68
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	10	4.68
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	14	4.68
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	14	4.68
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	14	4.68
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	12	4.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	14	4.68
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	5	4.68
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	5	4.68
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	10	4.68
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	10	4.68
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	6	4.68
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	6	4.68
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	6	4.68
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	16	4.68
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	16	4.68
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	16	4.68
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	5	4.68
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	5	4.68
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	5	4.68
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	5	4.68
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	5	4.68
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	5	4.68
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	5	4.68
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	5	4.68
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	5	4.68
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	18	4.68
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	18	4.68
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	3	4.68
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	12	4.68
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	2	4.68
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	1	4.68
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	5	4.68
(1,479)	1:38:A:THR:H	1:40:A:ASN:HD22	12	4.68
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	10	4.68
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	10	4.68
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	14	4.68
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	14	4.68
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	3	4.68
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	3	4.68
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	3	4.68
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	6	4.68
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	6	4.68
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	6	4.68
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	15	4.68
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	15	4.68
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	15	4.68
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	17	4.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	17	4.68
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	17	4.68
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	15	4.68
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	7	4.67
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	7	4.67
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	8	4.67
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	11	4.67
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	20	4.67
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	3	4.67
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	9	4.67
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	9	4.67
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	8	4.67
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	8	4.67
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	7	4.67
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	7	4.67
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	7	4.67
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	7	4.67
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	1	4.67
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	19	4.67
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	19	4.67
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	19	4.67
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	11	4.67
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	11	4.67
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	14	4.67
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	14	4.67
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	14	4.67
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	14	4.67
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	15	4.67
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	2	4.67
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	2	4.67
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	2	4.67
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	15	4.66
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	17	4.66
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	17	4.66
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	16	4.66
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	4	4.66
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	17	4.66
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	17	4.66
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	17	4.66
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	17	4.66
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	13	4.66
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	13	4.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	13	4.66
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	13	4.66
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	2	4.66
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	2	4.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	10	4.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	10	4.66
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	10	4.66
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	7	4.66
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	7	4.66
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	11	4.66
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	11	4.66
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	4.66
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	17	4.66
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	11	4.66
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	11	4.66
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	13	4.66
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	13	4.66
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	1	4.66
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	13	4.66
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	6	4.66
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	6	4.66
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	6	4.66
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	8	4.66
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	14	4.66
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	6	4.66
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	4	4.66
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	4	4.66
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	15	4.66
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	15	4.66
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	15	4.66
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	15	4.66
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	11	4.66
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	13	4.65
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	6	4.65
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	6	4.65
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	10	4.65
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	10	4.65
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	20	4.65
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	20	4.65
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	9	4.65
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	2	4.65
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	2	4.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	2	4.65
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	1	4.65
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	1	4.65
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	1	4.65
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	1	4.65
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	1	4.65
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	17	4.65
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	17	4.65
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	17	4.65
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	4	4.65
(1,529)	1:26:A:GLN:H	1:36:A:CYS:HB2	10	4.65
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	13	4.65
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	13	4.65
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	13	4.65
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	13	4.65
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	13	4.65
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	13	4.65
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	5	4.65
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	5	4.65
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	5	4.65
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	2	4.64
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	2	4.64
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	2	4.64
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	20	4.64
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	18	4.64
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	18	4.64
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	12	4.64
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	12	4.64
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	10	4.64
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	10	4.64
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	11	4.64
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	11	4.64
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	11	4.64
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	7	4.64
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	7	4.64
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	2	4.64
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	2	4.64
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	2	4.64
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	2	4.64
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	7	4.64
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	7	4.64
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	7	4.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	9	4.64
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	8	4.64
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	20	4.64
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	14	4.64
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	14	4.64
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	14	4.64
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	10	4.64
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	10	4.64
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	17	4.63
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	3	4.63
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	3	4.63
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	3	4.63
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	12	4.63
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	12	4.63
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	12	4.63
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	17	4.63
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	8	4.63
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	8	4.63
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	8	4.63
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	3	4.63
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	3	4.63
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	3	4.63
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	15	4.63
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	15	4.63
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	15	4.63
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	16	4.63
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	2	4.63
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	15	4.63
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	17	4.63
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	17	4.63
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	17	4.63
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	17	4.63
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	17	4.63
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	17	4.63
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	17	4.63
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	17	4.63
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	17	4.63
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	2	4.63
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	2	4.63
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	2	4.63
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	2	4.63
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	2	4.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	2	4.63
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	7	4.63
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	7	4.63
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	7	4.63
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	3	4.63
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	3	4.63
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	5	4.62
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	5	4.62
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	5	4.62
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	5	4.62
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	20	4.62
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	3	4.62
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	3	4.62
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	14	4.62
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	14	4.62
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	14	4.62
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	2	4.62
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	6	4.62
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	6	4.62
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	10	4.62
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	10	4.62
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	10	4.62
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	8	4.62
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	8	4.62
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	15	4.62
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	1	4.62
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	1	4.62
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	1	4.62
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	18	4.62
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	18	4.62
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	18	4.62
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	18	4.62
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	18	4.62
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	18	4.62
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	12	4.62
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	12	4.62
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	12	4.62
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	12	4.62
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	12	4.62
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	12	4.62
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	17	4.62
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	17	4.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	18	4.62
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	18	4.62
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	18	4.62
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	10	4.62
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	10	4.62
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	10	4.62
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	14	4.62
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	14	4.62
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	20	4.62
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	16	4.61
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	16	4.61
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	16	4.61
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	16	4.61
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	16	4.61
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	1	4.61
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	1	4.61
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	16	4.61
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	16	4.61
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	9	4.61
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	9	4.61
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	9	4.61
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	9	4.61
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	1	4.61
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	17	4.61
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	17	4.61
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	17	4.61
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	7	4.61
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	7	4.61
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	7	4.61
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	2	4.61
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	13	4.61
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	4.61
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	8	4.61
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	2	4.61
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	9	4.61
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	9	4.61
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	9	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	3	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	3	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	3	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	3	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	12	4.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	12	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	12	4.61
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	12	4.61
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	2	4.61
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	18	4.6
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	10	4.6
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	13	4.6
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	13	4.6
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	8	4.6
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	8	4.6
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	1	4.6
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	1	4.6
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	1	4.6
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	1	4.6
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	1	4.6
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	1	4.6
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	1	4.6
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	1	4.6
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	1	4.6
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	14	4.6
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	14	4.6
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	20	4.6
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	20	4.6
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	20	4.6
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	1	4.6
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	1	4.6
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	19	4.6
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	19	4.6
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	6	4.6
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	10	4.6
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	17	4.6
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	7	4.6
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	13	4.6
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	13	4.6
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	13	4.6
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	13	4.6
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	14	4.59
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	14	4.59
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	14	4.59
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	4	4.59
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	9	4.59
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	18	4.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	18	4.59
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	4	4.59
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	4	4.59
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	19	4.59
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	19	4.59
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	17	4.59
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	17	4.59
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	17	4.59
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	17	4.59
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	17	4.59
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	17	4.59
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	17	4.59
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	17	4.59
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	17	4.59
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	14	4.59
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	14	4.59
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	14	4.59
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	14	4.59
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	14	4.59
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	5	4.59
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	19	4.59
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	7	4.59
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	20	4.59
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	15	4.59
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	15	4.59
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	16	4.59
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	16	4.59
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	20	4.58
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	14	4.58
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	14	4.58
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	14	4.58
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	4	4.58
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	4	4.58
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	5	4.58
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	18	4.58
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	6	4.58
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	6	4.58
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	6	4.58
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	6	4.58
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	6	4.58
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	6	4.58
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	16	4.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	16	4.58
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	15	4.58
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	15	4.58
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	9	4.58
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	9	4.58
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	10	4.58
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	10	4.58
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	10	4.58
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	10	4.58
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	10	4.58
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	10	4.58
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	17	4.58
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	17	4.58
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	17	4.58
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	2	4.58
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	12	4.58
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	12	4.58
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	19	4.58
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	19	4.58
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	14	4.57
(1,1097)	1:40:A:ASN:HB2	1:67:A:LYS:HA	14	4.57
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	1	4.57
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	20	4.57
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	20	4.57
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	4.57
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	4.57
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	17	4.57
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	17	4.57
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	20	4.57
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	20	4.57
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	20	4.57
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	11	4.57
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	15	4.57
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	15	4.57
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	14	4.57
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	14	4.57
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	14	4.57
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	14	4.57
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	14	4.57
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	2	4.57
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	2	4.57
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	13	4.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	13	4.57
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	8	4.57
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	15	4.57
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	3	4.57
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	3	4.57
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	11	4.57
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	1	4.57
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	1	4.57
(1,92)	1:11:A:THR:HA	1:14:A:CYS:H	19	4.57
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	14	4.57
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	1	4.56
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	1	4.56
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	14	4.56
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	14	4.56
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	1	4.56
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	1	4.56
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	2	4.56
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	2	4.56
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	2	4.56
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	2	4.56
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	2	4.56
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	2	4.56
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	2	4.56
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	2	4.56
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	2	4.56
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	17	4.56
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	7	4.56
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	6	4.56
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	6	4.56
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	6	4.56
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	6	4.56
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	7	4.56
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	9	4.56
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	9	4.56
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	9	4.56
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	9	4.56
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	9	4.56
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	8	4.56
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	8	4.56
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	12	4.56
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	12	4.56
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	6	4.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	13	4.56
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	3	4.56
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	2	4.56
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	2	4.56
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	2	4.56
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	2	4.56
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	2	4.56
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	2	4.56
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	5	4.56
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	5	4.56
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	5	4.56
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	14	4.56
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	14	4.56
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	14	4.56
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	20	4.56
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	20	4.56
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	20	4.56
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	4	4.56
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	4	4.56
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	2	4.56
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	2	4.56
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	14	4.55
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	14	4.55
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	14	4.55
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	14	4.55
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	1	4.55
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	20	4.55
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	18	4.55
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	18	4.55
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	18	4.55
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	10	4.55
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	10	4.55
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	10	4.55
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	10	4.55
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	3	4.55
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	3	4.55
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	14	4.55
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	14	4.55
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	6	4.55
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	6	4.55
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	6	4.55
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	16	4.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	16	4.55
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	16	4.55
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	12	4.55
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	12	4.55
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	4.55
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	4.55
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	4.55
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	4.55
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	16	4.55
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	4	4.55
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	7	4.55
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	7	4.55
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	7	4.55
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	7	4.55
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	7	4.55
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	7	4.55
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	16	4.55
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	16	4.55
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	16	4.55
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	5	4.54
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	5	4.54
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	5	4.54
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	12	4.54
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	12	4.54
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	7	4.54
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	13	4.54
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	13	4.54
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	7	4.54
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	7	4.54
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	1	4.54
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	19	4.54
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	19	4.54
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	19	4.54
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	20	4.54
(1,836)	1:37:A:LYS:HE2	1:38:A:THR:HA	18	4.54
(1,836)	1:37:A:LYS:HE3	1:38:A:THR:HA	18	4.54
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	5	4.54
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	1	4.54
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	1	4.54
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	1	4.54
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	13	4.54
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	13	4.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	13	4.54
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	12	4.54
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	12	4.54
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	12	4.54
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	13	4.54
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	12	4.54
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	12	4.54
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	3	4.54
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	3	4.54
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	20	4.54
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	9	4.54
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	9	4.54
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	9	4.54
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	1	4.54
(1,118)	1:39:A:CYS:HB2	1:57:A:SER:H	1	4.54
(1,118)	1:39:A:CYS:HB3	1:57:A:SER:H	1	4.54
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	19	4.53
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG2	19	4.53
(1,1062)	1:50:A:LYS:H	1:51:A:GLU:HG3	19	4.53
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	2	4.53
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	2	4.53
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	10	4.53
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	10	4.53
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	10	4.53
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	10	4.53
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	8	4.53
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	8	4.53
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	8	4.53
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	8	4.53
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	8	4.53
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	8	4.53
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	7	4.53
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	7	4.53
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	7	4.53
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	19	4.53
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	17	4.53
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	17	4.53
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	17	4.53
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	9	4.53
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	15	4.53
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	15	4.53
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	15	4.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	15	4.53
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	4.53
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	10	4.53
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	10	4.53
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	10	4.53
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	7	4.53
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	7	4.53
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	7	4.53
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	10	4.53
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	10	4.53
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	10	4.53
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	10	4.53
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	10	4.53
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	14	4.53
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	14	4.53
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	14	4.53
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	6	4.53
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	6	4.53
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	6	4.53
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	6	4.53
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	6	4.53
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	6	4.53
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	6	4.53
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	14	4.53
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	14	4.53
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	15	4.52
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	2	4.52
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	2	4.52
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	20	4.52
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	10	4.52
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	2	4.52
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	2	4.52
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	8	4.52
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	8	4.52
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	8	4.52
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	9	4.52
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	9	4.52
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	9	4.52
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	3	4.52
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	3	4.52
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	3	4.52
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	3	4.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	4	4.52
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	4	4.52
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	6	4.52
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	1	4.52
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	1	4.52
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	14	4.52
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	16	4.52
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	16	4.52
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	16	4.52
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	10	4.52
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	6	4.52
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	6	4.52
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	6	4.52
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	12	4.52
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	12	4.52
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	12	4.52
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	11	4.52
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	11	4.52
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	11	4.52
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	5	4.52
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	5	4.52
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	5	4.52
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	4	4.52
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	4	4.52
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	14	4.51
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	3	4.51
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	3	4.51
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	17	4.51
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	17	4.51
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	3	4.51
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	3	4.51
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	8	4.51
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	8	4.51
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	17	4.51
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	17	4.51
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	2	4.51
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	2	4.51
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	2	4.51
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	20	4.51
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	20	4.51
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	20	4.51
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	19	4.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	19	4.51
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	19	4.51
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	20	4.51
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	20	4.51
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	20	4.51
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	17	4.51
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	17	4.51
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	8	4.51
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	13	4.51
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	13	4.51
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	13	4.51
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	11	4.5
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	11	4.5
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	16	4.5
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	16	4.5
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	16	4.5
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	3	4.5
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	3	4.5
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	5	4.5
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	5	4.5
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	1	4.5
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	1	4.5
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	14	4.5
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	14	4.5
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	11	4.5
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	11	4.5
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	8	4.5
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	8	4.5
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	8	4.5
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	8	4.5
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	5	4.5
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	5	4.5
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	5	4.5
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	5	4.5
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	5	4.5
(1,652)	1:38:A:THR:HB	1:55:A:PRO:HG3	2	4.5
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	3	4.5
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	4.5
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	4.5
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	4.5
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	4.5
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	17	4.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	7	4.5
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	17	4.5
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	2	4.5
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	2	4.5
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	2	4.5
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	2	4.5
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	2	4.5
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	2	4.5
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	8	4.49
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	8	4.49
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	14	4.49
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	12	4.49
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	12	4.49
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	11	4.49
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	11	4.49
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	11	4.49
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	11	4.49
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	7	4.49
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	7	4.49
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	7	4.49
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	7	4.49
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	7	4.49
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	5	4.49
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	5	4.49
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	7	4.49
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	7	4.49
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	7	4.49
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	7	4.49
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	6	4.49
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	6	4.49
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	6	4.49
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	17	4.49
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	17	4.49
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	15	4.48
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	8	4.48
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	8	4.48
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	8	4.48
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	8	4.48
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	17	4.48
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	9	4.48
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	9	4.48
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	9	4.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	9	4.48
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	12	4.48
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	12	4.48
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	14	4.48
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	14	4.48
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	14	4.48
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	14	4.48
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	14	4.48
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	14	4.48
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	1	4.48
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	1	4.48
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	1	4.48
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	1	4.48
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	5	4.48
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	5	4.48
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	5	4.48
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	15	4.48
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	15	4.48
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	15	4.48
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	6	4.48
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	7	4.48
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	7	4.48
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	7	4.48
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	15	4.48
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	15	4.48
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	15	4.48
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	15	4.48
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	16	4.48
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	16	4.48
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	16	4.48
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	10	4.48
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	15	4.48
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	1	4.48
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	19	4.48
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	11	4.48
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	11	4.48
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	4	4.48
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	4	4.48
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	4	4.48
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	8	4.48
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	8	4.48
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	8	4.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	9	4.48
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	12	4.48
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	12	4.48
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	12	4.47
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	12	4.47
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	12	4.47
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	12	4.47
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	2	4.47
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	9	4.47
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	17	4.47
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	5	4.47
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	5	4.47
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	5	4.47
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	5	4.47
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	6	4.47
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	6	4.47
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	3	4.47
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	10	4.47
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	17	4.47
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	7	4.47
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	14	4.47
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	14	4.47
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	14	4.47
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	14	4.47
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	14	4.47
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	14	4.47
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	13	4.47
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	13	4.47
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	13	4.47
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	13	4.47
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	13	4.47
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	13	4.47
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	13	4.47
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	13	4.47
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	13	4.47
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	3	4.47
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	3	4.47
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	3	4.47
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	11	4.47
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	11	4.47
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	11	4.47
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	15	4.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	15	4.47
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	15	4.47
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	1	4.46
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	1	4.46
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	19	4.46
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	19	4.46
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	8	4.46
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	4	4.46
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	4	4.46
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	4	4.46
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	4	4.46
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	7	4.46
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	7	4.46
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	7	4.46
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	15	4.46
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	5	4.46
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	4	4.46
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	8	4.46
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	8	4.46
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	8	4.46
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	8	4.46
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	8	4.46
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	8	4.46
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	3	4.46
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	5	4.46
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	3	4.46
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	3	4.46
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	11	4.46
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	11	4.46
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	11	4.46
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	13	4.46
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	13	4.46
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	13	4.46
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	3	4.45
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	2	4.45
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	2	4.45
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	2	4.45
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	3	4.45
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	3	4.45
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	20	4.45
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	20	4.45
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	19	4.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	19	4.45
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	18	4.45
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	13	4.45
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	9	4.45
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	2	4.45
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	20	4.45
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	20	4.45
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	20	4.45
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	20	4.45
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	7	4.45
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	7	4.45
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	7	4.45
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	7	4.45
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	7	4.45
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	7	4.45
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	13	4.45
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	20	4.45
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	13	4.45
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	13	4.45
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	4	4.45
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	4	4.45
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	4	4.45
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	10	4.45
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	10	4.45
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	9	4.44
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	9	4.44
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	9	4.44
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	9	4.44
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	9	4.44
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	15	4.44
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	15	4.44
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	11	4.44
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	11	4.44
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	11	4.44
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	11	4.44
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	4	4.44
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	4	4.44
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	18	4.44
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	18	4.44
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	6	4.44
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	19	4.44
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	19	4.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	6	4.44
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	6	4.44
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	16	4.44
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	16	4.44
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	20	4.44
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	20	4.44
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	7	4.43
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	7	4.43
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	7	4.43
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	10	4.43
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	10	4.43
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	13	4.43
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	13	4.43
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	9	4.43
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	19	4.43
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	7	4.43
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	7	4.43
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	7	4.43
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	7	4.43
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	1	4.43
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	7	4.43
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	7	4.43
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	16	4.43
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	1	4.43
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	1	4.43
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	1	4.43
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	1	4.43
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	5	4.43
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	18	4.43
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	12	4.43
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	15	4.43
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	3	4.43
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	11	4.43
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	8	4.43
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	12	4.43
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	12	4.43
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	12	4.43
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	1	4.43
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	1	4.43
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	6	4.43
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	2	4.43
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	2	4.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	2	4.43
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	20	4.43
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	20	4.43
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	9	4.42
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	9	4.42
(1,1076)	1:51:A:GLU:HA	1:52:A:CYS:HA	5	4.42
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	2	4.42
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	2	4.42
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	6	4.42
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	6	4.42
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	17	4.42
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	17	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	1	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	1	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	1	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	1	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	12	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	12	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	12	4.42
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	12	4.42
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	12	4.42
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	15	4.42
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	1	4.42
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	20	4.42
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	1	4.42
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	1	4.42
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	1	4.42
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	1	4.42
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	6	4.42
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	13	4.42
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	13	4.42
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	20	4.42
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	20	4.42
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	20	4.42
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	20	4.42
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	13	4.42
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	13	4.42
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	13	4.42
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	13	4.42
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	13	4.42
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	13	4.42
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	15	4.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	15	4.42
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	15	4.42
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	15	4.42
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	15	4.42
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	7	4.42
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	14	4.42
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	2	4.42
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	20	4.42
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	9	4.42
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	9	4.42
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	16	4.42
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	16	4.42
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	16	4.42
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	16	4.42
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	16	4.42
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	16	4.42
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	18	4.42
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	18	4.42
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	18	4.42
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	18	4.42
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	18	4.42
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	18	4.42
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	19	4.42
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	14	4.42
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	14	4.42
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	19	4.42
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	19	4.42
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	19	4.42
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	1	4.42
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	7	4.42
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	18	4.42
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	18	4.42
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	8	4.41
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	8	4.41
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	11	4.41
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	11	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	10	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	10	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	10	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	10	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	16	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	16	4.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	16	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	16	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	17	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	17	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	17	4.41
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	17	4.41
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	11	4.41
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	18	4.41
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	3	4.41
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	3	4.41
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	20	4.41
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	4.41
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	17	4.41
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	17	4.41
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	17	4.41
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	17	4.41
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	14	4.41
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	14	4.41
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	4.41
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	3	4.41
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	12	4.41
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	4	4.41
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	11	4.41
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	20	4.41
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	1	4.41
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	12	4.41
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	10	4.41
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	10	4.41
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	10	4.41
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	16	4.41
(1,226)	1:19:A:CYS:HB2	1:34:A:ALA:H	11	4.41
(1,226)	1:19:A:CYS:HB3	1:34:A:ALA:H	11	4.41
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	6	4.41
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	6	4.41
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	6	4.41
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	20	4.41
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	20	4.41
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	20	4.41
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	16	4.41
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	16	4.41
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	11	4.41
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	11	4.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	16	4.41
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	16	4.41
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	16	4.41
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	16	4.41
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	2	4.4
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	2	4.4
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	14	4.4
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	14	4.4
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	16	4.4
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	16	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	6	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	6	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	6	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	6	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	8	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	8	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	8	4.4
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	8	4.4
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	3	4.4
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	3	4.4
(1,951)	1:9:A:LYS:HG2	1:10:A:CYS:H	13	4.4
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	7	4.4
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	11	4.4
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	11	4.4
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	11	4.4
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	4.4
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	4.4
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	4.4
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	19	4.4
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	19	4.4
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	11	4.4
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	11	4.4
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	11	4.4
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	11	4.4
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	12	4.4
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	12	4.4
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	12	4.4
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	12	4.4
(1,783)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	15	4.4
(1,783)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	15	4.4
(1,783)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	15	4.4
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	7	4.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	14	4.4
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	14	4.4
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	14	4.4
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	6	4.4
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	6	4.4
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	18	4.4
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	18	4.4
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	18	4.4
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	3	4.4
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	8	4.4
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	16	4.4
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	10	4.4
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	6	4.39
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	7	4.39
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	7	4.39
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	18	4.39
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	18	4.39
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	4	4.39
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	4	4.39
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	4	4.39
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	4	4.39
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	20	4.39
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	20	4.39
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	1	4.39
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	1	4.39
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	1	4.39
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	1	4.39
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	1	4.39
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	1	4.39
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	13	4.39
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	13	4.39
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	18	4.39
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	18	4.39
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	18	4.39
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	7	4.39
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	7	4.39
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	3	4.39
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	3	4.39
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	3	4.39
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	3	4.39
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	13	4.39
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	13	4.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	13	4.39
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	13	4.39
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	13	4.39
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	13	4.39
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	13	4.39
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	12	4.39
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	12	4.39
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	12	4.39
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	3	4.39
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	6	4.39
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	18	4.39
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	17	4.39
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	6	4.39
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	6	4.39
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	6	4.39
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	6	4.39
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	6	4.39
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	6	4.39
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	3	4.39
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	3	4.39
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	3	4.39
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	3	4.39
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	3	4.39
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	3	4.39
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	18	4.39
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	16	4.39
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	18	4.39
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	9	4.39
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	9	4.39
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	9	4.39
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	2	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	2	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	2	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	2	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	19	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	19	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	19	4.38
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	19	4.38
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	5	4.38
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	5	4.38
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	16	4.38
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	17	4.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	17	4.38
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	17	4.38
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	20	4.38
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	20	4.38
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	16	4.38
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	16	4.38
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	16	4.38
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	18	4.38
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	18	4.38
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	9	4.38
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	18	4.38
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	16	4.38
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	16	4.38
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	16	4.38
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	5	4.38
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	5	4.38
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	18	4.38
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	13	4.38
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	7	4.38
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	7	4.38
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	7	4.38
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	3	4.38
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	3	4.38
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	13	4.37
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	3	4.37
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	3	4.37
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	3	4.37
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	20	4.37
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	20	4.37
(1,1074)	1:51:A:GLU:HG2	1:52:A:CYS:H	5	4.37
(1,1074)	1:51:A:GLU:HG3	1:52:A:CYS:H	5	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	9	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	9	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	9	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	9	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	15	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	15	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	15	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	15	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	18	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	18	4.37
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	18	4.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	18	4.37
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	2	4.37
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	2	4.37
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	14	4.37
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	15	4.37
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	8	4.37
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	20	4.37
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	16	4.37
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	16	4.37
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	16	4.37
(1,668)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	10	4.37
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	18	4.37
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	18	4.37
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	18	4.37
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	6	4.37
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	20	4.37
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	9	4.37
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	9	4.37
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	9	4.37
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	9	4.37
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	9	4.37
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	9	4.37
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	15	4.37
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	15	4.37
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	4	4.37
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	1	4.37
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	1	4.37
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	15	4.37
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	7	4.37
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	7	4.37
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	11	4.37
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	11	4.37
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	15	4.37
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	15	4.37
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	16	4.37
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	5	4.37
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	5	4.37
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	6	4.36
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	6	4.36
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	6	4.36
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	6	4.36
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	3	4.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	3	4.36
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	3	4.36
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	3	4.36
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	4	4.36
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	4	4.36
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	4	4.36
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	20	4.36
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	20	4.36
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	20	4.36
(1,794)	1:13:A:ALA:HB1	1:14:A:CYS:HB3	4	4.36
(1,794)	1:13:A:ALA:HB2	1:14:A:CYS:HB3	4	4.36
(1,794)	1:13:A:ALA:HB3	1:14:A:CYS:HB3	4	4.36
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	17	4.36
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	18	4.36
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	18	4.36
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	18	4.36
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	10	4.36
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	19	4.36
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	11	4.36
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	16	4.36
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	16	4.36
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	16	4.36
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	16	4.36
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	16	4.36
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	16	4.36
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	12	4.36
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	4	4.36
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	4	4.36
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	4	4.36
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	8	4.36
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	8	4.36
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	1	4.36
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	1	4.36
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	20	4.35
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	20	4.35
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	11	4.35
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	3	4.35
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	5	4.35
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	8	4.35
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	6	4.35
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	6	4.35
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	7	4.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	7	4.35
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	7	4.35
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	7	4.35
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	7	4.35
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	7	4.35
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	19	4.35
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	19	4.35
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	19	4.35
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	19	4.35
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	19	4.35
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	19	4.35
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	14	4.35
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	8	4.35
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	8	4.35
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	8	4.35
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	2	4.35
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	2	4.35
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	2	4.35
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	15	4.35
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	15	4.35
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	1	4.35
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	1	4.35
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	1	4.35
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	17	4.34
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	17	4.34
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	17	4.34
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	3	4.34
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	3	4.34
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	9	4.34
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	9	4.34
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	9	4.34
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	9	4.34
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	19	4.34
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	19	4.34
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	15	4.34
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	19	4.34
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	6	4.34
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	9	4.34
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	7	4.34
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	9	4.34
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	17	4.34
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	16	4.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	9	4.34
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	17	4.34
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	17	4.34
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	17	4.34
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	5	4.33
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	5	4.33
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	5	4.33
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	5	4.33
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	6	4.33
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	6	4.33
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	18	4.33
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	18	4.33
(1,982)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	19	4.33
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	2	4.33
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	14	4.33
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	20	4.33
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	20	4.33
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	20	4.33
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	20	4.33
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	20	4.33
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	20	4.33
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	4	4.33
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	4	4.33
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	4	4.33
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	18	4.33
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	18	4.33
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	18	4.33
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	6	4.33
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	6	4.33
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	6	4.33
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	2	4.33
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	5	4.33
(1,584)	1:20:A:GLN:HB3	1:21:A:CYS:H	14	4.33
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	19	4.33
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	6	4.33
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	6	4.33
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	6	4.32
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	6	4.32
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	6	4.32
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	6	4.32
(1,1105)	1:9:A:LYS:H	1:27:A:CYS:HB2	9	4.32
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	13	4.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	13	4.32
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	13	4.32
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	13	4.32
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	17	4.32
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	17	4.32
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	16	4.32
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	16	4.32
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	12	4.32
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	15	4.32
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	15	4.32
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	15	4.32
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	15	4.32
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	15	4.32
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	15	4.32
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	16	4.32
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	16	4.32
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	4.32
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	4.32
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	4.32
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	4.32
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	8	4.32
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	1	4.32
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	1	4.32
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	12	4.32
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	1	4.32
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	4.32
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	4.32
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	20	4.32
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	8	4.32
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	8	4.32
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	5	4.31
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	5	4.31
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	2	4.31
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	2	4.31
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	10	4.31
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	10	4.31
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	20	4.31
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	20	4.31
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	8	4.31
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	8	4.31
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	8	4.31
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	8	4.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	9	4.31
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	9	4.31
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	9	4.31
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	9	4.31
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	9	4.31
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	11	4.31
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	11	4.31
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	11	4.31
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	16	4.31
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	4	4.31
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	4	4.31
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	5	4.31
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	10	4.31
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	16	4.31
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	18	4.31
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	18	4.31
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	18	4.31
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	18	4.31
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	15	4.31
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	15	4.31
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	15	4.31
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	3	4.31
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	4	4.3
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	4	4.3
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	4	4.3
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	3	4.3
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	3	4.3
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	12	4.3
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	12	4.3
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	19	4.3
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	10	4.3
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	13	4.3
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	16	4.3
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	16	4.3
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	16	4.3
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	16	4.3
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	4	4.3
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	4	4.3
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	5	4.3
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	5	4.3
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	6	4.3
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	6	4.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	15	4.3
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	15	4.3
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	4	4.3
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	8	4.3
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	8	4.3
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	8	4.3
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	16	4.3
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	16	4.3
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	16	4.3
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	16	4.3
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	2	4.3
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	18	4.3
(1,573)	1:50:A:LYS:HG3	1:60:A:CYS:HA	19	4.3
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	19	4.3
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	19	4.3
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	19	4.3
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	19	4.3
(1,151)	1:39:A:CYS:HB3	1:56:A:ASP:H	19	4.3
(1,151)	1:39:A:CYS:HB2	1:56:A:ASP:H	19	4.3
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	8	4.3
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	8	4.3
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	8	4.3
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	8	4.3
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	8	4.3
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	12	4.29
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	11	4.29
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	11	4.29
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	3	4.29
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	3	4.29
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	12	4.29
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	12	4.29
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	16	4.29
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	16	4.29
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	20	4.29
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	20	4.29
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	4	4.29
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	4	4.29
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	4	4.29
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	4	4.29
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	17	4.29
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	12	4.29
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	13	4.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	16	4.29
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	16	4.29
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	16	4.29
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	16	4.29
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	15	4.29
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	2	4.29
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	16	4.29
(1,446)	1:48:A:CYS:H	1:66:A:CYS:HB2	18	4.29
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	13	4.29
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	13	4.29
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	13	4.29
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	5	4.29
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	5	4.29
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	5	4.29
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	6	4.29
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	15	4.29
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	10	4.29
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	10	4.29
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	18	4.29
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	6	4.29
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	6	4.29
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	9	4.29
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	9	4.29
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	9	4.29
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	14	4.29
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	14	4.29
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	14	4.29
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	14	4.29
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	1	4.28
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	1	4.28
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	7	4.28
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	7	4.28
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	7	4.28
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	7	4.28
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	7	4.28
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	7	4.28
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	16	4.28
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	16	4.28
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	18	4.28
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	13	4.28
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	13	4.28
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	13	4.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	6	4.28
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	6	4.28
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	19	4.28
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	5	4.28
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	5	4.28
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	5	4.28
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	5	4.28
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	5	4.28
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	5	4.28
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	20	4.28
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	20	4.28
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	20	4.28
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	20	4.28
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	20	4.28
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	20	4.28
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	17	4.28
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	17	4.28
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	17	4.28
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	1	4.28
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	1	4.28
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	1	4.28
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	1	4.28
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	1	4.28
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	1	4.28
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	4.28
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	12	4.28
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	12	4.28
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	12	4.28
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	17	4.28
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	19	4.28
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	19	4.28
(1,253)	1:41:A:CYS:H	1:55:A:PRO:HD3	6	4.28
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	2	4.28
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	2	4.28
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	2	4.28
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	14	4.28
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	14	4.28
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	14	4.28
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	16	4.28
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	16	4.28
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	16	4.28
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	3	4.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	3	4.27
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	1	4.27
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	1	4.27
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	2	4.27
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB2	18	4.27
(1,965)	1:11:A:THR:HG21	1:12:A:SER:HB3	18	4.27
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB2	18	4.27
(1,965)	1:11:A:THR:HG22	1:12:A:SER:HB3	18	4.27
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB2	18	4.27
(1,965)	1:11:A:THR:HG23	1:12:A:SER:HB3	18	4.27
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	10	4.27
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	10	4.27
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	10	4.27
(1,958)	1:9:A:LYS:HG3	1:29:A:GLU:H	15	4.27
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	1	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	1	4.27
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	2	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	2	4.27
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	9	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	9	4.27
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	10	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	10	4.27
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	11	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	11	4.27
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	18	4.27
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	18	4.27
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	1	4.27
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	1	4.27
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	4	4.27
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	4	4.27
(1,839)	1:37:A:LYS:HB3	1:38:A:THR:HA	5	4.27
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	14	4.27
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	14	4.27
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	14	4.27
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	14	4.27
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	19	4.27
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	19	4.27
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	19	4.27
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	19	4.27
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	5	4.27
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	5	4.27
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	3	4.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	3	4.27
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	12	4.27
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	12	4.27
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	12	4.27
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	12	4.27
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	9	4.27
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	2	4.27
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	11	4.27
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	5	4.27
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	5	4.27
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	5	4.27
(1,31)	1:17:A:GLU:H	1:20:A:GLN:HE21	6	4.27
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	13	4.26
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	13	4.26
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	19	4.26
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	19	4.26
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	10	4.26
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	18	4.26
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	18	4.26
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	19	4.26
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	19	4.26
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	12	4.26
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	12	4.26
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	12	4.26
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	12	4.26
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	17	4.26
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	17	4.26
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	19	4.26
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	19	4.26
(1,829)	1:50:A:LYS:HB2	1:52:A:CYS:HB2	12	4.26
(1,829)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	12	4.26
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	9	4.26
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	9	4.26
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	11	4.26
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	11	4.26
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	8	4.26
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	10	4.26
(1,670)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	10	4.26
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	4.26
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	4.26
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	4.26
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	4.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	3	4.26
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	13	4.26
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	13	4.26
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	12	4.26
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	12	4.26
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	12	4.26
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	11	4.26
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	11	4.26
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	11	4.26
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	15	4.26
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	15	4.26
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	15	4.26
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	2	4.26
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	2	4.26
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	7	4.26
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	19	4.26
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	19	4.26
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	1	4.25
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	1	4.25
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	10	4.25
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	10	4.25
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	10	4.25
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	10	4.25
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	7	4.25
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	7	4.25
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	9	4.25
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	9	4.25
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	17	4.25
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	4	4.25
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	4	4.25
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	4	4.25
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	18	4.25
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	18	4.25
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	13	4.25
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	13	4.25
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	13	4.25
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	13	4.25
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	13	4.25
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	13	4.25
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	13	4.25
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	13	4.25
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	13	4.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	3	4.25
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	3	4.25
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	3	4.25
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	20	4.25
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	20	4.25
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	20	4.25
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	4	4.25
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	4	4.25
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	13	4.25
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	13	4.25
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	19	4.24
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	19	4.24
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	19	4.24
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	7	4.24
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	7	4.24
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	7	4.24
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	7	4.24
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	19	4.24
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	19	4.24
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	8	4.24
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	8	4.24
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	5	4.24
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	5	4.24
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	5	4.24
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	6	4.24
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	6	4.24
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	6	4.24
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	3	4.24
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	3	4.24
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	4	4.24
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG2	4	4.24
(1,636)	1:10:A:CYS:HA	1:15:A:ARG:HG3	4	4.24
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	4	4.24
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	4.24
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	5	4.24
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	10	4.24
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	10	4.24
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	20	4.24
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	20	4.24
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	20	4.24
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	20	4.24
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	4	4.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	4	4.24
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	14	4.24
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	14	4.24
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	4	4.24
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	4	4.24
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	4	4.24
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	17	4.24
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	17	4.24
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	20	4.23
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB2	20	4.23
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	20	4.23
(1,1069)	1:51:A:GLU:H	1:52:A:CYS:HB3	20	4.23
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	8	4.23
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	8	4.23
(1,933)	1:8:A:GLU:H	1:9:A:LYS:HB2	2	4.23
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	10	4.23
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	10	4.23
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	18	4.23
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	18	4.23
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	18	4.23
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	18	4.23
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	18	4.23
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	18	4.23
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	18	4.23
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	18	4.23
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	18	4.23
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	18	4.23
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	18	4.23
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	18	4.23
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	18	4.23
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	18	4.23
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	18	4.23
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	1	4.23
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	1	4.23
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	1	4.23
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	7	4.23
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	7	4.23
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	1	4.23
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	9	4.22
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	9	4.22
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	12	4.22
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	12	4.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	12	4.22
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	9	4.22
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	9	4.22
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	9	4.22
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	18	4.22
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	18	4.22
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	18	4.22
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	13	4.22
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	13	4.22
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	1	4.22
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	1	4.22
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	1	4.22
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	18	4.22
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	18	4.22
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	9	4.22
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	10	4.22
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	10	4.22
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	20	4.22
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	20	4.22
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	1	4.22
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	1	4.22
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	4	4.21
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	2	4.21
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	2	4.21
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	17	4.21
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	17	4.21
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	17	4.21
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	4	4.21
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	4	4.21
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	4	4.21
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	4	4.21
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	4	4.21
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	4	4.21
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	1	4.21
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	1	4.21
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	14	4.21
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	14	4.21
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	1	4.21
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	8	4.21
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	8	4.21
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	2	4.21
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	2	4.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	4	4.21
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	4	4.2
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	4	4.2
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	4	4.2
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	4	4.2
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	8	4.2
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	8	4.2
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	18	4.2
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	18	4.2
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	6	4.2
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	6	4.2
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	20	4.2
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	4.2
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	4.2
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	14	4.2
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	14	4.2
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	1	4.2
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	1	4.2
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	15	4.2
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	15	4.2
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	9	4.2
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	9	4.2
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	4	4.2
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	7	4.2
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	7	4.2
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	3	4.2
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	5	4.2
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	8	4.2
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	9	4.2
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	16	4.2
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	6	4.2
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	6	4.2
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	6	4.2
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	6	4.2
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	6	4.2
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	6	4.2
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	6	4.2
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	6	4.2
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	6	4.2
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	12	4.2
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	12	4.2
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	13	4.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	13	4.2
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	4	4.2
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	4	4.2
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	4	4.2
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	4	4.2
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	12	4.19
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	12	4.19
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	12	4.19
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	12	4.19
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	3	4.19
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	3	4.19
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	3	4.19
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	3	4.19
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	13	4.19
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	13	4.19
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	13	4.19
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	13	4.19
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	12	4.19
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	12	4.19
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	2	4.19
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	2	4.19
(1,774)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	3	4.19
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	3	4.19
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	15	4.19
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	15	4.19
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	15	4.19
(1,613)	1:16:A:SER:H	1:20:A:GLN:HB2	17	4.19
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	18	4.19
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	4	4.19
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	19	4.19
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	19	4.19
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	19	4.19
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	19	4.19
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	19	4.19
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	19	4.19
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	17	4.19
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	17	4.19
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	7	4.19
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	7	4.19
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	13	4.19
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	13	4.19
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	13	4.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	9	4.19
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	9	4.19
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	20	4.18
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	20	4.18
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	19	4.18
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	19	4.18
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	17	4.18
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	17	4.18
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	9	4.18
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	5	4.18
(1,961)	1:15:A:ARG:HD2	1:16:A:SER:H	5	4.18
(1,961)	1:15:A:ARG:HD3	1:16:A:SER:H	5	4.18
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	19	4.18
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	19	4.18
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	19	4.18
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	19	4.18
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	8	4.18
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	8	4.18
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	16	4.18
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	6	4.18
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	6	4.18
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	6	4.18
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	4	4.18
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	18	4.18
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	14	4.18
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	19	4.18
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	19	4.18
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	9	4.18
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	9	4.18
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	12	4.18
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	12	4.18
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	12	4.18
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	19	4.17
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	19	4.17
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	19	4.17
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	19	4.17
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	4	4.17
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	4	4.17
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	4	4.17
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	4	4.17
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	12	4.17
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	12	4.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	12	4.17
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	12	4.17
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	4.17
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	4.17
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	16	4.17
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	16	4.17
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	2	4.17
(1,828)	1:39:A:CYS:HB2	1:52:A:CYS:HB3	2	4.17
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	2	4.17
(1,828)	1:39:A:CYS:HB3	1:52:A:CYS:HB3	2	4.17
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	12	4.17
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	3	4.17
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	3	4.17
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	3	4.17
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	6	4.17
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	6	4.17
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	6	4.17
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	6	4.17
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	6	4.17
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	3	4.17
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	3	4.17
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	1	4.17
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	1	4.17
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	1	4.17
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	2	4.17
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	2	4.17
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	2	4.17
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	19	4.17
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	19	4.17
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	19	4.17
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	9	4.17
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	9	4.17
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	6	4.17
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	6	4.17
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	6	4.17
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	7	4.17
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	7	4.17
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	7	4.17
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	12	4.17
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	8	4.16
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	13	4.16
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	13	4.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	17	4.16
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	17	4.16
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	15	4.16
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	15	4.16
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	16	4.16
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	16	4.16
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	16	4.16
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	7	4.16
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	7	4.16
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	7	4.16
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	17	4.16
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	17	4.16
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	17	4.16
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	14	4.16
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	18	4.16
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	18	4.16
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	18	4.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	7	4.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	7	4.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	7	4.16
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	7	4.16
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	5	4.15
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	5	4.15
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	20	4.15
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	20	4.15
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	10	4.15
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	10	4.15
(1,997)	1:30:A:GLY:H	1:31:A:CYS:HB2	18	4.15
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	13	4.15
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	4.15
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	4.15
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	4.15
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	4.15
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	11	4.15
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	11	4.15
(1,674)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	11	4.15
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	13	4.15
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	13	4.15
(1,614)	1:14:A:CYS:H	1:26:A:GLN:HB2	8	4.15
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	3	4.15
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	3	4.15
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	3	4.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	1	4.15
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	1	4.15
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	1	4.15
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	1	4.15
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	1	4.15
(1,263)	1:32:A:THR:H	1:33:A:CYS:HA	20	4.15
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB2	19	4.15
(1,97)	1:14:A:CYS:H	1:15:A:ARG:HB3	19	4.15
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	18	4.14
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	18	4.14
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	10	4.14
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	10	4.14
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	13	4.14
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	13	4.14
(1,1066)	1:24:A:LYS:HA	1:25:A:CYS:HB2	8	4.14
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	15	4.14
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	15	4.14
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	18	4.14
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	18	4.14
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	5	4.14
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	5	4.14
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	5	4.14
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	5	4.14
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	15	4.14
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	15	4.14
(1,882)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	15	4.14
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	15	4.14
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	15	4.14
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	15	4.14
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	20	4.14
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	19	4.14
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	19	4.14
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	19	4.14
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	1	4.14
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	4	4.14
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	4	4.14
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	10	4.14
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	10	4.14
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	10	4.14
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	10	4.14
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	10	4.14
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	1	4.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	3	4.13
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	13	4.13
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	2	4.13
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	2	4.13
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	2	4.13
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	2	4.13
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	18	4.13
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	18	4.13
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	18	4.13
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	18	4.13
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	4.13
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	4.13
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	11	4.13
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	11	4.13
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	11	4.13
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	11	4.13
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	11	4.13
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	11	4.13
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	11	4.13
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	11	4.13
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	17	4.13
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	17	4.13
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	17	4.13
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	17	4.13
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	17	4.13
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	17	4.13
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	5	4.13
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	5	4.13
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	7	4.13
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	7	4.13
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	7	4.13
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	19	4.13
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB2	11	4.13
(1,728)	1:9:A:LYS:HB3	1:27:A:CYS:HB3	11	4.13
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	5	4.13
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	5	4.13
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	5	4.13
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	2	4.13
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	2	4.13
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	13	4.13
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	13	4.13
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	13	4.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	9	4.13
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	9	4.13
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	5	4.13
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	5	4.13
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	5	4.13
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	5	4.13
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	5	4.13
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	5	4.13
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	6	4.13
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	6	4.13
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	6	4.13
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	4	4.13
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	4	4.13
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	17	4.13
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	6	4.13
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	6	4.13
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	10	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	10	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	10	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	10	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	20	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	20	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	20	4.12
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	20	4.12
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	11	4.12
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	11	4.12
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	8	4.12
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	8	4.12
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	1	4.12
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	16	4.12
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	16	4.12
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	20	4.12
(1,841)	1:37:A:LYS:HB2	1:38:A:THR:HA	19	4.12
(1,841)	1:37:A:LYS:HB3	1:38:A:THR:HA	19	4.12
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	1	4.12
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	1	4.12
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	1	4.12
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	10	4.12
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	10	4.12
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	10	4.12
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	11	4.12
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	11	4.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	11	4.12
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	9	4.12
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	1	4.12
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	1	4.12
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	1	4.12
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	1	4.12
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	15	4.11
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	15	4.11
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	5	4.11
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	5	4.11
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	5	4.11
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	4	4.11
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	18	4.11
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	18	4.11
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	18	4.11
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	4	4.11
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	4	4.11
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	13	4.11
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	10	4.11
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	16	4.1
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	20	4.1
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	20	4.1
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	20	4.1
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	20	4.1
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	4.1
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	4.1
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	6	4.1
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	6	4.1
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	4	4.1
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	4	4.1
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	4	4.1
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	4	4.1
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	4	4.1
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	4	4.1
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	9	4.1
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	9	4.1
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	9	4.1
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB2	3	4.1
(1,776)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	3	4.1
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	16	4.1
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	16	4.1
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	9	4.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	9	4.1
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	9	4.1
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	3	4.1
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	3	4.1
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	3	4.1
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	10	4.1
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	10	4.1
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	10	4.1
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	2	4.1
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	16	4.09
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	8	4.09
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	4.09
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	4.09
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	8	4.09
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	8	4.09
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	4.09
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	4.09
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	15	4.09
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	15	4.09
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	12	4.09
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	1	4.09
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	1	4.09
(1,811)	1:40:A:ASN:HB2	1:41:A:CYS:HA	12	4.09
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	17	4.09
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	17	4.09
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	17	4.09
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	18	4.08
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	18	4.08
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	18	4.08
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	19	4.08
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	5	4.08
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	5	4.08
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	7	4.08
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	7	4.08
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	7	4.08
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	7	4.08
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	7	4.08
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	20	4.08
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	15	4.08
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	15	4.08
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	20	4.08
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	20	4.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	20	4.08
(1,134)	1:13:A:ALA:H	1:26:A:GLN:HB2	4	4.08
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	7	4.07
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	9	4.07
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	9	4.07
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	12	4.07
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	12	4.07
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB2	11	4.07
(1,676)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	11	4.07
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB2	11	4.07
(1,676)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	11	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	3	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	3	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	3	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	8	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	8	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	8	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	15	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	15	4.07
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	15	4.07
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	5	4.07
(1,457)	1:61:A:GLY:HA2	1:64:A:CYS:H	8	4.07
(1,457)	1:61:A:GLY:HA3	1:64:A:CYS:H	8	4.07
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	18	4.06
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	18	4.06
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	18	4.06
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	15	4.06
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	15	4.06
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	8	4.06
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	1	4.06
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	14	4.06
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	14	4.06
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	14	4.06
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	14	4.06
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	20	4.06
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	20	4.06
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	20	4.06
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	20	4.06
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	6	4.06
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	6	4.06
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	6	4.06
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	8	4.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	8	4.06
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	8	4.06
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	20	4.06
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	9	4.06
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	9	4.06
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	9	4.06
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	16	4.06
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	16	4.06
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	16	4.06
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	7	4.06
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	10	4.06
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	4.06
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	4.06
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	4.06
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	4.06
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	5	4.06
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	12	4.06
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	12	4.06
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	12	4.06
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	12	4.06
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	12	4.06
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	5	4.06
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	5	4.06
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	5	4.06
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	5	4.06
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	5	4.06
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	5	4.06
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	8	4.06
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	10	4.06
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	12	4.06
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	12	4.06
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	12	4.06
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	16	4.05
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	16	4.05
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	16	4.05
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	7	4.05
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	7	4.05
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	7	4.05
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	7	4.05
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	2	4.05
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	5	4.05
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	20	4.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	20	4.05
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	20	4.05
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	4.05
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	20	4.05
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	4.05
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	5	4.05
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	5	4.05
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	5	4.05
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	5	4.05
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	5	4.05
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	5	4.05
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	18	4.05
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	18	4.05
(1,823)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	11	4.05
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	11	4.05
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	11	4.05
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	11	4.05
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	11	4.05
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	11	4.05
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	11	4.05
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	11	4.05
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	11	4.05
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	11	4.05
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	2	4.05
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	5	4.05
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	9	4.05
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	9	4.05
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	9	4.05
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	19	4.05
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	19	4.05
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	2	4.05
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	8	4.05
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	11	4.05
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	11	4.05
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	11	4.05
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	11	4.05
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	12	4.04
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	12	4.04
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	12	4.04
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	12	4.04
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	12	4.04
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	18	4.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	18	4.04
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	18	4.04
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	10	4.04
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	10	4.04
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	2	4.04
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	2	4.04
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	2	4.04
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	14	4.04
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	14	4.04
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	14	4.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	2	4.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	2	4.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	2	4.04
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	4	4.04
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	13	4.04
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	13	4.04
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	13	4.04
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	13	4.04
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	8	4.03
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	8	4.03
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	8	4.03
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	8	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	4	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	4	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	7	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	7	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	16	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	16	4.03
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	2	4.03
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	2	4.03
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	2	4.03
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	2	4.03
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	15	4.03
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	15	4.03
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	4	4.03
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	4	4.03
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	4	4.03
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	18	4.03
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	18	4.03
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	14	4.03
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE2	15	4.03
(1,316)	1:6:A:LYS:H	1:6:A:LYS:HE3	15	4.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	14	4.03
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	14	4.03
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	14	4.03
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB2	14	4.03
(1,276)	1:39:A:CYS:H	1:58:A:CYS:HB3	14	4.03
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	1	4.02
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	1	4.02
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	12	4.02
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	12	4.02
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB2	7	4.02
(1,1032)	1:55:A:PRO:HB2	1:58:A:CYS:HB3	7	4.02
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	2	4.02
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	14	4.02
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	14	4.02
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	14	4.02
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	14	4.02
(1,950)	1:6:A:LYS:HG2	1:10:A:CYS:H	9	4.02
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	6	4.02
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	6	4.02
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	20	4.02
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	20	4.02
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	6	4.02
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	9	4.02
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	14	4.02
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	14	4.02
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	14	4.02
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	14	4.02
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	14	4.02
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	14	4.02
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	17	4.02
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	17	4.02
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	17	4.02
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	17	4.02
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	17	4.02
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	17	4.02
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	15	4.02
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	15	4.02
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	15	4.02
(1,96)	1:14:A:CYS:H	1:15:A:ARG:HG3	18	4.02
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	10	4.01
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	18	4.01
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	4	4.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	4	4.01
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	4	4.01
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	4	4.01
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	4	4.01
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	4	4.01
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	18	4.01
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	9	4.01
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	9	4.01
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	17	4.01
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	17	4.01
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	17	4.01
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	6	4.01
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	6	4.01
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	6	4.01
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	6	4.01
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	7	4.01
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	7	4.01
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	7	4.01
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	8	4.0
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	8	4.0
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	13	4.0
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	13	4.0
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	15	4.0
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	15	4.0
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	15	4.0
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	15	4.0
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	12	4.0
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	12	4.0
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	4	4.0
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	4	4.0
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	4	4.0
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	4	4.0
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	9	4.0
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	9	4.0
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	9	4.0
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	9	4.0
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	9	4.0
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	9	4.0
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	1	4.0
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	1	4.0
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	1	4.0
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	3	4.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	3	4.0
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	3	4.0
(1,726)	1:60:A:CYS:HB2	1:64:A:CYS:H	18	4.0
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	6	4.0
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	6	4.0
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	6	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	6	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	6	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	6	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	10	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	10	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	10	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	18	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	18	4.0
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	18	4.0
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	13	4.0
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	14	4.0
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	14	4.0
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	14	4.0
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	13	4.0
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	13	4.0
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	13	4.0
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	12	4.0
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	12	4.0
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	12	3.99
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	12	3.99
(1,1127)	1:6:A:LYS:HG2	1:9:A:LYS:HA	9	3.99
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	9	3.99
(1,1127)	1:6:A:LYS:HG3	1:9:A:LYS:HA	9	3.99
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	2	3.99
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	2	3.99
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	3	3.99
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	3	3.99
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	1	3.99
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	9	3.99
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	9	3.99
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	9	3.99
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	9	3.99
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	3	3.99
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	8	3.99
(1,922)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	8	3.99
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	3	3.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	3	3.99
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	3	3.99
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	3	3.99
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	15	3.99
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	15	3.99
(1,884)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	15	3.99
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB1	15	3.99
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB2	15	3.99
(1,884)	1:33:A:CYS:HB3	1:34:A:ALA:HB3	15	3.99
(1,868)	1:67:A:LYS:HB2	1:67:A:LYS:HE3	4	3.99
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	12	3.99
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	12	3.99
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	12	3.99
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	17	3.99
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	17	3.99
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	17	3.99
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	17	3.99
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	17	3.99
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	17	3.99
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	14	3.99
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	2	3.99
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	2	3.99
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	2	3.99
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	4	3.99
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	4	3.99
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	4	3.99
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	2	3.99
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	2	3.99
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	2	3.99
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	6	3.99
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	6	3.99
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	10	3.99
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	10	3.99
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	10	3.99
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	10	3.99
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	10	3.99
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	14	3.99
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	14	3.99
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	14	3.99
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	14	3.99
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	14	3.99
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	18	3.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	18	3.99
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	18	3.99
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	6	3.99
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	6	3.99
(1,32)	1:19:A:CYS:H	1:20:A:GLN:HE21	17	3.99
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	7	3.98
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	3	3.98
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	3	3.98
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	13	3.98
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	13	3.98
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	13	3.98
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	13	3.98
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	14	3.98
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	14	3.98
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	14	3.98
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	14	3.98
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	19	3.98
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	19	3.98
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	19	3.98
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	19	3.98
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	19	3.98
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	13	3.98
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	5	3.98
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	5	3.98
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	5	3.98
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	14	3.98
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	14	3.98
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	14	3.98
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	10	3.98
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	10	3.98
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	13	3.98
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	5	3.98
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	5	3.98
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	5	3.98
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	5	3.98
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	17	3.97
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	17	3.97
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	17	3.97
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	17	3.97
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	2	3.97
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	4	3.97
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	4	3.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	4	3.97
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	6	3.97
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	6	3.97
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	8	3.97
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	8	3.97
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	9	3.97
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	9	3.97
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	9	3.97
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	19	3.97
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	3	3.97
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	3	3.97
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	3	3.97
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	3	3.97
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	3	3.97
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	3	3.97
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	16	3.97
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	16	3.97
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	5	3.96
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	5	3.96
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	5	3.96
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	5	3.96
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	18	3.96
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	3.96
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	18	3.96
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	18	3.96
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	5	3.96
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	5	3.96
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	7	3.96
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	7	3.96
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	4	3.96
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	4	3.96
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	4	3.96
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	4	3.96
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	4	3.96
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	12	3.96
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	12	3.96
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	2	3.96
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	2	3.96
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	15	3.96
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	15	3.96
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	14	3.95
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	14	3.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	14	3.95
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	14	3.95
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	3	3.95
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	3	3.95
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	9	3.95
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	9	3.95
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	9	3.95
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	5	3.95
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	5	3.95
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	5	3.95
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	8	3.95
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	20	3.95
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	20	3.95
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	20	3.95
(1,338)	1:47:A:LYS:H	1:66:A:CYS:HB3	17	3.95
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	3	3.95
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	3	3.95
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	18	3.95
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	18	3.95
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	18	3.95
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	1	3.94
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	1	3.94
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	1	3.94
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	1	3.94
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	1	3.94
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	13	3.94
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	4	3.94
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	4	3.94
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	4	3.94
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	4	3.94
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	10	3.94
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	10	3.94
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	10	3.94
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	10	3.94
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	10	3.94
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	10	3.94
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	10	3.94
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	10	3.94
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	19	3.94
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	19	3.94
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	4	3.94
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	4	3.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	4	3.94
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	4	3.94
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	4	3.94
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	4	3.94
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	13	3.94
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	13	3.94
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	7	3.94
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	7	3.94
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	16	3.94
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	16	3.94
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	16	3.94
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	14	3.94
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	14	3.94
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	14	3.94
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	10	3.93
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	10	3.93
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	3	3.93
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	3	3.93
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	3	3.93
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	1	3.93
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	1	3.93
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	1	3.93
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	1	3.93
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	1	3.93
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	1	3.93
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	3	3.93
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	3	3.93
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	3	3.93
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	3	3.93
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	3	3.93
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	3	3.93
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	1	3.93
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	1	3.93
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	9	3.93
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	9	3.93
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	3	3.93
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	3	3.93
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	3	3.93
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	3	3.93
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	3	3.93
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	19	3.93
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	2	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	2	3.93
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	2	3.93
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	2	3.93
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	3	3.93
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	3	3.93
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	3	3.93
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	6	3.93
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	6	3.93
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	6	3.93
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	9	3.92
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	9	3.92
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	8	3.92
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	8	3.92
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	8	3.92
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	9	3.92
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	9	3.92
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	16	3.92
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	4	3.92
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	4	3.92
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	8	3.92
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	3.92
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	3.92
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	7	3.92
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	7	3.92
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	4	3.92
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	4	3.92
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	4	3.92
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	4	3.92
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	3	3.92
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	3	3.92
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	3	3.92
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	2	3.92
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	2	3.92
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	11	3.92
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	11	3.92
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	4	3.92
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	4	3.92
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	20	3.92
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	20	3.92
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	14	3.92
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	14	3.92
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	14	3.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	3	3.92
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	13	3.92
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	13	3.92
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	11	3.92
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	11	3.92
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	11	3.92
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	15	3.92
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	15	3.92
(1,14)	1:19:A:CYS:HB2	1:35:A:ALA:H	11	3.92
(1,14)	1:19:A:CYS:HB3	1:35:A:ALA:H	11	3.92
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	6	3.91
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	19	3.91
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	19	3.91
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	6	3.91
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	9	3.91
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	9	3.91
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	9	3.91
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	9	3.91
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	17	3.91
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	17	3.91
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	16	3.91
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	16	3.91
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	16	3.91
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	16	3.91
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	16	3.91
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	16	3.91
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	11	3.91
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	11	3.91
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	1	3.91
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	1	3.91
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	1	3.91
(1,540)	1:42:A:THR:HA	1:53:A:THR:HA	11	3.91
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE2	14	3.91
(1,143)	1:61:A:GLY:H	1:67:A:LYS:HE3	14	3.91
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	10	3.91
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	10	3.91
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	10	3.91
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	10	3.91
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	9	3.9
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	9	3.9
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE2	14	3.9
(1,1058)	1:50:A:LYS:H	1:50:A:LYS:HE3	14	3.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	9	3.9
(1,947)	1:6:A:LYS:HG2	1:9:A:LYS:HA	9	3.9
(1,947)	1:6:A:LYS:HG3	1:9:A:LYS:HA	9	3.9
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	4	3.9
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	4	3.9
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	4	3.9
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	14	3.9
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	14	3.9
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	18	3.9
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	18	3.9
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	18	3.9
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	16	3.9
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	16	3.9
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	2	3.9
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	5	3.9
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	1	3.9
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	1	3.9
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	4	3.9
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	4	3.9
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	18	3.9
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	18	3.9
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	18	3.9
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	18	3.9
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	17	3.9
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	17	3.9
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	14	3.89
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	14	3.89
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	3.89
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	3.89
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	20	3.89
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	14	3.89
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	14	3.89
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	9	3.89
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	18	3.89
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	1	3.89
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	1	3.89
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	1	3.89
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	3	3.89
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	3	3.89
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	7	3.89
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	14	3.89
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	16	3.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	9	3.89
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	9	3.89
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	9	3.89
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	9	3.89
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	9	3.89
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	9	3.89
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	9	3.89
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	9	3.89
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	9	3.89
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	9	3.89
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	9	3.89
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	17	3.89
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	17	3.89
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	17	3.89
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	14	3.89
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	14	3.89
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	14	3.89
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	12	3.89
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	12	3.89
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	14	3.88
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	14	3.88
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	10	3.88
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	10	3.88
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	14	3.88
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	8	3.88
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	8	3.88
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	8	3.88
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	8	3.88
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	8	3.88
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	8	3.88
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	9	3.88
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	9	3.88
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	9	3.88
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	9	3.88
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	18	3.88
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	18	3.88
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	18	3.88
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	18	3.88
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	18	3.88
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	18	3.88
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	20	3.88
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	20	3.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	20	3.88
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	14	3.88
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	14	3.88
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	19	3.88
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	19	3.88
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	19	3.88
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	2	3.88
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	18	3.88
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	18	3.88
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	18	3.88
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	6	3.88
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	6	3.88
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	6	3.88
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	6	3.88
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	6	3.88
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	4	3.88
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	4	3.88
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	3	3.88
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	3	3.88
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	16	3.88
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	16	3.88
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	8	3.88
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	7	3.87
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	7	3.87
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	7	3.87
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	20	3.87
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	8	3.87
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	8	3.87
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	8	3.87
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	8	3.87
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	2	3.87
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	2	3.87
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	2	3.87
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	2	3.87
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	2	3.87
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	2	3.87
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	9	3.87
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	9	3.87
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	5	3.87
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	5	3.87
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	5	3.87
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	8	3.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	8	3.87
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	8	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	3	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	3	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	3	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	7	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	7	3.87
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	7	3.87
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	11	3.87
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	17	3.87
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	19	3.87
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	19	3.87
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	19	3.87
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	6	3.87
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	6	3.87
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	6	3.87
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	15	3.87
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	15	3.87
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	15	3.87
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	19	3.87
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	19	3.87
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	19	3.87
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	15	3.87
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	15	3.87
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	15	3.87
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	6	3.87
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	6	3.87
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	16	3.87
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	16	3.87
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	16	3.87
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	13	3.87
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	13	3.87
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	14	3.86
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	14	3.86
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	5	3.86
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	10	3.86
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	17	3.86
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	2	3.86
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	2	3.86
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	2	3.86
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	3	3.86
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	3	3.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	10	3.86
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	10	3.86
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	10	3.86
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	10	3.86
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	10	3.86
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	10	3.86
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	10	3.86
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	10	3.86
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	10	3.86
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	1	3.86
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	3	3.86
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	4	3.86
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	5	3.86
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	5	3.86
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	5	3.86
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	10	3.86
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	10	3.86
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	10	3.86
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	10	3.86
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	2	3.86
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	2	3.86
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	2	3.86
(1,311)	1:7:A:GLY:H	1:10:A:CYS:H	7	3.86
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	2	3.86
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	2	3.86
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	7	3.86
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	7	3.86
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	20	3.86
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	20	3.86
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	6	3.85
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	6	3.85
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	6	3.85
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	2	3.85
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	16	3.85
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	17	3.85
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	19	3.85
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	19	3.85
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	4	3.85
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	7	3.85
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	15	3.85
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	17	3.85
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	4	3.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	4	3.85
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	4	3.85
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	10	3.85
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	10	3.85
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	10	3.85
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	17	3.85
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	17	3.85
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	17	3.85
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	14	3.85
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	14	3.85
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	14	3.85
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	14	3.85
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	14	3.85
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	14	3.85
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	18	3.85
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	18	3.85
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	18	3.85
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	18	3.85
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	18	3.85
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	18	3.85
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	18	3.85
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	18	3.85
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	18	3.85
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	9	3.85
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	13	3.85
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	13	3.85
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	20	3.85
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	20	3.85
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	20	3.85
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	18	3.85
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	18	3.85
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	18	3.85
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	18	3.85
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	18	3.85
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	9	3.85
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	9	3.85
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	18	3.85
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	18	3.85
(1,1163)	1:9:A:LYS:HG2	1:29:A:GLU:H	7	3.84
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	6	3.84
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	6	3.84
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	6	3.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	15	3.84
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	15	3.84
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	15	3.84
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	19	3.84
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	19	3.84
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	19	3.84
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	19	3.84
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	19	3.84
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	15	3.84
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	11	3.84
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	11	3.84
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	11	3.84
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	12	3.84
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	9	3.84
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	9	3.84
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	9	3.84
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	2	3.84
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	2	3.84
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	8	3.84
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	19	3.84
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	12	3.84
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	12	3.84
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	19	3.83
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	19	3.83
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	19	3.83
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	19	3.83
(1,983)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	17	3.83
(1,983)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	17	3.83
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	15	3.83
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	15	3.83
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	15	3.83
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	15	3.83
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	11	3.83
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	11	3.83
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	11	3.83
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	14	3.83
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	14	3.83
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	14	3.83
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	4	3.83
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	4	3.83
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	8	3.83
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	7	3.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	7	3.83
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	7	3.83
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	12	3.83
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	12	3.83
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	12	3.83
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	14	3.83
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	14	3.83
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	3	3.82
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	15	3.82
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	4	3.82
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	1	3.82
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	1	3.82
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	1	3.82
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	1	3.82
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	3	3.82
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	3	3.82
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	3	3.82
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	7	3.82
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	4	3.82
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	19	3.82
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	19	3.82
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	12	3.82
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	12	3.82
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	12	3.82
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	20	3.82
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB3	20	3.82
(1,644)	1:58:A:CYS:HA	1:59:A:LYS:HB2	20	3.82
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	5	3.82
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	5	3.82
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	5	3.82
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	3	3.82
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	3	3.82
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	5	3.82
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	5	3.82
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	5	3.82
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	5	3.82
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	5	3.82
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	5	3.82
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	5	3.82
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	5	3.82
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	5	3.82
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	1	3.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	1	3.82
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	1	3.82
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	13	3.81
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	19	3.81
(1,905)	1:54:A:GLY:HA3	1:55:A:PRO:HG3	14	3.81
(1,905)	1:54:A:GLY:HA2	1:55:A:PRO:HG3	14	3.81
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	10	3.81
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	10	3.81
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	10	3.81
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	10	3.81
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	10	3.81
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	10	3.81
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	7	3.81
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	7	3.81
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	7	3.81
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	7	3.81
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	7	3.81
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	7	3.81
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	19	3.81
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	17	3.81
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	17	3.81
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	17	3.81
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	1	3.81
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	1	3.81
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	1	3.81
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	14	3.81
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	14	3.81
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	14	3.81
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	7	3.81
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	7	3.81
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	4	3.81
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	4	3.81
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	4	3.81
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	6	3.81
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	6	3.81
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	11	3.81
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	11	3.81
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	13	3.8
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	19	3.8
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	12	3.8
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	12	3.8
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	12	3.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	18	3.8
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	18	3.8
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	18	3.8
(1,852)	1:11:A:THR:HG21	1:14:A:CYS:HA	19	3.8
(1,852)	1:11:A:THR:HG22	1:14:A:CYS:HA	19	3.8
(1,852)	1:11:A:THR:HG23	1:14:A:CYS:HA	19	3.8
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	11	3.8
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	11	3.8
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	11	3.8
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	11	3.8
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	11	3.8
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	14	3.8
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	14	3.8
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	14	3.8
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	14	3.8
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	14	3.8
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	14	3.8
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	12	3.8
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	12	3.8
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	12	3.8
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	9	3.79
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	9	3.79
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	9	3.79
(1,1137)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	4	3.79
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	14	3.79
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	14	3.79
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	14	3.79
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	1	3.79
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	7	3.79
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	11	3.79
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	17	3.79
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	19	3.79
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	7	3.79
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	7	3.79
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	7	3.79
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	13	3.79
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	13	3.79
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	13	3.79
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	15	3.79
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	15	3.79
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	15	3.79
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	7	3.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	7	3.79
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	2	3.79
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	2	3.79
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	2	3.79
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	2	3.79
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	2	3.79
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	2	3.79
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	6	3.79
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	6	3.79
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	6	3.79
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	6	3.79
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	6	3.79
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	6	3.79
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	11	3.79
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE21	6	3.79
(1,440)	1:11:A:THR:HG21	1:26:A:GLN:HE22	6	3.79
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE21	6	3.79
(1,440)	1:11:A:THR:HG22	1:26:A:GLN:HE22	6	3.79
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE21	6	3.79
(1,440)	1:11:A:THR:HG23	1:26:A:GLN:HE22	6	3.79
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	1	3.79
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	1	3.79
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	1	3.79
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	11	3.78
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	11	3.78
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	11	3.78
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	14	3.78
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	10	3.78
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	6	3.78
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	12	3.78
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	12	3.78
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	13	3.78
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	13	3.78
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	3.78
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	20	3.78
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	8	3.78
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	8	3.78
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	8	3.78
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	8	3.78
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	8	3.78
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	8	3.78
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	6	3.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	4	3.78
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	4	3.78
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	4	3.78
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	7	3.78
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	7	3.78
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	16	3.78
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	16	3.78
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	16	3.78
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	17	3.78
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	17	3.78
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	17	3.78
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	19	3.78
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	19	3.78
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	19	3.78
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	18	3.77
(1,1000)	1:31:A:CYS:H	1:37:A:LYS:HG2	15	3.77
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	3	3.77
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	3	3.77
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	16	3.77
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	16	3.77
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	16	3.77
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	16	3.77
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	16	3.77
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	16	3.77
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	9	3.77
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	9	3.77
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	9	3.77
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	9	3.77
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	9	3.77
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	9	3.77
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	10	3.77
(1,1154)	1:37:A:LYS:HG2	1:62:A:SER:HA	20	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	13	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	13	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	13	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	16	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	16	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	16	3.76
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	7	3.76
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	13	3.76
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	19	3.76
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	19	3.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	19	3.76
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	7	3.76
(1,574)	1:59:A:LYS:HB2	1:60:A:CYS:HA	8	3.76
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	8	3.76
(1,574)	1:59:A:LYS:HB3	1:60:A:CYS:HA	8	3.76
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	17	3.76
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	17	3.76
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	20	3.76
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	20	3.76
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	6	3.76
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	6	3.76
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	6	3.76
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	8	3.76
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	8	3.76
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	8	3.76
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	3	3.76
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	3	3.76
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	3	3.75
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	3	3.75
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	3	3.75
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE2	8	3.75
(1,1106)	1:9:A:LYS:H	1:9:A:LYS:HE3	8	3.75
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	15	3.75
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	15	3.75
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	12	3.75
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	12	3.75
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	3	3.75
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	3	3.75
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	3	3.75
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	3	3.75
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	3	3.75
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	3	3.75
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	3	3.75
(1,827)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	3	3.75
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	19	3.75
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	19	3.75
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	19	3.75
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	19	3.75
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	19	3.75
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	19	3.75
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	19	3.75
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	19	3.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	19	3.75
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	12	3.75
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	12	3.75
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	13	3.75
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	13	3.75
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	13	3.75
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	20	3.75
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	20	3.75
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	20	3.75
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	11	3.75
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	11	3.75
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	19	3.74
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	19	3.74
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	19	3.74
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	1	3.74
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	1	3.74
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	1	3.74
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	13	3.74
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	13	3.74
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	13	3.74
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	1	3.74
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	2	3.74
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	2	3.74
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	2	3.74
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	12	3.74
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	12	3.74
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	12	3.74
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	3	3.74
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	3	3.74
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	3	3.74
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	18	3.74
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	12	3.73
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	13	3.73
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	13	3.73
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	13	3.73
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	13	3.73
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	9	3.73
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	17	3.73
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	17	3.73
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	17	3.73
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	17	3.73
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	17	3.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	17	3.73
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	1	3.73
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	1	3.73
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	9	3.73
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	9	3.73
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	9	3.73
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	9	3.73
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	9	3.73
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	9	3.73
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	9	3.73
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	9	3.73
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	9	3.73
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	17	3.73
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	17	3.73
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	19	3.72
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	11	3.72
(1,954)	1:9:A:LYS:HG3	1:28:A:GLY:H	11	3.72
(1,859)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	16	3.72
(1,859)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	16	3.72
(1,859)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	16	3.72
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	15	3.72
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	1	3.72
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	6	3.72
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	10	3.72
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	7	3.72
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	20	3.72
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	20	3.72
(1,305)	1:7:A:GLY:HA2	1:10:A:CYS:H	19	3.72
(1,305)	1:7:A:GLY:HA3	1:10:A:CYS:H	19	3.72
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	10	3.71
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	10	3.71
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	10	3.71
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	1	3.71
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	1	3.71
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	1	3.71
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	1	3.71
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	3	3.71
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	3	3.71
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	3	3.71
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	3	3.71
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	12	3.71
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	12	3.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	12	3.71
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	12	3.71
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	13	3.71
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	13	3.71
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	13	3.71
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	13	3.71
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	13	3.71
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	1	3.71
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	1	3.71
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	2	3.71
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	2	3.71
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	7	3.71
(1,350)	1:26:A:GLN:HG2	1:27:A:CYS:H	7	3.71
(1,350)	1:26:A:GLN:HG3	1:27:A:CYS:H	7	3.71
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	19	3.7
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	19	3.7
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	19	3.7
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	19	3.7
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	12	3.7
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	18	3.7
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	18	3.7
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	18	3.7
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	18	3.7
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	3	3.7
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	3	3.7
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	3	3.7
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	3	3.7
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	3	3.7
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	3	3.7
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	3	3.7
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	3	3.7
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	3	3.7
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	1	3.7
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	7	3.7
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	7	3.7
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	17	3.7
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	17	3.7
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	10	3.7
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	10	3.7
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	11	3.7
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	11	3.7
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	5	3.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	5	3.7
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	19	3.69
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	19	3.69
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	1	3.69
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	18	3.69
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	20	3.69
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	12	3.69
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	12	3.69
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	12	3.69
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	12	3.69
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	1	3.69
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	1	3.69
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	1	3.69
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	1	3.69
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	1	3.69
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	1	3.69
(1,703)	1:13:A:ALA:HB1	1:26:A:GLN:HB3	10	3.69
(1,703)	1:13:A:ALA:HB2	1:26:A:GLN:HB3	10	3.69
(1,703)	1:13:A:ALA:HB3	1:26:A:GLN:HB3	10	3.69
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	8	3.69
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	8	3.69
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	7	3.69
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	7	3.69
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	7	3.69
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	7	3.69
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	7	3.69
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	9	3.69
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	9	3.69
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	14	3.69
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	14	3.69
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	1	3.69
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	1	3.69
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	8	3.68
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	20	3.68
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	17	3.68
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	17	3.68
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	10	3.68
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	17	3.68
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	17	3.68
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	17	3.68
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	11	3.68
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	11	3.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	5	3.68
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	5	3.68
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	10	3.68
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	10	3.68
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	10	3.68
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	4	3.67
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	6	3.67
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	6	3.67
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	6	3.67
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	6	3.67
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	9	3.67
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	9	3.67
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	20	3.67
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	20	3.67
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	20	3.67
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	20	3.67
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	20	3.67
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	2	3.67
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	2	3.67
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	11	3.67
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	14	3.67
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	17	3.67
(1,81)	1:11:A:THR:HG21	1:15:A:ARG:H	19	3.67
(1,81)	1:11:A:THR:HG22	1:15:A:ARG:H	19	3.67
(1,81)	1:11:A:THR:HG23	1:15:A:ARG:H	19	3.67
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	17	3.66
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	17	3.66
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	17	3.66
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	3	3.66
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	13	3.66
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	19	3.66
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	3	3.66
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	6	3.66
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	6	3.66
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	6	3.66
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	6	3.66
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	16	3.66
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	16	3.66
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	13	3.66
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	13	3.66
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	13	3.66
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	13	3.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	13	3.66
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	13	3.66
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	3	3.66
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	8	3.66
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	8	3.66
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	8	3.66
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	3.66
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	3.66
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	5	3.66
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	5	3.66
(1,1024)	1:41:A:CYS:H	1:47:A:LYS:HB2	5	3.65
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	9	3.65
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	9	3.65
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	8	3.65
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	17	3.65
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	5	3.65
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	12	3.65
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	12	3.65
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	2	3.65
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	2	3.65
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	2	3.65
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	20	3.65
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	20	3.65
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	16	3.65
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	16	3.65
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	14	3.65
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	14	3.65
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	14	3.65
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	14	3.65
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	14	3.65
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	14	3.65
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	14	3.65
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	14	3.65
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	14	3.65
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	13	3.65
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	6	3.65
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	14	3.64
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	6	3.64
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	14	3.64
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	20	3.64
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD2	2	3.64
(1,934)	1:8:A:GLU:H	1:9:A:LYS:HD3	2	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	6	3.64
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	6	3.64
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	6	3.64
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	6	3.64
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	19	3.64
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	19	3.64
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	19	3.64
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	20	3.64
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	12	3.64
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	12	3.64
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	12	3.64
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	20	3.64
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	20	3.64
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	20	3.64
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	16	3.64
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	3	3.63
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	3	3.63
(1,1055)	1:50:A:LYS:H	1:50:A:LYS:HG3	6	3.63
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	7	3.63
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	9	3.63
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	8	3.63
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	15	3.63
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	18	3.63
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	5	3.63
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	8	3.63
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	15	3.63
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	18	3.63
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	2	3.63
(1,673)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	2	3.63
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	20	3.63
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	3.63
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	20	3.63
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	20	3.63
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	20	3.63
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	20	3.63
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	14	3.63
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	9	3.63
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	9	3.63
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	9	3.63
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	9	3.63
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	8	3.63
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	8	3.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	16	3.63
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	18	3.63
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	18	3.63
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	7	3.62
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	7	3.62
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	2	3.62
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	4	3.62
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	10	3.62
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	3.62
(1,921)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	3.62
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	2	3.62
(1,921)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	2	3.62
(1,751)	1:13:A:ALA:HA	1:20:A:GLN:HG2	18	3.62
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	10	3.62
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	15	3.62
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	15	3.62
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	15	3.62
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	15	3.62
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	15	3.62
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	15	3.62
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	14	3.62
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	14	3.62
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	14	3.62
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	14	3.62
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	14	3.62
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	12	3.62
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	10	3.62
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	10	3.62
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	4	3.62
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	5	3.61
(1,1168)	1:37:A:LYS:HD3	1:38:A:THR:H	5	3.61
(1,1168)	1:37:A:LYS:HD2	1:38:A:THR:H	5	3.61
(1,1117)	1:6:A:LYS:HG2	1:10:A:CYS:H	9	3.61
(1,1117)	1:6:A:LYS:HG3	1:10:A:CYS:H	9	3.61
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	8	3.61
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	8	3.61
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	8	3.61
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	8	3.61
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	12	3.61
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	12	3.61
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	12	3.61
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	12	3.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	12	3.61
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	12	3.61
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	20	3.61
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD2	20	3.61
(1,741)	1:39:A:CYS:H	1:67:A:LYS:HD3	20	3.61
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	9	3.61
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	11	3.61
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	11	3.61
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	11	3.61
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	11	3.61
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	11	3.61
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	6	3.61
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	16	3.61
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	16	3.61
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	16	3.61
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	16	3.61
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	16	3.61
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	16	3.61
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	15	3.61
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	15	3.61
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	4	3.61
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	4	3.61
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	4	3.61
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	8	3.61
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	11	3.61
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	19	3.61
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	19	3.61
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	19	3.61
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	14	3.61
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	14	3.61
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	11	3.6
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	11	3.6
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	11	3.6
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	13	3.6
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	7	3.6
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	7	3.6
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	16	3.6
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	16	3.6
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	13	3.6
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	3	3.6
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	3	3.6
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	3	3.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	8	3.6
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	8	3.6
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	8	3.6
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	1	3.6
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	7	3.6
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	14	3.6
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	18	3.6
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	3	3.6
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	3	3.6
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	3	3.6
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	18	3.6
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	18	3.6
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	18	3.6
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	5	3.59
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	15	3.59
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	1	3.59
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	1	3.59
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	1	3.59
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	4	3.59
(1,739)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	4	3.59
(1,739)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	4	3.59
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	1	3.59
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	16	3.59
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	16	3.59
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	16	3.59
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	20	3.59
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	20	3.59
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	20	3.59
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	12	3.59
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	12	3.59
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	2	3.59
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	3	3.59
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	16	3.59
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	12	3.58
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	12	3.58
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	12	3.58
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	12	3.58
(1,938)	1:9:A:LYS:H	1:9:A:LYS:HB3	11	3.58
(1,730)	1:9:A:LYS:H	1:9:A:LYS:HB3	11	3.58
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	13	3.58
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	13	3.58
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	13	3.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	11	3.58
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	11	3.58
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	11	3.58
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	11	3.58
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	11	3.58
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	11	3.58
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	18	3.58
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	15	3.58
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	15	3.58
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	4	3.58
(1,526)	1:36:A:CYS:HB3	1:37:A:LYS:HG2	4	3.58
(1,526)	1:36:A:CYS:HB2	1:37:A:LYS:HG2	4	3.58
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	3	3.58
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	3	3.58
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	10	3.58
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	10	3.58
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	6	3.58
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	10	3.58
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	13	3.58
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	15	3.58
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	19	3.58
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	20	3.58
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	2	3.58
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	2	3.58
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	2	3.58
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	4	3.57
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	8	3.57
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	8	3.57
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	8	3.57
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	16	3.57
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	4	3.57
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	4	3.57
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	4	3.57
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	4	3.57
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	4	3.57
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	4	3.57
(1,654)	1:38:A:THR:HB	1:39:A:CYS:H	5	3.57
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	13	3.57
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	13	3.57
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	13	3.57
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	14	3.57
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	14	3.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	14	3.57
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	14	3.57
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	7	3.57
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	17	3.57
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	4	3.57
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	9	3.57
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	17	3.57
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	6	3.57
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	8	3.56
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	8	3.56
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	8	3.56
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	8	3.56
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	8	3.56
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	17	3.56
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	12	3.56
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	12	3.56
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	12	3.56
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	12	3.56
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	12	3.56
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	12	3.56
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	20	3.56
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	20	3.56
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	20	3.56
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	20	3.56
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	20	3.56
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	20	3.56
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	20	3.56
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	20	3.56
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	20	3.56
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	2	3.56
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	8	3.56
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	8	3.56
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	8	3.56
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	8	3.56
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	8	3.56
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	1	3.56
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	1	3.56
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	8	3.56
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	8	3.56
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	8	3.56
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	13	3.56
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	13	3.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	13	3.56
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	1	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	1	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	1	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	1	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	11	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	11	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	11	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	11	3.55
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	19	3.55
(1,930)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	19	3.55
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	19	3.55
(1,930)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	19	3.55
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	9	3.55
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	11	3.55
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	15	3.55
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	20	3.55
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	8	3.55
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	8	3.55
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	8	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	9	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	9	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	9	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	9	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	9	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	9	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	12	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	12	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	12	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	12	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	12	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	12	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	14	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	14	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	14	3.55
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	14	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	14	3.55
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	14	3.55
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	13	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	13	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	13	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	13	3.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	2	3.54
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	2	3.54
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	2	3.54
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	2	3.54
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	2	3.54
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	2	3.54
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	9	3.54
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	9	3.54
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	7	3.54
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	7	3.54
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	7	3.54
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	7	3.54
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	8	3.54
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	20	3.54
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	5	3.54
(1,255)	1:41:A:CYS:H	1:41:A:CYS:HB3	12	3.54
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	10	3.53
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	10	3.53
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	10	3.53
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	10	3.53
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	5	3.53
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	10	3.53
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	10	3.53
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	10	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	7	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	7	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	7	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	7	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	7	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	7	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	19	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	19	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	19	3.53
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	19	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	19	3.53
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	19	3.53
(1,615)	1:11:A:THR:H	1:26:A:GLN:HB2	8	3.53
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	6	3.53
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	6	3.53
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	15	3.53
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	15	3.53
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	15	3.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	15	3.53
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	17	3.53
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	17	3.53
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	17	3.53
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	17	3.53
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	7	3.53
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	7	3.53
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	9	3.53
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	14	3.53
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	14	3.53
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	14	3.53
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	17	3.53
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	17	3.53
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	17	3.53
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	7	3.53
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	10	3.53
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	10	3.53
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	10	3.53
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	3	3.52
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	3	3.52
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	3	3.52
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	3	3.52
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	17	3.52
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	17	3.52
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	17	3.52
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	17	3.52
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	2	3.52
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	2	3.52
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	2	3.52
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	3	3.52
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	9	3.52
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	11	3.52
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	11	3.52
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	11	3.52
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	17	3.52
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	17	3.52
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB2	9	3.52
(1,307)	1:10:A:CYS:H	1:27:A:CYS:HB3	9	3.52
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	15	3.52
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	20	3.52
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	20	3.52
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	16	3.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	5	3.51
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	5	3.51
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	7	3.51
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	7	3.51
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	7	3.51
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	7	3.51
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	11	3.51
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	11	3.51
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	11	3.51
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	13	3.51
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	13	3.51
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	13	3.51
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	18	3.51
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	18	3.51
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	18	3.51
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	18	3.51
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	18	3.51
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	18	3.51
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	3.51
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	3.51
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	3.51
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	3.51
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	3.51
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	11	3.51
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	11	3.51
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	19	3.51
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	14	3.51
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	14	3.51
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	14	3.51
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	12	3.51
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	12	3.51
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	12	3.51
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	12	3.51
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	20	3.51
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	20	3.51
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	20	3.51
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	20	3.51
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	18	3.51
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	18	3.51
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	6	3.5
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	6	3.5
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	14	3.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	14	3.5
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	11	3.5
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	3.5
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	20	3.5
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	20	3.5
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	20	3.5
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	3.5
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	15	3.5
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	15	3.5
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	15	3.5
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	15	3.5
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	15	3.5
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	15	3.5
(1,323)	1:60:A:CYS:HB2	1:62:A:SER:H	19	3.5
(1,323)	1:60:A:CYS:HB3	1:62:A:SER:H	19	3.5
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	10	3.5
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	15	3.5
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	19	3.5
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	11	3.5
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	5	3.5
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	5	3.5
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	5	3.5
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	11	3.5
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	11	3.5
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	11	3.5
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	19	3.49
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	18	3.49
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	18	3.49
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	18	3.49
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	13	3.49
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	13	3.49
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	2	3.49
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	14	3.49
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	15	3.49
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	17	3.49
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	8	3.49
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	8	3.49
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	8	3.49
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	8	3.49
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	8	3.49
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	2	3.49
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	2	3.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	2	3.49
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	2	3.49
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	2	3.49
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	2	3.49
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	11	3.49
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	11	3.49
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	11	3.49
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	11	3.49
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	19	3.49
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	19	3.49
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	19	3.49
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	19	3.49
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	10	3.49
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	3	3.49
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	15	3.48
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	15	3.48
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	15	3.48
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	15	3.48
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	16	3.48
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	16	3.48
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	16	3.48
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	15	3.48
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	15	3.48
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	1	3.48
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	8	3.48
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	10	3.48
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	10	3.48
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	10	3.48
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	5	3.48
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	6	3.48
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	6	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	1	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	1	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	1	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	1	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	2	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	2	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	2	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	2	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	3	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	3	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	3	3.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	3	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	4	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	4	3.48
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	4	3.48
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	4	3.48
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	12	3.48
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	12	3.48
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	12	3.48
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	20	3.48
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	14	3.48
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	5	3.48
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	1	3.47
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	1	3.47
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	10	3.47
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	2	3.47
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD2	2	3.47
(1,675)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	2	3.47
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD2	2	3.47
(1,675)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	2	3.47
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	2	3.47
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	2	3.47
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	2	3.47
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	2	3.47
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	2	3.47
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	2	3.47
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	13	3.47
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	13	3.47
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	13	3.47
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	13	3.47
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	13	3.47
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	13	3.47
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	19	3.47
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	19	3.47
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	10	3.47
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	10	3.47
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	10	3.47
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	6	3.47
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	6	3.47
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	6	3.47
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	6	3.47
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	16	3.47
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	16	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	16	3.47
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	16	3.47
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	18	3.47
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	18	3.47
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	18	3.47
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	18	3.47
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	20	3.46
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	20	3.46
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	20	3.46
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	8	3.46
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	9	3.46
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	9	3.46
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	9	3.46
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	9	3.46
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	18	3.46
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	3	3.46
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	3	3.45
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	6	3.45
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	10	3.45
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	11	3.45
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	12	3.45
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	2	3.45
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	7	3.45
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	7	3.45
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	7	3.45
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	7	3.45
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	9	3.45
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	9	3.45
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	12	3.45
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	1	3.45
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	1	3.45
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	1	3.45
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	1	3.45
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	1	3.45
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	1	3.45
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	8	3.45
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	8	3.45
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	8	3.45
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	8	3.45
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	8	3.45
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	8	3.45
(1,564)	1:6:A:LYS:HD2	1:9:A:LYS:HA	9	3.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,564)	1:6:A:LYS:HD3	1:9:A:LYS:HA	9	3.45
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	5	3.45
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	7	3.45
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	7	3.45
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	7	3.45
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	15	3.45
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	15	3.45
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	15	3.45
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	2	3.45
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	2	3.45
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	11	3.45
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	11	3.45
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	13	3.45
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	2	3.45
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	1	3.45
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	18	3.45
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	1	3.45
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	1	3.45
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	14	3.44
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	15	3.44
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	20	3.44
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	6	3.44
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	11	3.44
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	2	3.44
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	2	3.44
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	14	3.44
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	3	3.44
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	3	3.44
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	3	3.44
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	3	3.44
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	3	3.44
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	3	3.44
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	9	3.44
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	9	3.44
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	9	3.44
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	10	3.44
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	6	3.44
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	12	3.44
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	12	3.44
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	4	3.43
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	10	3.43
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	6	3.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	6	3.43
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	8	3.43
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	8	3.43
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	8	3.43
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	5	3.42
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	11	3.42
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	11	3.42
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	19	3.42
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	19	3.42
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	19	3.42
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	19	3.42
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	18	3.42
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	18	3.42
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	18	3.42
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	18	3.42
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	6	3.42
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	6	3.42
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	14	3.42
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	14	3.42
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	14	3.42
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	12	3.42
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	12	3.42
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	20	3.42
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	20	3.42
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	13	3.42
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	1	3.41
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	14	3.41
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	14	3.41
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	17	3.41
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	17	3.41
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	17	3.41
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	17	3.41
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	4	3.41
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	4	3.41
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	11	3.41
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	11	3.41
(1,791)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	11	3.41
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	8	3.41
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	8	3.41
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	8	3.41
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	8	3.41
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	8	3.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	8	3.41
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	8	3.41
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	8	3.41
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	8	3.41
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	5	3.41
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	5	3.41
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	5	3.41
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	5	3.41
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	4	3.41
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	4	3.41
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	8	3.41
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	9	3.41
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	9	3.41
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	5	3.4
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	5	3.4
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	5	3.4
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	5	3.4
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	5	3.4
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	5	3.4
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	6	3.4
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	15	3.4
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	15	3.4
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	8	3.4
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	8	3.4
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	8	3.4
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	8	3.4
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	10	3.4
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	10	3.4
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	10	3.4
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	10	3.4
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	11	3.4
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	11	3.4
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	11	3.4
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	11	3.4
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	11	3.4
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	11	3.4
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	16	3.4
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	16	3.4
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	10	3.4
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	10	3.4
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	18	3.39
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	20	3.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	20	3.39
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	13	3.39
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	18	3.39
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	10	3.39
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	2	3.39
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	2	3.39
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	11	3.39
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	19	3.39
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	19	3.39
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	3	3.39
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	2	3.38
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	14	3.38
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	14	3.38
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB2	14	3.38
(1,1153)	1:37:A:LYS:HG2	1:62:A:SER:HB3	14	3.38
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	1	3.38
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	1	3.38
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	1	3.38
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	1	3.38
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	1	3.38
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	1	3.38
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	1	3.38
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	1	3.38
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	6	3.38
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	6	3.38
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	6	3.38
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	6	3.38
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	6	3.38
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	6	3.38
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	18	3.38
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	18	3.38
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	19	3.38
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	19	3.38
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	16	3.38
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	9	3.37
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	9	3.37
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	9	3.37
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	9	3.37
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	9	3.37
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	9	3.37
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	9	3.37
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	17	3.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	4	3.37
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	4	3.37
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	4	3.37
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	4	3.37
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	19	3.37
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	19	3.37
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	17	3.37
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	17	3.37
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	7	3.37
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	9	3.37
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	9	3.37
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	9	3.37
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	9	3.37
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	9	3.37
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	9	3.37
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	9	3.37
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	9	3.37
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	9	3.37
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	3	3.37
(1,422)	1:19:A:CYS:HB2	1:22:A:GLY:H	5	3.37
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	5	3.37
(1,422)	1:19:A:CYS:HB3	1:22:A:GLY:H	5	3.37
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	19	3.37
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	2	3.37
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	2	3.37
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	2	3.37
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	2	3.37
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	2	3.37
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	2	3.37
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	2	3.37
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	2	3.37
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	2	3.37
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	3	3.37
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	3	3.37
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	6	3.37
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	6	3.37
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	13	3.37
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	13	3.37
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	4	3.36
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	2	3.36
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	2	3.36
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	2	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	10	3.36
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	10	3.36
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	3	3.36
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	3	3.36
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	3	3.36
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	13	3.36
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	13	3.36
(1,391)	1:66:A:CYS:HB2	1:67:A:LYS:H	13	3.36
(1,391)	1:66:A:CYS:HB3	1:67:A:LYS:H	13	3.36
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	2	3.36
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	12	3.35
(1,778)	1:31:A:CYS:HB3	1:37:A:LYS:HB2	18	3.35
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	16	3.35
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	16	3.35
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	13	3.35
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	13	3.35
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	8	3.34
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	9	3.34
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	13	3.34
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	17	3.34
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	12	3.34
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	12	3.34
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	12	3.34
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	12	3.34
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	3	3.34
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	3	3.34
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	19	3.34
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	19	3.34
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	19	3.34
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	19	3.34
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	19	3.34
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	19	3.34
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	5	3.34
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	5	3.34
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	14	3.34
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	14	3.34
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	14	3.34
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	14	3.34
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	14	3.34
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	14	3.34
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	14	3.34
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	14	3.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	14	3.34
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	15	3.34
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	15	3.34
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	7	3.34
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	7	3.34
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	7	3.34
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	7	3.33
(1,1161)	1:43:A:SER:HA	1:44:A:ASP:H	16	3.33
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	5	3.33
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	16	3.32
(1,1007)	1:37:A:LYS:HG2	1:38:A:THR:HA	16	3.32
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	12	3.32
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	12	3.32
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	10	3.32
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	10	3.32
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	19	3.32
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	1	3.32
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	7	3.32
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	20	3.32
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	13	3.32
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	13	3.32
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	8	3.32
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	8	3.32
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	8	3.32
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	8	3.32
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	8	3.32
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	8	3.32
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	1	3.32
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	1	3.32
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	11	3.32
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	11	3.32
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	11	3.32
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	20	3.32
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	15	3.31
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	15	3.31
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	15	3.31
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	7	3.31
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	8	3.31
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	16	3.31
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB2	16	3.31
(1,720)	1:26:A:GLN:H	1:27:A:CYS:HB3	16	3.31
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	12	3.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	11	3.31
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	12	3.31
(1,55)	1:7:A:GLY:HA2	1:9:A:LYS:H	16	3.31
(1,55)	1:7:A:GLY:HA3	1:9:A:LYS:H	16	3.31
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	16	3.3
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	13	3.3
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	13	3.3
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	13	3.3
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	13	3.3
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	12	3.3
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	12	3.3
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	12	3.3
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	18	3.3
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	18	3.3
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	8	3.3
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	10	3.3
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	10	3.3
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	8	3.29
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	8	3.29
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	8	3.29
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	8	3.29
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	17	3.29
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	14	3.29
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	14	3.29
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	4	3.29
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	4	3.29
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	9	3.29
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	17	3.29
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	17	3.29
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	17	3.29
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	17	3.29
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	1	3.28
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	1	3.28
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	16	3.28
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	16	3.28
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	16	3.28
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	16	3.28
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	16	3.28
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	16	3.28
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	7	3.28
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	7	3.28
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	7	3.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	8	3.28
(1,295)	1:39:A:CYS:HA	1:40:A:ASN:HD21	14	3.28
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	7	3.28
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	7	3.28
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	9	3.27
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	13	3.27
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	13	3.27
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	13	3.27
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	16	3.27
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	8	3.27
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	8	3.27
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	5	3.27
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	5	3.27
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	5	3.27
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	5	3.27
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	5	3.27
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	7	3.27
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	7	3.27
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	7	3.27
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	19	3.27
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	16	3.27
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	16	3.27
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	4	3.26
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	4	3.26
(1,1005)	1:37:A:LYS:HG2	1:38:A:THR:HA	16	3.26
(1,1005)	1:37:A:LYS:HG3	1:38:A:THR:HA	16	3.26
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	14	3.26
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	1	3.26
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	1	3.26
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	1	3.26
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	10	3.26
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	10	3.26
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	9	3.26
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	9	3.26
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	9	3.26
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	9	3.26
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	9	3.26
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	2	3.25
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	2	3.25
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	2	3.25
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	2	3.25
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	3	3.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	5	3.25
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	15	3.25
(1,916)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	15	3.25
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	15	3.25
(1,916)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	15	3.25
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	19	3.25
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	13	3.25
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	19	3.25
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	17	3.25
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	17	3.25
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	17	3.25
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	3	3.25
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	4	3.25
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	4	3.25
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	4	3.25
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	11	3.25
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	8	3.25
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	8	3.25
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	18	3.25
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	18	3.25
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	19	3.25
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	19	3.25
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	20	3.25
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	20	3.25
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	18	3.24
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	18	3.24
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	6	3.24
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	6	3.24
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	6	3.24
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	6	3.24
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	6	3.24
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	6	3.24
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	6	3.24
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	6	3.24
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	6	3.24
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	17	3.24
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	17	3.24
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	17	3.24
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	16	3.24
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	16	3.24
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	11	3.24
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	11	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	10	3.24
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	17	3.24
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	17	3.24
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	6	3.23
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	6	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	9	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	9	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	9	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	16	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	16	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	16	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	18	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	18	3.23
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	18	3.23
(1,789)	1:50:A:LYS:HB2	1:51:A:GLU:H	20	3.23
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	3	3.23
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	3	3.23
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	6	3.23
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	7	3.23
(1,264)	1:30:A:GLY:HA2	1:32:A:THR:H	16	3.23
(1,264)	1:30:A:GLY:HA3	1:32:A:THR:H	16	3.23
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	3	3.23
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	3	3.23
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	4	3.23
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	4	3.23
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	3	3.22
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	6	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	1	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	1	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	1	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	2	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	2	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	2	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	3	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	3	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	3	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	4	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	4	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	4	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	5	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	5	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	5	3.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	7	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	7	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	7	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	8	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	8	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	8	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	10	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	10	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	10	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	11	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	11	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	11	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	12	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	12	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	12	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	13	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	13	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	13	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	14	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	14	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	14	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	17	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	17	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	17	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	19	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	19	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	19	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	20	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	20	3.22
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	20	3.22
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	8	3.22
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	8	3.22
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	8	3.22
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	8	3.22
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	8	3.22
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	8	3.22
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	8	3.22
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	8	3.22
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	8	3.22
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	6	3.22
(1,330)	1:37:A:LYS:HG3	1:62:A:SER:H	13	3.22
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	5	3.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	5	3.22
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	16	3.22
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	16	3.22
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	18	3.21
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	18	3.21
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	18	3.21
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	18	3.21
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	6	3.21
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	6	3.21
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	6	3.21
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	18	3.21
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	14	3.21
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	7	3.2
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG21	15	3.2
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG22	15	3.2
(1,843)	1:38:A:THR:HA	1:38:A:THR:HG23	15	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	8	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	8	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	8	3.2
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	8	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	8	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	16	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	16	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	16	3.2
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	16	3.2
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	16	3.2
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	19	3.2
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	19	3.2
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	7	3.2
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	7	3.2
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	7	3.2
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	7	3.2
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	7	3.2
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	7	3.2
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	7	3.2
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE22	7	3.2
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	7	3.2
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE22	7	3.2
(1,388)	1:24:A:LYS:HG2	1:26:A:GLN:HE21	7	3.2
(1,388)	1:24:A:LYS:HG3	1:26:A:GLN:HE21	7	3.2
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	5	3.2
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	17	3.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	6	3.2
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	6	3.2
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	1	3.19
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	1	3.19
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	1	3.19
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	16	3.19
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	16	3.19
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	16	3.19
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	16	3.19
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	2	3.19
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	2	3.19
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	2	3.19
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	2	3.19
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	2	3.19
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	2	3.19
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	2	3.19
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	2	3.19
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	2	3.19
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	1	3.19
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	1	3.19
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	1	3.19
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	1	3.19
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	1	3.19
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	1	3.19
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	1	3.19
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	3	3.19
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	5	3.19
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	5	3.19
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	2	3.19
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	2	3.19
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	19	3.19
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	14	3.18
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	7	3.18
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	9	3.18
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	9	3.18
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	9	3.18
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	8	3.18
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	12	3.18
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	1	3.18
(1,187)	1:37:A:LYS:HG2	1:38:A:THR:H	16	3.18
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	13	3.17
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	13	3.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	13	3.17
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	13	3.17
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	1	3.17
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	1	3.17
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	7	3.17
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	7	3.17
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	20	3.17
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	20	3.17
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	6	3.17
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	6	3.17
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	6	3.17
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	6	3.17
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	6	3.17
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	9	3.17
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	11	3.17
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	17	3.17
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	9	3.17
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	12	3.17
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	12	3.17
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	15	3.16
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	15	3.16
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	15	3.16
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	15	3.16
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	15	3.16
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	15	3.16
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	15	3.16
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	15	3.16
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	15	3.16
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	15	3.16
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	18	3.16
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	5	3.16
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	5	3.16
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	15	3.16
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	6	3.16
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	6	3.16
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	6	3.16
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	18	3.15
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	18	3.15
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	19	3.15
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	19	3.15
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	19	3.15
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	8	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	8	3.15
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	10	3.15
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	2	3.15
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	2	3.15
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	2	3.15
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	5	3.15
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	17	3.15
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	17	3.15
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	18	3.15
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	18	3.15
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	16	3.14
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	19	3.14
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	19	3.14
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	13	3.14
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	5	3.14
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	7	3.14
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	13	3.14
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	2	3.14
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	2	3.14
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	13	3.13
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	13	3.13
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	13	3.13
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	13	3.13
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	13	3.13
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	13	3.13
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	13	3.13
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	19	3.13
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	19	3.13
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	19	3.13
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	19	3.13
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	19	3.13
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	19	3.13
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	2	3.13
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	2	3.13
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	2	3.13
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	2	3.13
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	2	3.13
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	14	3.13
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	14	3.13
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	3	3.13
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	12	3.12
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	12	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	12	3.12
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	15	3.12
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	15	3.12
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	15	3.12
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	15	3.12
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	10	3.12
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	10	3.12
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB2	10	3.12
(1,666)	1:39:A:CYS:HB2	1:66:A:CYS:HB3	10	3.12
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB2	10	3.12
(1,666)	1:39:A:CYS:HB3	1:66:A:CYS:HB3	10	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	10	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	10	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	10	3.12
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	10	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	10	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	15	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	15	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	15	3.12
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	15	3.12
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	15	3.12
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	7	3.12
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	2	3.12
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	7	3.12
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	17	3.12
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	10	3.12
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	10	3.12
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	10	3.12
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	10	3.12
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	10	3.12
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	10	3.12
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	1	3.12
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	1	3.12
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	5	3.12
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	5	3.12
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	5	3.12
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	14	3.12
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	14	3.12
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	14	3.12
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	20	3.11
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	20	3.11
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	20	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	12	3.11
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	12	3.11
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	12	3.11
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	12	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	11	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	11	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	11	3.11
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	11	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	11	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	18	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	18	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	18	3.11
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	18	3.11
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	18	3.11
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	19	3.11
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	19	3.11
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	19	3.11
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	19	3.11
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	19	3.11
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	4	3.11
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	4	3.11
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	4	3.11
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	9	3.11
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	9	3.11
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	2	3.11
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	15	3.11
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	15	3.11
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	8	3.1
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	1	3.1
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	1	3.1
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	1	3.1
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	11	3.1
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	8	3.1
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	8	3.1
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	6	3.1
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	6	3.1
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	6	3.1
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	6	3.1
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	6	3.1
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	6	3.1
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	15	3.1
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	7	3.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	7	3.1
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	7	3.1
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	7	3.1
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	7	3.1
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	7	3.1
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	7	3.1
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	7	3.1
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	7	3.1
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	19	3.1
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	19	3.09
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	19	3.09
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	19	3.09
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	9	3.09
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	9	3.09
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	9	3.09
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	9	3.09
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	9	3.09
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	9	3.09
(1,669)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	11	3.09
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	13	3.09
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	13	3.09
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	1	3.09
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	1	3.09
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	1	3.09
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	1	3.09
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	1	3.09
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	11	3.09
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	11	3.09
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	11	3.09
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	6	3.09
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	6	3.09
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	17	3.09
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	17	3.09
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	19	3.08
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	14	3.08
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	14	3.08
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	16	3.08
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	16	3.08
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	17	3.08
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	17	3.08
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	19	3.08
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	19	3.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	19	3.08
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	19	3.08
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	19	3.08
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	11	3.08
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	11	3.08
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	11	3.08
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	14	3.08
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	9	3.08
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	9	3.08
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	9	3.08
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	9	3.08
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	2	3.07
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	2	3.07
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	18	3.07
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	18	3.07
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	5	3.07
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	5	3.07
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	5	3.07
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	16	3.07
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	16	3.07
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	20	3.07
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	7	3.07
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	3	3.06
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	3	3.06
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	3	3.06
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	4	3.06
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	4	3.06
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	4	3.06
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	4	3.06
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	4	3.06
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	4	3.06
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	14	3.06
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	10	3.06
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	10	3.06
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	10	3.06
(1,569)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	11	3.06
(1,569)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	11	3.06
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	12	3.06
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	12	3.06
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	12	3.06
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	15	3.06
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	15	3.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	15	3.06
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	5	3.05
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	1	3.05
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	1	3.05
(1,605)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	16	3.05
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	14	3.05
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	4	3.05
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	3	3.05
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	3	3.05
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	3	3.05
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	8	3.05
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	10	3.04
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	7	3.04
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	7	3.04
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	7	3.04
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	7	3.04
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	7	3.04
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	7	3.04
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	10	3.04
(1,792)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	10	3.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	15	3.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	15	3.04
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	15	3.04
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	18	3.04
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	18	3.04
(1,149)	1:54:A:GLY:HA3	1:56:A:ASP:H	13	3.04
(1,149)	1:54:A:GLY:HA2	1:56:A:ASP:H	13	3.04
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	12	3.03
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	12	3.03
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	12	3.03
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	4	3.03
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	4	3.03
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	4	3.03
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	4	3.03
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	4	3.03
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	4	3.03
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	4	3.03
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	4	3.03
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	4	3.03
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	9	3.03
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	9	3.03
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	16	3.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	12	3.03
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	15	3.03
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	15	3.03
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	15	3.03
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	5	3.03
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	19	3.02
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	19	3.02
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	19	3.02
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	2	3.02
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	18	3.02
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	18	3.02
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	17	3.02
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	17	3.02
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	17	3.02
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	17	3.02
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	17	3.02
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	4	3.02
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	3	3.02
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	5	3.02
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	5	3.02
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	15	3.01
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	15	3.01
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	4	3.01
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	4	3.01
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	13	3.01
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	13	3.01
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	17	3.01
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	7	3.01
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	7	3.01
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	20	3.01
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	20	3.01
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	9	3.01
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	9	3.01
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	9	3.01
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	10	3.01
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	10	3.01
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG2	18	3.0
(1,784)	1:11:A:THR:HG21	1:26:A:GLN:HG3	18	3.0
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG2	18	3.0
(1,784)	1:11:A:THR:HG22	1:26:A:GLN:HG3	18	3.0
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG2	18	3.0
(1,784)	1:11:A:THR:HG23	1:26:A:GLN:HG3	18	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	7	3.0
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	7	3.0
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	7	3.0
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG2	7	3.0
(1,758)	1:13:A:ALA:HB1	1:26:A:GLN:HG3	7	3.0
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG2	7	3.0
(1,758)	1:13:A:ALA:HB2	1:26:A:GLN:HG3	7	3.0
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	7	3.0
(1,758)	1:13:A:ALA:HB3	1:26:A:GLN:HG3	7	3.0
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	8	3.0
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	7	3.0
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	7	3.0
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	7	3.0
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	7	2.99
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	20	2.99
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	20	2.99
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	5	2.99
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	5	2.99
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	15	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	2	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	2	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	5	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	5	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	6	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	6	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	9	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	9	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	18	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	18	2.99
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	17	2.99
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	17	2.99
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	17	2.99
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	17	2.99
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	17	2.99
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	17	2.99
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	6	2.99
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	6	2.99
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	6	2.99
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	3	2.99
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	3	2.99
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	15	2.99
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	15	2.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	2	2.99
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	8	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	8	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	10	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	10	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	11	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	11	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	15	2.98
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	15	2.98
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	15	2.97
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE2	6	2.97
(1,1067)	1:50:A:LYS:HA	1:50:A:LYS:HE3	6	2.97
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	7	2.97
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	7	2.97
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	7	2.97
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	7	2.97
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	7	2.97
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	7	2.97
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	7	2.97
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	17	2.97
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	17	2.97
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB2	11	2.97
(1,667)	1:47:A:LYS:HB2	1:66:A:CYS:HB3	11	2.97
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	4	2.97
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	4	2.97
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	4	2.97
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	4	2.97
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	4	2.97
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	7	2.97
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	7	2.97
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	12	2.97
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	10	2.97
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	10	2.97
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	9	2.97
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	19	2.97
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	11	2.96
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	2	2.96
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	7	2.96
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	7	2.96
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	14	2.96
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	14	2.96
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	14	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	14	2.96
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	14	2.96
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	14	2.96
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	12	2.96
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	12	2.96
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	5	2.96
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	5	2.96
(1,458)	1:63:A:SER:HB2	1:64:A:CYS:H	18	2.96
(1,458)	1:63:A:SER:HB3	1:64:A:CYS:H	18	2.96
(1,371)	1:61:A:GLY:HA2	1:63:A:SER:H	8	2.96
(1,371)	1:61:A:GLY:HA3	1:63:A:SER:H	8	2.96
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	1	2.96
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	1	2.96
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	1	2.96
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	11	2.96
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	4	2.96
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	7	2.95
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	16	2.95
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	16	2.95
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	17	2.95
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	5	2.95
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	5	2.95
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	5	2.95
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	5	2.95
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	5	2.95
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	5	2.95
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	17	2.95
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	17	2.95
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	2.95
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	20	2.95
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	20	2.95
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	20	2.95
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	20	2.95
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	16	2.95
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	4	2.95
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	5	2.94
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	1	2.94
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	1	2.94
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	2	2.94
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	11	2.94
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	20	2.94
(1,1100)	1:6:A:LYS:HE2	1:29:A:GLU:H	8	2.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:6:A:LYS:HE3	1:29:A:GLU:H	8	2.94
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB2	14	2.94
(1,993)	1:51:A:GLU:H	1:51:A:GLU:HB3	14	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	3	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	3	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	3	2.94
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	3	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	3	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	7	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	7	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	7	2.94
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	7	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	7	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	13	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	13	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	13	2.94
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	13	2.94
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	13	2.94
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	18	2.94
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	10	2.94
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	10	2.94
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	10	2.94
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	12	2.93
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	20	2.93
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	2.93
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	20	2.93
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	15	2.93
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	9	2.93
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	10	2.93
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	10	2.93
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	10	2.93
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	10	2.93
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	10	2.93
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	10	2.93
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	10	2.93
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	10	2.93
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	10	2.93
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	9	2.93
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	5	2.93
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	5	2.93
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	2	2.92
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	19	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	19	2.92
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	19	2.92
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	15	2.92
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	15	2.92
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	12	2.92
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	12	2.92
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB2	12	2.92
(1,631)	1:50:A:LYS:HB2	1:52:A:CYS:HB3	12	2.92
(1,631)	1:50:A:LYS:HB3	1:52:A:CYS:HB3	12	2.92
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	4	2.92
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	4	2.92
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	12	2.92
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	12	2.92
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	19	2.92
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	19	2.92
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	19	2.92
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	3	2.91
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	14	2.91
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	11	2.91
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	2	2.91
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	2	2.91
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	2	2.91
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	1	2.91
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD2	3	2.91
(1,186)	1:38:A:THR:H	1:67:A:LYS:HD3	3	2.91
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	8	2.9
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	8	2.9
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	17	2.9
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	17	2.9
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	20	2.9
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	20	2.9
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	6	2.9
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	6	2.9
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	6	2.9
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	6	2.9
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	6	2.9
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	15	2.9
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	11	2.89
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	11	2.89
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	9	2.89
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	5	2.89
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	5	2.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	5	2.89
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	5	2.89
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	5	2.89
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	5	2.89
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD2	19	2.89
(1,899)	1:7:A:GLY:HA2	1:15:A:ARG:HD3	19	2.89
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD2	19	2.89
(1,899)	1:7:A:GLY:HA3	1:15:A:ARG:HD3	19	2.89
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	4	2.89
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	4	2.89
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	4	2.89
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	4	2.89
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	4	2.89
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	4	2.89
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	8	2.89
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	8	2.89
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	8	2.89
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	20	2.89
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	20	2.89
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	20	2.89
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	8	2.89
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	11	2.89
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	1	2.89
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	3	2.88
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	3	2.88
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	15	2.88
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	8	2.88
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	8	2.88
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	8	2.88
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	8	2.88
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	8	2.88
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	8	2.88
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	8	2.88
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	11	2.88
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	11	2.88
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	11	2.88
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	11	2.88
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	11	2.88
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	11	2.88
(1,444)	1:48:A:CYS:H	1:66:A:CYS:HB3	11	2.88
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG2	19	2.88
(1,412)	1:7:A:GLY:H	1:8:A:GLU:HG3	19	2.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	16	2.88
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	13	2.88
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	13	2.88
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	13	2.88
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	17	2.88
(1,273)	1:22:A:GLY:HA3	1:24:A:LYS:H	17	2.88
(1,273)	1:22:A:GLY:HA2	1:24:A:LYS:H	17	2.88
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	1	2.88
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	2	2.88
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	7	2.88
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	2	2.87
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	2	2.87
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	7	2.87
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	7	2.87
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	13	2.87
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	13	2.87
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	10	2.87
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	14	2.87
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	14	2.87
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	14	2.87
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	14	2.87
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	17	2.87
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	17	2.87
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	17	2.87
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	17	2.87
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	17	2.87
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	17	2.87
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	17	2.87
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	3	2.87
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	9	2.87
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	14	2.87
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	16	2.87
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	18	2.87
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	3	2.86
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	3	2.86
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	1	2.86
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	20	2.86
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	20	2.86
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	20	2.86
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	20	2.86
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	19	2.86
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	19	2.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	4	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	6	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	10	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	13	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	15	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	17	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	19	2.86
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	20	2.86
(1,244)	1:33:A:CYS:HB2	1:36:A:CYS:H	15	2.86
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	8	2.85
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	13	2.85
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	4	2.85
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	4	2.85
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	18	2.85
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	6	2.85
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	20	2.85
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	10	2.84
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	10	2.84
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	10	2.84
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	16	2.84
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	16	2.84
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	8	2.84
(1,883)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	2	2.84
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	1	2.84
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	19	2.84
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	10	2.84
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	12	2.83
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	12	2.83
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	17	2.83
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	10	2.83
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	8	2.83
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	8	2.83
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	8	2.83
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	8	2.83
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	8	2.83
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	8	2.83
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	15	2.83
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	15	2.83
(1,439)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	15	2.83
(1,439)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	15	2.83
(1,439)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	15	2.83
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	11	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	12	2.83
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	4	2.83
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	4	2.83
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	4	2.83
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	8	2.83
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	8	2.83
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA2	8	2.83
(1,53)	1:9:A:LYS:H	1:28:A:GLY:HA3	8	2.83
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE21	17	2.82
(1,981)	1:24:A:LYS:HD2	1:26:A:GLN:HE22	17	2.82
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	17	2.82
(1,981)	1:24:A:LYS:HD3	1:26:A:GLN:HE22	17	2.82
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	7	2.82
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	7	2.82
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	7	2.82
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	7	2.82
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	7	2.82
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	16	2.82
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	8	2.82
(1,251)	1:41:A:CYS:H	1:41:A:CYS:HA	5	2.82
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	9	2.82
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	19	2.82
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	19	2.82
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	19	2.82
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	2	2.81
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	2	2.81
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	6	2.81
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	6	2.81
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	18	2.81
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	18	2.81
(1,989)	1:26:A:GLN:H	1:26:A:GLN:HB3	12	2.81
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	15	2.81
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	15	2.81
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	15	2.81
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	15	2.81
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	15	2.81
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	15	2.81
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	15	2.81
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	15	2.81
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	15	2.81
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	15	2.81
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	9	2.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	9	2.81
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	9	2.81
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	6	2.81
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	11	2.81
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	3	2.81
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	20	2.81
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	19	2.8
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	4	2.8
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	4	2.8
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	4	2.8
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	6	2.8
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	6	2.8
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	6	2.8
(1,587)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	20	2.8
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	13	2.8
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	6	2.8
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	13	2.79
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG2	12	2.79
(1,1149)	1:5:A:GLY:H	1:6:A:LYS:HG3	12	2.79
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	10	2.79
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	15	2.79
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	15	2.79
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	15	2.79
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	1	2.79
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	17	2.79
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	16	2.79
(1,185)	1:37:A:LYS:HG2	1:38:A:THR:H	16	2.79
(1,185)	1:37:A:LYS:HG3	1:38:A:THR:H	16	2.79
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	16	2.78
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	16	2.78
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	16	2.78
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	16	2.78
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	16	2.78
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	16	2.78
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	16	2.78
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	3	2.78
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	6	2.78
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	6	2.78
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	4	2.78
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	4	2.78
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	4	2.78
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	4	2.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	4	2.78
(1,567)	1:9:A:LYS:HD2	1:29:A:GLU:H	4	2.78
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	15	2.78
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	19	2.78
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	15	2.77
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	15	2.77
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	15	2.77
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	15	2.77
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	15	2.77
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	15	2.77
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	15	2.77
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	2	2.77
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	6	2.77
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	6	2.77
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	5	2.77
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	7	2.77
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	3	2.76
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	18	2.76
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	5	2.76
(1,996)	1:7:A:GLY:H	1:10:A:CYS:HB2	9	2.76
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	10	2.76
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	16	2.76
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	2	2.76
(1,181)	1:38:A:THR:H	1:38:A:THR:HB	7	2.76
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	2	2.76
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	2	2.76
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	17	2.75
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	17	2.75
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	17	2.75
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	17	2.75
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	13	2.75
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	13	2.75
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	13	2.75
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	7	2.75
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	2	2.75
(1,881)	1:33:A:CYS:HB3	1:37:A:LYS:HG3	2	2.75
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	18	2.75
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	18	2.75
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	18	2.75
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	4	2.75
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	4	2.75
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	4	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	4	2.75
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	4	2.75
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	4	2.75
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	4	2.75
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	4	2.75
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	4	2.75
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	4	2.74
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	17	2.74
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	17	2.74
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	4	2.74
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	4	2.74
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	4	2.74
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	7	2.74
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	20	2.74
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	20	2.74
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	16	2.74
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	3	2.74
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	2	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	2	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	2	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	5	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	5	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	5	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	6	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	6	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	6	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	9	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	9	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	9	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	18	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	18	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	18	2.73
(1,1070)	1:27:A:CYS:HB2	1:29:A:GLU:H	11	2.73
(1,1070)	1:27:A:CYS:HB3	1:29:A:GLU:H	11	2.73
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	12	2.73
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	12	2.73
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	12	2.73
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	12	2.73
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	12	2.73
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	12	2.73
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	12	2.73
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	1	2.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	10	2.73
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	10	2.73
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	10	2.73
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	18	2.73
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	8	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	8	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	8	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	10	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	10	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	10	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	15	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	15	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	15	2.72
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	3	2.72
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	3	2.72
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	3	2.72
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	3	2.72
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	3	2.72
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	3	2.72
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	3	2.72
(1,941)	1:9:A:LYS:HB3	1:10:A:CYS:H	11	2.72
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	20	2.72
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	20	2.72
(1,885)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	20	2.72
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	20	2.72
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	20	2.72
(1,885)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	20	2.72
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	9	2.72
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	9	2.72
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	6	2.72
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	4	2.72
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	2	2.72
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	15	2.72
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	7	2.72
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	7	2.72
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	11	2.71
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	11	2.71
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	11	2.71
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	1	2.71
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	14	2.71
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	14	2.71
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	14	2.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	15	2.71
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	15	2.71
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	15	2.71
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	15	2.71
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	15	2.71
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	15	2.71
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	15	2.71
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	15	2.71
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	15	2.71
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	9	2.71
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	1	2.7
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	17	2.7
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	17	2.7
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	17	2.7
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	12	2.7
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	19	2.7
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	19	2.7
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	19	2.7
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	19	2.7
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	19	2.7
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	19	2.7
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	19	2.7
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	9	2.7
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	11	2.7
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	11	2.7
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	14	2.7
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	5	2.7
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	5	2.7
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	5	2.7
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	7	2.69
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	7	2.69
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	7	2.69
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	19	2.69
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	19	2.69
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	3	2.69
(1,441)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	3	2.69
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	3	2.69
(1,441)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	3	2.69
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	3	2.69
(1,441)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	3	2.69
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	16	2.69
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	14	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	14	2.68
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	14	2.68
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	16	2.68
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB2	16	2.68
(1,1072)	1:51:A:GLU:H	1:51:A:GLU:HB3	16	2.68
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	12	2.68
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	12	2.68
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	12	2.68
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	12	2.68
(1,925)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	12	2.68
(1,925)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	12	2.68
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	5	2.68
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	5	2.68
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	5	2.68
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	20	2.68
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	4	2.68
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	4	2.67
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	4	2.67
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	4	2.67
(1,610)	1:13:A:ALA:HB1	1:26:A:GLN:HB2	15	2.67
(1,610)	1:13:A:ALA:HB2	1:26:A:GLN:HB2	15	2.67
(1,610)	1:13:A:ALA:HB3	1:26:A:GLN:HB2	15	2.67
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	9	2.67
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	9	2.67
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	9	2.67
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	9	2.67
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	9	2.67
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	13	2.67
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	13	2.67
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	13	2.67
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	2	2.66
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	2	2.66
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	2	2.66
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	2	2.66
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	5	2.66
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	13	2.66
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	4	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	4	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	4	2.65
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	4	2.65
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	4	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	4	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	4	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	19	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	19	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	19	2.65
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	19	2.65
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	19	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	19	2.65
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	19	2.65
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	18	2.64
(1,537)	1:42:A:THR:H	1:47:A:LYS:HG2	20	2.64
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	20	2.64
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	9	2.63
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	16	2.63
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	5	2.63
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	5	2.63
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	5	2.63
(1,256)	1:41:A:CYS:H	1:66:A:CYS:HB2	12	2.63
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	1	2.62
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	1	2.62
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	1	2.62
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	1	2.62
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	1	2.62
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	1	2.62
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	1	2.62
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	15	2.62
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	15	2.62
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	15	2.62
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	15	2.62
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	15	2.62
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	15	2.62
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	15	2.62
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	15	2.62
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	15	2.62
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	13	2.62
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	13	2.62
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	2	2.61
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	2	2.61
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	15	2.61
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	15	2.61
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	10	2.6
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	10	2.6
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	10	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	10	2.6
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	10	2.6
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	10	2.6
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	10	2.6
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	6	2.6
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	18	2.6
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	3	2.6
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	13	2.6
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	6	2.59
(1,889)	1:33:A:CYS:H	1:33:A:CYS:HB3	18	2.59
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	8	2.59
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	17	2.59
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	12	2.58
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	10	2.58
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB2	10	2.58
(1,685)	1:21:A:CYS:HA	1:26:A:GLN:HB3	10	2.58
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	3	2.58
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	3	2.58
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	3	2.58
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	20	2.58
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	20	2.58
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	20	2.58
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	3	2.56
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	3	2.56
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	3	2.56
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	3	2.56
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	8	2.56
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	11	2.56
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	14	2.56
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	10	2.56
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	10	2.56
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	15	2.56
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	15	2.56
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	2	2.55
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	2	2.55
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	11	2.55
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	11	2.55
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	2	2.54
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	2	2.54
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	2	2.54
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	12	2.54
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	11	2.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	5	2.53
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	10	2.53
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	14	2.52
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	4	2.52
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	4	2.52
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	5	2.52
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	13	2.52
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	9	2.52
(1,245)	1:19:A:CYS:HB3	1:36:A:CYS:H	9	2.52
(1,245)	1:19:A:CYS:HB2	1:36:A:CYS:H	9	2.52
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	1	2.52
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	1	2.52
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	1	2.52
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	2	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	2	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	2	2.51
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	2	2.51
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	2	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	2	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	2	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	18	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	18	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	18	2.51
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	18	2.51
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	18	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	18	2.51
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	18	2.51
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	4	2.51
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	14	2.51
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	14	2.51
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	7	2.51
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	7	2.51
(1,296)	1:40:A:ASN:HD21	1:67:A:LYS:HA	14	2.51
(1,271)	1:39:A:CYS:H	1:55:A:PRO:HD3	4	2.51
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	16	2.5
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	16	2.5
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	16	2.5
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	16	2.5
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	11	2.5
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	11	2.5
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	11	2.5
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	11	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	11	2.5
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	11	2.5
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	11	2.5
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	17	2.5
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	8	2.5
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	8	2.5
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.49
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.49
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	20	2.49
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	20	2.49
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	20	2.49
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.49
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	20	2.49
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	4	2.49
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	4	2.49
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	4	2.49
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	4	2.49
(1,886)	1:33:A:CYS:HB2	1:37:A:LYS:HG2	2	2.49
(1,886)	1:33:A:CYS:HB3	1:37:A:LYS:HG2	2	2.49
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	6	2.49
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	6	2.49
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	6	2.49
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	1	2.49
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	1	2.49
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	1	2.49
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	20	2.49
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	20	2.49
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	10	2.48
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	7	2.48
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	7	2.48
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	7	2.48
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	7	2.48
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	7	2.48
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	7	2.48
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	9	2.48
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	9	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	8	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	8	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	8	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	8	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	11	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	11	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	11	2.48
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	11	2.48
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	17	2.47
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	6	2.47
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	6	2.47
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	6	2.47
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	6	2.47
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	6	2.47
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	6	2.47
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	6	2.47
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	11	2.47
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	7	2.47
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	13	2.46
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	13	2.46
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	13	2.46
(1,942)	1:8:A:GLU:HB2	1:10:A:CYS:H	6	2.46
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	12	2.46
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	6	2.46
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	6	2.46
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	6	2.46
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	2	2.46
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	3	2.46
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	3	2.46
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	3	2.46
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE21	3	2.46
(1,387)	1:13:A:ALA:HB1	1:26:A:GLN:HE22	3	2.46
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE21	3	2.46
(1,387)	1:13:A:ALA:HB2	1:26:A:GLN:HE22	3	2.46
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE21	3	2.46
(1,387)	1:13:A:ALA:HB3	1:26:A:GLN:HE22	3	2.46
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	17	2.46
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	17	2.46
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	5	2.45
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	5	2.45
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	5	2.45
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	5	2.45
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	5	2.45
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	5	2.45
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	5	2.45
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	20	2.45
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	20	2.45
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	20	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	20	2.45
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	8	2.45
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	8	2.45
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	8	2.45
(1,372)	1:63:A:SER:H	1:63:A:SER:HB2	14	2.45
(1,372)	1:63:A:SER:H	1:63:A:SER:HB3	14	2.45
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	16	2.43
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	16	2.43
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	16	2.43
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	15	2.43
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	15	2.43
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	15	2.43
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	15	2.43
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	3	2.43
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	3	2.43
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	3	2.43
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	14	2.43
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	14	2.43
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	14	2.43
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	10	2.42
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	15	2.42
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	17	2.42
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	17	2.42
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	20	2.42
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	20	2.42
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	2	2.41
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	2	2.41
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	2	2.41
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	6	2.41
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	4	2.4
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	4	2.4
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	15	2.4
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	11	2.4
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	9	2.4
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	9	2.4
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	9	2.4
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	16	2.4
(1,471)	1:40:A:ASN:HD22	1:67:A:LYS:HA	14	2.4
(1,471)	1:40:A:ASN:HD21	1:67:A:LYS:HA	14	2.4
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	4	2.39
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	14	2.39
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	14	2.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	14	2.39
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	18	2.39
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	15	2.39
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	19	2.38
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	19	2.38
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	18	2.38
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	18	2.38
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	18	2.38
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	19	2.37
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	19	2.37
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	19	2.37
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	8	2.37
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	19	2.37
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	19	2.37
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	19	2.37
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	8	2.37
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	2	2.36
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	2	2.36
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	2	2.36
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	12	2.36
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	12	2.36
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	12	2.36
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	9	2.36
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	4	2.36
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	4	2.36
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	4	2.36
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	15	2.36
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	15	2.36
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	6	2.36
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	6	2.36
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	14	2.36
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	14	2.36
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	14	2.36
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	14	2.36
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	19	2.35
(1,1182)	1:10:A:CYS:HB3	1:11:A:THR:H	20	2.35
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	1	2.35
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	4	2.35
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	4	2.35
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	4	2.35
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	14	2.35
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	3	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	3	2.35
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	3	2.35
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	7	2.35
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	7	2.35
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	14	2.34
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	14	2.34
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	10	2.34
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	10	2.34
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	10	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	1	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	1	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	1	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	13	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	13	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	13	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	15	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	15	2.34
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	15	2.34
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	8	2.34
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	8	2.34
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	2	2.33
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	2	2.33
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	2	2.33
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	5	2.33
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	15	2.33
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	14	2.33
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	14	2.33
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	14	2.33
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	14	2.33
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	2	2.33
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	10	2.33
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	10	2.33
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	10	2.33
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	10	2.33
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	10	2.33
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	2	2.32
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	11	2.32
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	11	2.32
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	11	2.32
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	11	2.32
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	1	2.32
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	1	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	12	2.32
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	12	2.32
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	12	2.32
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	12	2.32
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	9	2.32
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	9	2.32
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG2	9	2.31
(1,1135)	1:47:A:LYS:HA	1:47:A:LYS:HG3	9	2.31
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.31
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.31
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	20	2.31
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	5	2.31
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	11	2.31
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	11	2.31
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	4	2.3
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	4	2.3
(1,499)	1:14:A:CYS:H	1:15:A:ARG:H	19	2.3
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	11	2.3
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	11	2.3
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	11	2.3
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	11	2.3
(1,715)	1:39:A:CYS:HA	1:67:A:LYS:HD3	20	2.29
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	8	2.29
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	8	2.29
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	8	2.29
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	2	2.29
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	2	2.29
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	3	2.29
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	3	2.29
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	8	2.28
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	8	2.28
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	8	2.28
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	13	2.28
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	8	2.27
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	8	2.27
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	8	2.27
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	8	2.27
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	12	2.27
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	12	2.27
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	17	2.27
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	17	2.27
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	19	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	19	2.27
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	16	2.27
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	16	2.27
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	16	2.27
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	16	2.27
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	5	2.26
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	6	2.26
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	12	2.26
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	16	2.26
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	17	2.26
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	17	2.26
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	17	2.26
(1,606)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	11	2.26
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	19	2.26
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	19	2.26
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	4	2.25
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	18	2.25
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	19	2.25
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	15	2.25
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	15	2.25
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	15	2.25
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	15	2.25
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	17	2.25
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	17	2.25
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	17	2.25
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	4	2.25
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	4	2.25
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	20	2.25
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	20	2.25
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	20	2.25
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	20	2.25
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	18	2.24
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	18	2.24
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	18	2.24
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	15	2.24
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	15	2.24
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	5	2.24
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	5	2.24
(1,604)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	11	2.24
(1,604)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	11	2.24
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	18	2.24
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	18	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	18	2.24
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	18	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	13	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	13	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	14	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	14	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	15	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	15	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	16	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	16	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	18	2.24
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	18	2.24
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	14	2.24
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	14	2.24
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	14	2.24
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	14	2.24
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	9	2.23
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	15	2.23
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	15	2.23
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	8	2.23
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	8	2.23
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	1	2.23
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	1	2.23
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	1	2.23
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	1	2.23
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	5	2.22
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	5	2.22
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA2	9	2.22
(1,364)	1:28:A:GLY:H	1:28:A:GLY:HA3	9	2.22
(1,137)	1:11:A:THR:HG21	1:13:A:ALA:H	18	2.22
(1,137)	1:11:A:THR:HG22	1:13:A:ALA:H	18	2.22
(1,137)	1:11:A:THR:HG23	1:13:A:ALA:H	18	2.22
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	13	2.21
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	13	2.21
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	6	2.21
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	6	2.21
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	6	2.21
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	6	2.21
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	17	2.21
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	17	2.21
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	12	2.21
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	12	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	12	2.21
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	1	2.21
(1,363)	1:10:A:CYS:HA	1:28:A:GLY:H	10	2.21
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	19	2.21
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	19	2.21
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	19	2.21
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	19	2.21
(1,1120)	1:62:A:SER:H	1:62:A:SER:HA	13	2.2
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	8	2.2
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	2	2.2
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	7	2.2
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	7	2.2
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	7	2.2
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	7	2.2
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	1	2.19
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	6	2.19
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	7	2.19
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	11	2.18
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	11	2.18
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	11	2.18
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	11	2.18
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	19	2.18
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	19	2.18
(1,1101)	1:9:A:LYS:HE2	1:29:A:GLU:H	19	2.18
(1,1101)	1:9:A:LYS:HE3	1:29:A:GLU:H	19	2.18
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	5	2.18
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	5	2.18
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	5	2.18
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	16	2.17
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	19	2.17
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	15	2.17
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	15	2.17
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	15	2.17
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	5	2.17
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	5	2.17
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	5	2.17
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	5	2.17
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	10	2.17
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	10	2.17
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	10	2.17
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	10	2.17
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	11	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	9	2.16
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	9	2.16
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	9	2.16
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE2	2	2.16
(1,1018)	1:37:A:LYS:HA	1:37:A:LYS:HE3	2	2.16
(1,1006)	1:32:A:THR:HA	1:37:A:LYS:HG2	1	2.16
(1,890)	1:33:A:CYS:HB2	1:34:A:ALA:H	9	2.16
(1,890)	1:33:A:CYS:HB3	1:34:A:ALA:H	9	2.16
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	7	2.16
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	7	2.16
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	7	2.16
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	14	2.15
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	14	2.15
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	14	2.15
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	14	2.15
(1,1033)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	14	2.15
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	14	2.15
(1,1033)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	14	2.15
(1,1030)	1:39:A:CYS:HB3	1:55:A:PRO:HA	14	2.15
(1,990)	1:26:A:GLN:H	1:26:A:GLN:HG3	7	2.15
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	11	2.15
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	11	2.15
(1,571)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	11	2.15
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	11	2.15
(1,571)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	11	2.15
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	9	2.15
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	9	2.15
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	9	2.15
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	5	2.14
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	5	2.14
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	5	2.14
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	1	2.14
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	1	2.14
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	1	2.14
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	19	2.14
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	19	2.14
(1,414)	1:29:A:GLU:HB2	1:30:A:GLY:H	7	2.14
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	4	2.13
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	4	2.13
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	4	2.13
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	4	2.13
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD2	3	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:9:A:LYS:H	1:9:A:LYS:HD3	3	2.13
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	14	2.12
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB2	14	2.12
(1,840)	1:32:A:THR:HA	1:37:A:LYS:HB3	14	2.12
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	11	2.12
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	11	2.12
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	11	2.12
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	1	2.12
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	1	2.12
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	1	2.12
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	7	2.12
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	7	2.12
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	13	2.12
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	13	2.12
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	13	2.12
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	13	2.12
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	9	2.11
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	8	2.11
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	13	2.11
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	13	2.11
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	3	2.1
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	12	2.1
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	16	2.1
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	16	2.1
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	16	2.1
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	19	2.1
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	19	2.1
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	19	2.1
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	3	2.1
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	3	2.1
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	18	2.1
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	18	2.1
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	18	2.1
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	12	2.09
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	12	2.09
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	12	2.09
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	12	2.09
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	13	2.09
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	16	2.09
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	16	2.09
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	4	2.09
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	4	2.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	4	2.09
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	8	2.08
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	8	2.08
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	8	2.08
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	8	2.08
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	4	2.08
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	18	2.08
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	2.08
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	2.08
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	12	2.08
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	2.08
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	12	2.08
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	2.08
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	2.08
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	2.08
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	14	2.08
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	14	2.08
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG2	12	2.08
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	12	2.08
(1,712)	1:26:A:GLN:HA	1:26:A:GLN:HG3	12	2.08
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	9	2.08
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	9	2.08
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	9	2.08
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	9	2.08
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	20	2.07
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	15	2.07
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	15	2.07
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	15	2.07
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	15	2.07
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	1	2.06
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	1	2.06
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	1	2.06
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	12	2.06
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	12	2.06
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	2	2.06
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	2	2.06
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	2	2.06
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	14	2.06
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG2	14	2.06
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	14	2.06
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	14	2.06
(1,520)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	14	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	15	2.05
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	15	2.05
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	18	2.05
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	18	2.05
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	15	2.05
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	15	2.05
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	18	2.05
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	18	2.05
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	17	2.04
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	2.04
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	2.04
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	2	2.04
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	2.04
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	2	2.04
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	2.04
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	2.04
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	2.04
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	10	2.04
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	10	2.04
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	1	2.04
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	1	2.04
(1,415)	1:6:A:LYS:HB2	1:7:A:GLY:H	8	2.04
(1,415)	1:6:A:LYS:HB3	1:7:A:GLY:H	8	2.04
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	9	2.03
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	15	2.03
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	8	2.03
(1,775)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	8	2.03
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	17	2.03
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	17	2.03
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	2	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	2	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	5	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	5	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	10	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	10	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	13	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	13	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	2.02
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	2	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	2	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	5	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	5	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	10	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	10	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	13	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	13	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	2.02
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	2.02
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	7	2.02
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	7	2.02
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	7	2.02
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	19	2.02
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	19	2.02
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	19	2.02
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	20	2.02
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD2	20	2.02
(1,681)	1:39:A:CYS:HA	1:67:A:LYS:HD3	20	2.02
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	12	2.01
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	12	2.01
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	6	2.01
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	6	2.01
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	6	2.01
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	6	2.01
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	6	2.0
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	20	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	2	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	2	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	2	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	2	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	3	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	3	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	3	2.0
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	3	2.0
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	6	1.99
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	6	1.99
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	6	1.99
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	6	1.99
(1,1029)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	7	1.99
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	4	1.99
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	1	1.98
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	1	1.98
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	1	1.98
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	1	1.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	14	1.98
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	14	1.98
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	7	1.97
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	7	1.97
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	7	1.97
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	7	1.97
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	17	1.97
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	17	1.97
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	17	1.97
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	17	1.97
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	3	1.96
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	3	1.96
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	9	1.96
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	9	1.96
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	9	1.96
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	3	1.96
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	3	1.96
(1,1124)	1:11:A:THR:HG21	1:26:A:GLN:H	18	1.96
(1,1124)	1:11:A:THR:HG22	1:26:A:GLN:H	18	1.96
(1,1124)	1:11:A:THR:HG23	1:26:A:GLN:H	18	1.96
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	1	1.96
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	1	1.96
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	1	1.96
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	19	1.96
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD2	17	1.94
(1,1134)	1:47:A:LYS:HA	1:47:A:LYS:HD3	17	1.94
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD2	17	1.94
(1,1132)	1:47:A:LYS:HA	1:47:A:LYS:HD3	17	1.94
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	1	1.91
(1,416)	1:29:A:GLU:HB2	1:30:A:GLY:H	5	1.91
(1,416)	1:29:A:GLU:HB3	1:30:A:GLY:H	5	1.91
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	18	1.9
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	11	1.9
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	11	1.9
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	11	1.9
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	5	1.88
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	5	1.88
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	5	1.88
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD2	5	1.88
(1,661)	1:15:A:ARG:HA	1:15:A:ARG:HD3	5	1.88
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	10	1.88
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	10	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	10	1.88
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	20	1.88
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	20	1.88
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	20	1.88
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	20	1.88
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	14	1.87
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	4	1.85
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD2	4	1.85
(1,1133)	1:37:A:LYS:HA	1:37:A:LYS:HD3	4	1.85
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	20	1.85
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	1.85
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	20	1.85
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	20	1.85
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	20	1.85
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	1.85
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	20	1.85
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	1.85
(1,939)	1:8:A:GLU:HB2	1:9:A:LYS:H	19	1.84
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	14	1.83
(1,1028)	1:39:A:CYS:HB2	1:55:A:PRO:HA	14	1.83
(1,1028)	1:39:A:CYS:HB3	1:55:A:PRO:HA	14	1.83
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	5	1.83
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	5	1.83
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	5	1.83
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	5	1.83
(4,782)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	7	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	2	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	2	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	2	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	2	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	11	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	11	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	11	1.82
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	11	1.82
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	19	1.82
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	19	1.82
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	19	1.82
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	2	1.81
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	2	1.81
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	5	1.8
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	5	1.8
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB2	5	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:11:A:THR:H	1:27:A:CYS:HB3	5	1.8
(1,99)	1:11:A:THR:HG21	1:14:A:CYS:H	1	1.8
(1,99)	1:11:A:THR:HG22	1:14:A:CYS:H	1	1.8
(1,99)	1:11:A:THR:HG23	1:14:A:CYS:H	1	1.8
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	16	1.77
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	16	1.77
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE2	16	1.77
(1,1017)	1:47:A:LYS:HA	1:47:A:LYS:HE3	16	1.77
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	2	1.77
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	19	1.75
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	19	1.75
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	13	1.74
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	12	1.73
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	12	1.73
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	12	1.73
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	12	1.73
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	14	1.73
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	14	1.73
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	14	1.73
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	14	1.7
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	5	1.7
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	16	1.68
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	16	1.68
(1,570)	1:9:A:LYS:HB2	1:28:A:GLY:HA3	16	1.68
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	11	1.67
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	1.65
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	1.65
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	1.65
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	1.65
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	1.65
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	1.65
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	1.65
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	1.65
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	1.65
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	1.65
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	15	1.6
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	15	1.6
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	19	1.6
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	19	1.6
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	19	1.6
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	19	1.6
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	1	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,782)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	11	1.57
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD3	19	1.57
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	8	1.57
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	8	1.57
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	8	1.57
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	8	1.57
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	15	1.56
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	15	1.56
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	15	1.56
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	15	1.56
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	13	1.51
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	13	1.51
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	1	1.51
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	14	1.5
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	1	1.49
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	1	1.49
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	1	1.49
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	19	1.48
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	8	1.47
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	8	1.47
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	8	1.47
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	10	1.44
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD3	14	1.44
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	17	1.44
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	17	1.44
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	17	1.44
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	17	1.44
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	10	1.44
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	10	1.44
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	10	1.44
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	10	1.44
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	7	1.43
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	10	1.43
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	10	1.43
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	10	1.43
(4,907)	1:9:A:LYS:HE2	1:29:A:GLU:H	16	1.42
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	15	1.41
(4,787)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	14	1.4
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	6	1.4
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	6	1.4
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	6	1.4
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	6	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	8	1.39
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	8	1.39
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	3	1.39
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	1.39
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	3	1.39
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	3	1.39
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	3	1.39
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	1.39
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	3	1.39
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	1.39
(4,907)	1:9:A:LYS:HE3	1:29:A:GLU:H	10	1.38
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	1	1.37
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	5	1.37
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	16	1.37
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	1	1.37
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	1	1.37
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	1	1.37
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	1	1.37
(4,787)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	4	1.36
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	8	1.36
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	8	1.36
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	13	1.36
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	13	1.36
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	13	1.36
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	2	1.35
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	2	1.35
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	2	1.35
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	2	1.35
(4,941)	1:6:A:LYS:HG3	1:9:A:LYS:H	7	1.34
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	11	1.33
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	5	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	11	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	11	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	11	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	11	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	13	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	13	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	13	1.33
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	13	1.33
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	20	1.32
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	20	1.32
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	20	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	20	1.32
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	17	1.31
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	11	1.3
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	11	1.3
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	2	1.3
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	2	1.3
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	2	1.3
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	12	1.29
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	12	1.29
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	12	1.29
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	12	1.29
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	12	1.29
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	5	1.28
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	5	1.28
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	5	1.28
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	5	1.28
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG2	17	1.27
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	17	1.26
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	17	1.26
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	18	1.26
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	18	1.26
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	18	1.26
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	17	1.25
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	6	1.25
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	6	1.25
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	6	1.25
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	6	1.25
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	8	1.25
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	8	1.25
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	8	1.25
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	8	1.25
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	8	1.25
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	8	1.25
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	19	1.25
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	19	1.25
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	19	1.25
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	16	1.24
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	13	1.23
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	1	1.23
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	1	1.23
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	6	1.23
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	6	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	6	1.23
(4,782)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	5	1.22
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	17	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	17	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	17	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	17	1.22
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	17	1.22
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	8	1.21
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	8	1.21
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	8	1.21
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	8	1.21
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	3	1.21
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	3	1.21
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	3	1.21
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	3	1.21
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	10	1.2
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	8	1.2
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	8	1.2
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	8	1.2
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	8	1.2
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	7	1.2
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	7	1.2
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	7	1.2
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	7	1.2
(4,907)	1:9:A:LYS:HE3	1:29:A:GLU:H	13	1.19
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG2	6	1.19
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	8	1.19
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	17	1.19
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	17	1.19
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	17	1.19
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	17	1.19
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	17	1.19
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	17	1.19
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	17	1.19
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	17	1.19
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	17	1.19
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	11	1.19
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG2	11	1.19
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	11	1.19
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	3	1.18
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	16	1.18
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	16	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	16	1.18
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	16	1.18
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	16	1.18
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	16	1.18
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	16	1.18
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	16	1.18
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	4	1.18
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	4	1.18
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	4	1.18
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	4	1.18
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	9	1.18
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	8	1.18
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	8	1.18
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	8	1.18
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	8	1.18
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG3	16	1.17
(4,805)	1:9:A:LYS:HG2	1:29:A:GLU:H	20	1.17
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	4	1.17
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	4	1.17
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	4	1.17
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	4	1.17
(4,907)	1:9:A:LYS:HE2	1:29:A:GLU:H	5	1.15
(4,907)	1:9:A:LYS:HE3	1:29:A:GLU:H	18	1.15
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	13	1.15
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	17	1.15
(1,366)	1:27:A:CYS:HB2	1:28:A:GLY:H	18	1.15
(1,366)	1:27:A:CYS:HB2	1:28:A:GLY:H	18	1.15
(1,366)	1:27:A:CYS:HB3	1:28:A:GLY:H	18	1.15
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	18	1.15
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	18	1.15
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	2	1.14
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	17	1.14
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	9	1.14
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	9	1.14
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	9	1.14
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	10	1.14
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	10	1.13
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	10	1.13
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	10	1.13
(1,262)	1:30:A:GLY:HA2	1:32:A:THR:H	20	1.13
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	16	1.12
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	4	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	4	1.12
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	2	1.12
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	2	1.12
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	2	1.12
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	11	1.12
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	11	1.12
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	11	1.12
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	4	1.12
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	12	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	9	1.11
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	9	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	9	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	15	1.11
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	15	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	15	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	17	1.11
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	17	1.11
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	17	1.11
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	16	1.1
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	11	1.1
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	11	1.1
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	12	1.1
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	12	1.1
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	12	1.1
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	1	1.1
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	1	1.1
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	1	1.1
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	1	1.1
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	1	1.1
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	1	1.1
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	1	1.1
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	1	1.1
(1,718)	1:10:A:CYS:HA	1:27:A:CYS:HB2	18	1.1
(1,718)	1:10:A:CYS:HA	1:27:A:CYS:HB2	18	1.1
(1,718)	1:10:A:CYS:HA	1:27:A:CYS:HB3	18	1.1
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG2	4	1.1
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG3	4	1.1
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	14	1.09
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	14	1.09
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	14	1.09
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	11	1.09
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	11	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	11	1.09
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	11	1.09
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	12	1.09
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	17	1.08
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	14	1.07
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	17	1.06
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	6	1.06
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	12	1.06
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	12	1.06
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	12	1.06
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	11	1.06
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	10	1.06
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	10	1.06
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	10	1.06
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	10	1.06
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	6	1.06
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	6	1.06
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	6	1.06
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	6	1.06
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	10	1.05
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	7	1.05
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	7	1.05
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	18	1.05
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	18	1.05
(1,671)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	18	1.05
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	20	1.05
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	20	1.05
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	20	1.05
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	7	1.05
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	7	1.05
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	7	1.05
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	8	1.05
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	13	1.04
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	13	1.04
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	18	1.04
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	18	1.04
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	16	1.03
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	16	1.03
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	10	1.03
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	10	1.03
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	10	1.03
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	10	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	10	1.03
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	19	1.03
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	11	1.03
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	11	1.03
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	11	1.03
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	9	1.02
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD3	12	1.02
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	10	1.02
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	20	1.01
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	4	1.01
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	4	1.01
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	17	1.01
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	17	1.01
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	17	1.01
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	17	1.01
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	19	1.01
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	19	1.01
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	19	1.01
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG2	9	1.01
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG3	9	1.01
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HB3	6	1.0
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	12	1.0
(4,907)	1:9:A:LYS:HE2	1:29:A:GLU:H	1	1.0
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	12	1.0
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	19	1.0
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	19	1.0
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	19	1.0
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	19	1.0
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	19	1.0
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	19	1.0
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	19	1.0
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	19	1.0
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	9	1.0
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	9	1.0
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	9	1.0
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	9	1.0
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG2	14	1.0
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG3	14	1.0
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG2	19	1.0
(1,258)	1:41:A:CYS:H	1:47:A:LYS:HG3	19	1.0
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	16	1.0
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	16	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	16	1.0
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	16	1.0
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	7	1.0
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE3	11	0.99
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	5	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	9	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	9	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	9	0.99
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	9	0.99
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	10	0.99
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	16	0.98
(4,782)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	9	0.98
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	2	0.98
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	2	0.98
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	2	0.98
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	2	0.98
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	5	0.98
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	5	0.98
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	5	0.98
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	12	0.98
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	1	0.97
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	6	0.97
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	6	0.97
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	6	0.97
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	6	0.97
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	6	0.97
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	6	0.97
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	6	0.97
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	6	0.97
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	6	0.97
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	1	0.97
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	11	0.96
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	11	0.96
(4,787)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	15	0.95
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	13	0.95
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	5	0.95
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	5	0.95
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	5	0.95
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	5	0.95
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	15	0.95
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	7	0.94
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	7	0.94
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	18	0.94
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	18	0.94
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	18	0.94
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	18	0.94
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	9	0.94
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	9	0.94
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	9	0.94
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	5	0.94
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	19	0.94
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	19	0.94
(4,907)	1:9:A:LYS:HE3	1:29:A:GLU:H	11	0.93
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	7	0.93
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	7	0.93
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	6	0.93
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	6	0.93
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB2	14	0.93
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB2	14	0.93
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB3	14	0.93
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	20	0.93
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	20	0.93
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	20	0.93
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	11	0.93
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	11	0.93
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	11	0.93
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	11	0.93
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	10	0.93
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	10	0.93
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	10	0.93
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	9	0.93
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	9	0.93
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	9	0.93
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HB3	3	0.92
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	9	0.92
(4,722)	1:32:A:THR:HA	1:37:A:LYS:HE2	3	0.91
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	8	0.91
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	8	0.91
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.91
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.91
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	0.91
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	14	0.91
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	14	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	14	0.91
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	14	0.91
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	14	0.91
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	14	0.91
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	14	0.91
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	14	0.91
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	3	0.91
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	3	0.91
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	3	0.91
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	3	0.91
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	3	0.91
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	3	0.91
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	3	0.91
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	3	0.91
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	3	0.91
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	3	0.91
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	3	0.91
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	3	0.91
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	7	0.91
(1,44)	1:19:A:CYS:H	1:20:A:GLN:HE21	19	0.91
(1,44)	1:19:A:CYS:H	1:20:A:GLN:HE22	19	0.91
(4,941)	1:6:A:LYS:HG2	1:9:A:LYS:H	11	0.9
(4,787)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	19	0.9
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	10	0.9
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	10	0.9
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	17	0.9
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	17	0.9
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	17	0.9
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	17	0.9
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	8	0.9
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	6	0.89
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	5	0.89
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	5	0.89
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	5	0.89
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	5	0.89
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	5	0.89
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	5	0.89
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	5	0.89
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	5	0.89
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	1	0.89
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	1	0.89
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	1	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	1	0.89
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	18	0.89
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD2	18	0.89
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	18	0.89
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	13	0.89
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	8	0.89
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	8	0.89
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	8	0.89
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	8	0.89
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	15	0.89
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	15	0.89
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	15	0.89
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	2	0.88
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	2	0.88
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	2	0.88
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	2	0.88
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	10	0.88
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	10	0.88
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	10	0.88
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	16	0.88
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	5	0.88
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	5	0.88
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	5	0.88
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	19	0.87
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	19	0.87
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	19	0.87
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	5	0.87
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	5	0.87
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	5	0.87
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	5	0.87
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	16	0.87
(4,477)	1:10:A:CYS:HB2	1:15:A:ARG:HG2	14	0.86
(1,1152)	1:37:A:LYS:HG2	1:62:A:SER:HA	2	0.86
(1,1152)	1:37:A:LYS:HG3	1:62:A:SER:HA	2	0.86
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	20	0.86
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	20	0.86
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	13	0.86
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	13	0.86
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	0.86
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	13	0.86
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	13	0.86
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	13	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	13	0.86
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	13	0.86
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	17	0.86
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	17	0.86
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	17	0.86
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	4	0.85
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	4	0.85
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	5	0.85
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	5	0.85
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	16	0.85
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	16	0.85
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	8	0.85
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	8	0.85
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	8	0.85
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	4	0.85
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	4	0.85
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	4	0.85
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	3	0.85
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	19	0.84
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	19	0.84
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD3	10	0.84
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	4	0.84
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	19	0.84
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	19	0.84
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	19	0.84
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	19	0.84
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	20	0.84
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	20	0.84
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	20	0.84
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	20	0.84
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HB3	17	0.83
(4,805)	1:9:A:LYS:HG2	1:29:A:GLU:H	1	0.83
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	8	0.83
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	7	0.83
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	7	0.83
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	7	0.83
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.83
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	4	0.83
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	18	0.83
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	20	0.82
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG2	10	0.82
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	15	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	15	0.82
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	17	0.82
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	17	0.82
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	15	0.82
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	15	0.82
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	15	0.82
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	15	0.82
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	8	0.82
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	8	0.82
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	8	0.82
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	5	0.81
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	5	0.81
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	11	0.81
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	11	0.81
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	5	0.81
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	5	0.81
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	5	0.81
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	5	0.81
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	14	0.81
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	14	0.81
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	10	0.81
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	10	0.81
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	0.81
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	10	0.81
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	10	0.81
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	10	0.81
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	10	0.81
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	10	0.81
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	17	0.81
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	17	0.81
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	17	0.81
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	17	0.81
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	17	0.81
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	17	0.81
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	17	0.81
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	17	0.81
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	14	0.81
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE2	14	0.81
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	14	0.81
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	15	0.81
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	15	0.81
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	15	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	15	0.81
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	7	0.81
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	7	0.81
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	12	0.81
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	12	0.81
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	12	0.81
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	12	0.8
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	18	0.8
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	18	0.8
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	7	0.8
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	7	0.8
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	3	0.8
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	3	0.8
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	8	0.8
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	8	0.8
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	8	0.8
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	8	0.8
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	11	0.8
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	11	0.8
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	19	0.8
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	14	0.8
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	14	0.8
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	14	0.8
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	4	0.79
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	4	0.79
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	8	0.79
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	8	0.79
(1,1136)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	5	0.79
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	15	0.79
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	15	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	4	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	4	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	4	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	4	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	8	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	8	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	8	0.79
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	8	0.79
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	17	0.79
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	17	0.79
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	17	0.79
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	18	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	18	0.79
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	18	0.79
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	18	0.79
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	11	0.79
(1,95)	1:14:A:CYS:H	1:15:A:ARG:HB2	14	0.79
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	13	0.79
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	2	0.79
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	2	0.79
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	2	0.79
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	11	0.78
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	6	0.78
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	6	0.78
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	9	0.78
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	9	0.78
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	9	0.78
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	9	0.78
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	18	0.78
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	18	0.78
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	18	0.78
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	9	0.78
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	9	0.78
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG3	9	0.78
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	19	0.78
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	19	0.78
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	19	0.78
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	8	0.78
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	8	0.78
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	8	0.78
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	8	0.78
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	8	0.78
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	17	0.77
(1,1152)	1:37:A:LYS:HG2	1:62:A:SER:HA	4	0.77
(1,1152)	1:37:A:LYS:HG3	1:62:A:SER:HA	4	0.77
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	12	0.77
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	20	0.76
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	5	0.76
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	3	0.76
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	3	0.76
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	9	0.76
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	9	0.76
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	12	0.76
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	12	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	2	0.76
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	2	0.76
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	12	0.76
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	12	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	3	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	3	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	3	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	3	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	9	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	9	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	9	0.76
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	9	0.76
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	12	0.76
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	12	0.76
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	12	0.76
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	4	0.76
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	4	0.76
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	4	0.76
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	4	0.76
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	13	0.76
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	13	0.76
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	11	0.76
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	9	0.75
(4,907)	1:9:A:LYS:HE2	1:29:A:GLU:H	3	0.75
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG2	7	0.75
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	5	0.75
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	5	0.75
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	9	0.75
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	19	0.75
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	19	0.75
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	2	0.75
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	2	0.75
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	11	0.75
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	11	0.75
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	19	0.75
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	19	0.75
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	2	0.75
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	2	0.75
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	2	0.75
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	6	0.75
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	6	0.75
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	6	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	6	0.75
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	15	0.75
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	15	0.75
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	15	0.75
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	19	0.75
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	19	0.75
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	19	0.75
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	2	0.75
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	20	0.75
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	2	0.74
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	10	0.74
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	10	0.74
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	14	0.74
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	14	0.74
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	19	0.74
(4,787)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	6	0.74
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	2	0.74
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	15	0.74
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	15	0.74
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	15	0.74
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	15	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	7	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	7	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	9	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	9	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	13	0.74
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	13	0.74
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	10	0.74
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	10	0.74
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	10	0.74
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	10	0.74
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	14	0.74
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	14	0.74
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	14	0.74
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	14	0.74
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	13	0.74
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	13	0.74
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	13	0.74
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	6	0.74
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	6	0.74
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	6	0.74
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	15	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	15	0.74
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	15	0.74
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	15	0.74
(1,279)	1:24:A:LYS:H	1:24:A:LYS:HB2	19	0.74
(1,279)	1:24:A:LYS:H	1:24:A:LYS:HB2	19	0.74
(1,279)	1:24:A:LYS:H	1:24:A:LYS:HB3	19	0.74
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	4	0.74
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD2	17	0.73
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	12	0.73
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	12	0.73
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	4	0.73
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	4	0.73
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	20	0.73
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	20	0.73
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	14	0.73
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	14	0.73
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	7	0.73
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	7	0.73
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	7	0.73
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	7	0.73
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	17	0.73
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	17	0.73
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	17	0.73
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	2	0.73
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	2	0.73
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	2	0.73
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	2	0.73
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	19	0.73
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	19	0.73
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	19	0.73
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	19	0.73
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	15	0.73
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	15	0.73
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	15	0.73
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	15	0.73
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	15	0.73
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	15	0.73
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	9	0.73
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	9	0.73
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	14	0.73
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	14	0.73
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	14	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	19	0.73
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	19	0.73
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	19	0.73
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	5	0.72
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	5	0.72
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	5	0.72
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	5	0.72
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	3	0.72
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	18	0.72
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	18	0.72
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	5	0.72
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	5	0.72
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	5	0.72
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	5	0.72
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	5	0.72
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	5	0.72
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	15	0.72
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	15	0.72
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	19	0.72
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	19	0.72
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	2	0.72
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	15	0.71
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	15	0.71
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	17	0.71
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	17	0.71
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	5	0.71
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	5	0.71
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	5	0.71
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	8	0.71
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	8	0.71
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	8	0.71
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	20	0.71
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	20	0.71
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	20	0.71
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	20	0.71
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	9	0.71
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	9	0.71
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	9	0.71
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	15	0.71
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	4	0.7
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	4	0.7
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	16	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	4	0.7
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	4	0.7
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	4	0.7
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	4	0.7
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG21	20	0.7
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG22	20	0.7
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG23	20	0.7
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG21	20	0.7
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG22	20	0.7
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG23	20	0.7
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG21	20	0.7
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG22	20	0.7
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG23	20	0.7
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	14	0.7
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	16	0.7
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	16	0.7
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	16	0.7
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	5	0.7
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	5	0.7
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	5	0.7
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	5	0.7
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	14	0.7
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	14	0.7
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	14	0.7
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	9	0.7
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	20	0.7
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	20	0.7
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	20	0.7
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	4	0.69
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	4	0.69
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	20	0.69
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	20	0.69
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	2	0.69
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	2	0.69
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	8	0.69
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	8	0.69
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	5	0.69
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	5	0.69
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	17	0.69
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	17	0.69
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	17	0.69
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	17	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	4	0.69
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	4	0.69
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	4	0.69
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	4	0.69
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	20	0.69
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	20	0.69
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	20	0.69
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	20	0.69
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	2	0.69
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	2	0.69
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	2	0.69
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	2	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	8	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	8	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	8	0.69
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	8	0.69
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	4	0.69
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	4	0.69
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	4	0.69
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	4	0.69
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	4	0.69
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	4	0.69
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	7	0.69
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.69
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	7	0.69
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	4	0.69
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	4	0.69
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	4	0.69
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	4	0.69
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	13	0.69
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	13	0.69
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	13	0.69
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	13	0.69
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	7	0.68
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	7	0.68
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	20	0.68
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	20	0.68
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	10	0.68
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	17	0.68
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	7	0.68
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	7	0.68
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	7	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	7	0.68
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	20	0.68
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	20	0.68
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	20	0.68
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	20	0.68
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	15	0.68
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	15	0.68
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	15	0.68
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	15	0.68
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	16	0.68
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	16	0.68
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	16	0.68
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	18	0.68
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB2	18	0.68
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	18	0.68
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	19	0.68
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	11	0.68
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	11	0.68
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	11	0.68
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	1	0.67
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	11	0.67
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	1	0.67
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	8	0.67
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	8	0.67
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	9	0.67
(1,892)	1:33:A:CYS:HB2	1:36:A:CYS:HA	9	0.67
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	9	0.67
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	9	0.67
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	14	0.67
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	14	0.67
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	14	0.67
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	14	0.67
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	19	0.67
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	19	0.67
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	19	0.67
(4,805)	1:9:A:LYS:HG2	1:29:A:GLU:H	9	0.66
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD3	5	0.66
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	5	0.66
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	5	0.66
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	5	0.66
(4,44)	1:19:A:CYS:H	1:20:A:GLN:HE22	19	0.66
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	17	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	17	0.66
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	17	0.66
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	17	0.66
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	4	0.66
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	4	0.66
(1,671)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	4	0.66
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	14	0.66
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	14	0.66
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	14	0.66
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	14	0.66
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	6	0.66
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	6	0.66
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	6	0.66
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	20	0.65
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	15	0.65
(4,722)	1:32:A:THR:HA	1:37:A:LYS:HE3	2	0.65
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	18	0.65
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	18	0.65
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	18	0.65
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	18	0.65
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	7	0.65
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	7	0.65
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	5	0.65
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	5	0.65
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	10	0.65
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	10	0.65
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	10	0.65
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	10	0.65
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	10	0.65
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	10	0.65
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	10	0.65
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	10	0.65
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	10	0.65
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	10	0.65
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	7	0.65
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	7	0.65
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	7	0.65
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	7	0.65
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	7	0.65
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	7	0.65
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	18	0.65
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	18	0.65
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	18	0.65
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	6	0.65
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	6	0.65
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	6	0.65
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	6	0.65
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	12	0.65
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	12	0.65
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	12	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	3	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	3	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	3	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	14	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	14	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	14	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	20	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	20	0.65
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	20	0.65
(4,830)	1:25:A:CYS:H	1:26:A:GLN:HG2	12	0.64
(4,830)	1:25:A:CYS:H	1:26:A:GLN:HG3	12	0.64
(4,807)	1:15:A:ARG:HD2	1:16:A:SER:H	2	0.64
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	13	0.64
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	13	0.64
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	13	0.64
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	13	0.64
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	13	0.64
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	13	0.64
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	13	0.64
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	13	0.64
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	13	0.64
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	13	0.64
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG2	12	0.64
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG3	12	0.64
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG3	12	0.64
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	7	0.64
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	7	0.64
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	7	0.64
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	7	0.64
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	12	0.64
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	12	0.64
(1,671)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	12	0.64
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	19	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	19	0.64
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	19	0.64
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	19	0.64
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	16	0.64
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	16	0.64
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	1	0.63
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	1	0.63
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	16	0.63
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	16	0.63
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	16	0.63
(4,787)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	3	0.63
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	10	0.63
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	10	0.63
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	10	0.63
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	10	0.63
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	3	0.63
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	3	0.63
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	16	0.63
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	16	0.63
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	1	0.63
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	1	0.63
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	1	0.63
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	1	0.63
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	13	0.63
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	13	0.63
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	16	0.63
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	16	0.63
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	16	0.63
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	0.63
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	0.63
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	0.63
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	0.63
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	0.63
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	17	0.63
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	0.63
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	0.63
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	0.63
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	17	0.63
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	5	0.63
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	5	0.63
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	5	0.63
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	5	0.63
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	5	0.63
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	5	0.63
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	5	0.63
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	5	0.63
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	17	0.63
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	17	0.63
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	17	0.63
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	20	0.63
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	20	0.63
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	20	0.63
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	18	0.63
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	18	0.63
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	18	0.63
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	18	0.63
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	18	0.63
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	6	0.63
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	6	0.63
(1,184)	1:38:A:THR:H	1:67:A:LYS:HD3	8	0.63
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	1	0.62
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	1	0.62
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	6	0.62
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	6	0.62
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	12	0.62
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.62
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	15	0.62
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	15	0.62
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	8	0.62
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	8	0.62
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG2	10	0.62
(1,1060)	1:50:A:LYS:H	1:51:A:GLU:HG3	10	0.62
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	1	0.62
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	1	0.62
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	1	0.62
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	1	0.62
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	6	0.62
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	6	0.62
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	6	0.62
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	6	0.62
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	12	0.62
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.62
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.62
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	15	0.62
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	15	0.62
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	15	0.62
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	15	0.62
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	9	0.62
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	9	0.62
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	9	0.62
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	11	0.62
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	11	0.62
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	11	0.62
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	11	0.62
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	11	0.62
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	11	0.62
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	20	0.62
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	15	0.62
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	15	0.62
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	15	0.62
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	15	0.62
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	9	0.62
(1,485)	1:21:A:CYS:HB3	1:26:A:GLN:H	12	0.62
(1,485)	1:21:A:CYS:HB2	1:26:A:GLN:H	12	0.62
(1,485)	1:21:A:CYS:HB3	1:26:A:GLN:H	12	0.62
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	11	0.62
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	11	0.62
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD3	11	0.62
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	17	0.62
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	17	0.62
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	8	0.62
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	8	0.62
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	5	0.62
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	7	0.61
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	14	0.61
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	18	0.61
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	14	0.61
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	14	0.61
(4,597)	1:47:A:LYS:HG3	1:66:A:CYS:HB3	4	0.61
(4,438)	1:39:A:CYS:H	1:40:A:ASN:HD22	1	0.61
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD22	1	0.61
(4,277)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	1	0.61
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	7	0.61
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	9	0.61
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	9	0.61
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB2	9	0.61
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	9	0.61
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB2	9	0.61
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	9	0.61
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	9	0.61
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	9	0.61
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	14	0.61
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	14	0.61
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	14	0.61
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	14	0.61
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	9	0.61
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	9	0.61
(1,956)	1:9:A:LYS:HG2	1:29:A:GLU:H	8	0.61
(1,956)	1:9:A:LYS:HG3	1:29:A:GLU:H	8	0.61
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	6	0.61
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	14	0.61
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	14	0.61
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG3	14	0.61
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	17	0.61
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	17	0.61
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE2	17	0.61
(1,325)	1:62:A:SER:H	1:67:A:LYS:HE3	17	0.61
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	1	0.61
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	1	0.61
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	1	0.61
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	1	0.61
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	15	0.61
(4,807)	1:15:A:ARG:HD2	1:16:A:SER:H	11	0.6
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	7	0.6
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	15	0.6
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	15	0.6
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	18	0.6
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	18	0.6
(1,1148)	1:6:A:LYS:HG2	1:9:A:LYS:H	11	0.6
(1,1148)	1:6:A:LYS:HG3	1:9:A:LYS:H	11	0.6
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	14	0.6
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	14	0.6
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	14	0.6
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	14	0.6
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	1	0.6
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	3	0.6
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	3	0.6
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	3	0.6
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	3	0.6
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	3	0.6
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	3	0.6
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	14	0.6
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	14	0.6
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	14	0.6
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	2	0.6
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	2	0.6
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	2	0.6
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	2	0.6
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	0.6
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	17	0.6
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	17	0.6
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	17	0.6
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	8	0.6
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	11	0.6
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	11	0.6
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	11	0.6
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	1	0.6
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	1	0.6
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	1	0.6
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	7	0.59
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	7	0.59
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	9	0.59
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	9	0.59
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	7	0.59
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	7	0.59
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	7	0.59
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	7	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	18	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	18	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	18	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	18	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	18	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	18	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	18	0.59
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	18	0.59
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	18	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	18	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	20	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	20	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	20	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	20	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	20	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	20	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	20	0.59
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	20	0.59
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	20	0.59
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	12	0.59
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	12	0.59
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	19	0.59
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	19	0.59
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	19	0.59
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	19	0.59
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	4	0.59
(1,892)	1:33:A:CYS:HB2	1:36:A:CYS:HA	4	0.59
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	4	0.59
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	10	0.59
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	10	0.59
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	10	0.59
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	10	0.59
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	10	0.59
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	10	0.59
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	0.59
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.59
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	0.59
(1,466)	1:52:A:CYS:HB3	1:54:A:GLY:H	5	0.59
(1,466)	1:52:A:CYS:HB2	1:54:A:GLY:H	5	0.59
(1,466)	1:52:A:CYS:HB3	1:54:A:GLY:H	5	0.59
(1,466)	1:52:A:CYS:HB2	1:54:A:GLY:H	5	0.59
(1,466)	1:52:A:CYS:HB2	1:54:A:GLY:H	5	0.59
(1,466)	1:52:A:CYS:HB2	1:54:A:GLY:H	5	0.59
(1,466)	1:52:A:CYS:HB3	1:54:A:GLY:H	5	0.59
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	20	0.59
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	1	0.59
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	1	0.59
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	1	0.59
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	1	0.59
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	2	0.59
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	8	0.59
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	8	0.59
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	12	0.59
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	14	0.58
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	14	0.58
(4,24)	1:19:A:CYS:HA	1:20:A:GLN:HE21	19	0.58
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	15	0.58
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	15	0.58
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	5	0.58
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	5	0.58
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	9	0.58
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	9	0.58
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	9	0.58
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	19	0.58
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	19	0.58
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	19	0.58
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	19	0.58
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	19	0.58
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	19	0.58
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	2	0.58
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	2	0.58
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	2	0.58
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	2	0.58
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	4	0.58
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	19	0.58
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	19	0.58
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	19	0.58
(1,38)	1:19:A:CYS:HA	1:20:A:GLN:HE21	19	0.58
(1,38)	1:19:A:CYS:HA	1:20:A:GLN:HE22	19	0.58
(1,38)	1:19:A:CYS:HA	1:20:A:GLN:HE21	19	0.58
(1,38)	1:19:A:CYS:HA	1:20:A:GLN:HE22	19	0.58
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	18	0.57
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	18	0.57
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	18	0.57
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	18	0.57
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	18	0.57
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	18	0.57
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	17	0.57
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	17	0.57
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	17	0.57
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	15	0.57
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	15	0.57
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	20	0.57
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	20	0.57
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	20	0.57
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	4	0.57
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	4	0.57
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	4	0.57
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	13	0.57
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	13	0.57
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	7	0.57
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	7	0.57
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	1	0.57
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	1	0.57
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	1	0.57
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	1	0.57
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	13	0.56
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG3	5	0.56
(4,907)	1:9:A:LYS:HE2	1:29:A:GLU:H	9	0.56
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	6	0.56
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	6	0.56
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG3	20	0.56
(4,731)	1:32:A:THR:H	1:37:A:LYS:HE2	18	0.56
(4,731)	1:32:A:THR:H	1:37:A:LYS:HE3	18	0.56
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	8	0.56
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	8	0.56
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	6	0.56
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	6	0.56
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	6	0.56
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	6	0.56
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	19	0.56
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	19	0.56
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	19	0.56
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	19	0.56
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	19	0.56
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	19	0.56
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	11	0.56
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	11	0.56
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	11	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	6	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	6	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	6	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	6	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	6	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	6	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	16	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	16	0.56
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	16	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	16	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	16	0.56
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	16	0.56
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	20	0.56
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	20	0.56
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD3	20	0.56
(1,262)	1:30:A:GLY:HA2	1:32:A:THR:H	8	0.56
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	3	0.55
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	3	0.55
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	3	0.55
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	3	0.55
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	10	0.55
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	16	0.55
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	16	0.55
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	3	0.55
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	3	0.55
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	3	0.55
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	3	0.55
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	4	0.55
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	4	0.55
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	4	0.55
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	11	0.55
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	11	0.55
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	11	0.55
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	11	0.55
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	11	0.55
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	11	0.55
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	11	0.55
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	11	0.55
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	12	0.55
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	12	0.55
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	12	0.55
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	12	0.55
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	2	0.55
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	2	0.55
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	2	0.55
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	2	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	2	0.55
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	2	0.55
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	19	0.55
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	4	0.55
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	4	0.55
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	4	0.55
(1,643)	1:50:A:LYS:HB2	1:58:A:CYS:HA	5	0.55
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	4	0.55
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	19	0.55
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	19	0.55
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	19	0.55
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	10	0.55
(4,58)	1:9:A:LYS:H	1:9:A:LYS:HG2	11	0.54
(4,57)	1:9:A:LYS:H	1:9:A:LYS:HG2	11	0.54
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	11	0.54
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	11	0.54
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	11	0.54
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	11	0.54
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	11	0.54
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	11	0.54
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	11	0.54
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	11	0.54
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	11	0.54
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	11	0.54
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	11	0.54
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	11	0.54
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	11	0.54
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	11	0.54
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	6	0.54
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	6	0.54
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	6	0.54
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	6	0.54
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	19	0.54
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	19	0.54
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	19	0.54
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	19	0.54
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	19	0.54
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	19	0.54
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	19	0.54
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	19	0.54
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	19	0.54
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	19	0.54
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	19	0.54
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	14	0.54
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	14	0.54
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	14	0.54
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	14	0.54
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	14	0.54
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	14	0.54
(1,487)	1:11:A:THR:H	1:26:A:GLN:H	10	0.54
(1,262)	1:30:A:GLY:HA2	1:32:A:THR:H	18	0.54
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	15	0.54
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE2	15	0.54
(1,182)	1:38:A:THR:H	1:67:A:LYS:HE3	15	0.54
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	16	0.54
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	6	0.54
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	20	0.54
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	20	0.54
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	20	0.54
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	11	0.54
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	11	0.54
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG3	11	0.54
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	3	0.54
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	3	0.54
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	6	0.54
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	6	0.54
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	6	0.54
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	6	0.54
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	15	0.54
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	15	0.54
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	15	0.54
(4,950)	1:14:A:CYS:H	1:20:A:GLN:HG2	19	0.53
(4,787)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	17	0.53
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	17	0.53
(4,199)	1:58:A:CYS:H	1:59:A:LYS:HD2	20	0.53
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	4	0.53
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	4	0.53
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	13	0.53
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	13	0.53
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	13	0.53
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	13	0.53
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	18	0.53
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	18	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	18	0.53
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	18	0.53
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	6	0.53
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	6	0.53
(1,858)	1:11:A:THR:HG21	1:14:A:CYS:HB2	4	0.53
(1,858)	1:11:A:THR:HG22	1:14:A:CYS:HB2	4	0.53
(1,858)	1:11:A:THR:HG23	1:14:A:CYS:HB2	4	0.53
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	17	0.53
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	2	0.53
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	2	0.53
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD3	2	0.53
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	17	0.53
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	13	0.53
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	13	0.53
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	3	0.53
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	3	0.53
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	17	0.53
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	20	0.53
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	16	0.53
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	16	0.53
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	20	0.53
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	20	0.53
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD2	20	0.53
(1,209)	1:58:A:CYS:H	1:59:A:LYS:HD3	20	0.53
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	8	0.53
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	18	0.53
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	18	0.53
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	18	0.53
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	18	0.53
(4,787)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	13	0.52
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	14	0.52
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	14	0.52
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	14	0.52
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	14	0.52
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	14	0.52
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	14	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	10	0.52
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	19	0.52
(1,304)	1:8:A:GLU:HA	1:10:A:CYS:H	14	0.52
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	11	0.52
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	6	0.52
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	6	0.52
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB2	4	0.51
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB3	4	0.51
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB2	4	0.51
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB3	4	0.51
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	6	0.51
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	6	0.51
(4,807)	1:15:A:ARG:HD2	1:16:A:SER:H	13	0.51
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB2	4	0.51
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB3	4	0.51
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	4	0.51
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	4	0.51
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	4	0.51
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	4	0.51
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	4	0.51
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	4	0.51
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	6	0.51
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	6	0.51
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	6	0.51
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	6	0.51
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	18	0.51
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	18	0.51
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	18	0.51
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	18	0.51
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	16	0.51
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	16	0.51
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	16	0.51
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	16	0.51
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	0.51
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	0.51
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	0.51
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	18	0.51
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	18	0.51
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	18	0.51
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	0.51
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	18	0.51
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	1	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	1	0.51
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	4	0.51
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	4	0.51
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	4	0.51
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	19	0.51
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	19	0.51
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	19	0.51
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	3	0.51
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	17	0.51
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	20	0.51
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	8	0.51
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	8	0.51
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	8	0.51
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	20	0.5
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	20	0.5
(4,826)	1:24:A:LYS:HD3	1:26:A:GLN:HE21	1	0.5
(4,405)	1:11:A:THR:HG21	1:26:A:GLN:HE21	1	0.5
(4,355)	1:11:A:THR:HG21	1:26:A:GLN:HE21	1	0.5
(4,282)	1:8:A:GLU:HA	1:10:A:CYS:H	11	0.5
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	20	0.5
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	20	0.5
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	20	0.5
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	20	0.5
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	10	0.5
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	10	0.5
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	20	0.5
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	20	0.5
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	12	0.5
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	12	0.5
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	12	0.5
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	8	0.5
(1,747)	1:21:A:CYS:HB2	1:25:A:CYS:HA	8	0.5
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	8	0.5
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	15	0.5
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	17	0.5
(1,304)	1:8:A:GLU:HA	1:10:A:CYS:H	11	0.5
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	10	0.5
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	1	0.49
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	1	0.49
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	1	0.49
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	1	0.49
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	11	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	11	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	11	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	11	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	18	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	18	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	18	0.49
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	18	0.49
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	4	0.49
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	4	0.49
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	1	0.49
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	1	0.49
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	1	0.49
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	1	0.49
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	1	0.49
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	1	0.49
(1,956)	1:9:A:LYS:HG2	1:29:A:GLU:H	20	0.49
(1,956)	1:9:A:LYS:HG3	1:29:A:GLU:H	20	0.49
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	5	0.49
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	5	0.49
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	5	0.49
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	0.49
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	18	0.49
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	0.49
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	0.49
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	18	0.49
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	18	0.49
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	0.49
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	18	0.49
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	18	0.49
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	18	0.49
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE2	18	0.49
(1,869)	1:6:A:LYS:HA	1:6:A:LYS:HE3	18	0.49
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	12	0.49
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	12	0.49
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	12	0.49
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	12	0.49
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	12	0.49
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	12	0.49
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	12	0.49
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	12	0.49
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	12	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	12	0.49
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	12	0.49
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	12	0.49
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	18	0.49
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	18	0.49
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	7	0.49
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	7	0.49
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	7	0.49
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	7	0.49
(4,303)	1:62:A:SER:H	1:67:A:LYS:HG2	15	0.48
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	10	0.48
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	10	0.48
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	15	0.48
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	15	0.48
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	15	0.48
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	15	0.48
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	15	0.48
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	15	0.48
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	15	0.48
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	15	0.48
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	15	0.48
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	15	0.48
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	15	0.48
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	15	0.48
(1,900)	1:15:A:ARG:H	1:15:A:ARG:HD2	19	0.48
(1,900)	1:15:A:ARG:H	1:15:A:ARG:HD2	19	0.48
(1,900)	1:15:A:ARG:H	1:15:A:ARG:HD3	19	0.48
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	20	0.48
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	20	0.48
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	20	0.48
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	20	0.48
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	20	0.48
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	20	0.48
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	11	0.48
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	11	0.48
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	14	0.48
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	14	0.48
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	16	0.48
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	16	0.48
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	16	0.48
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	15	0.48
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	18	0.48
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	10	0.48
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	10	0.48
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	10	0.48
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	10	0.48
(4,850)	1:37:A:LYS:HG2	1:38:A:THR:H	2	0.47
(4,850)	1:37:A:LYS:HG3	1:38:A:THR:H	2	0.47
(4,430)	1:52:A:CYS:HB2	1:54:A:GLY:H	5	0.47
(4,430)	1:52:A:CYS:HB3	1:54:A:GLY:H	5	0.47
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	9	0.47
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	9	0.47
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	2	0.47
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	2	0.47
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	2	0.47
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	2	0.47
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	13	0.47
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	13	0.47
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	13	0.47
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	13	0.47
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	7	0.47
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	7	0.47
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	7	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	2	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	2	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	3	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	3	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	8	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	8	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	9	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	9	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	10	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	10	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	15	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	15	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	16	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	16	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	18	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	18	0.47
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	19	0.47
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	19	0.47
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	9	0.47
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	4	0.47
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD2	4	0.47
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	4	0.47
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	8	0.47
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	18	0.47
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	9	0.47
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	9	0.47
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	9	0.47
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	2	0.46
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	2	0.46
(4,797)	1:8:A:GLU:HB2	1:10:A:CYS:HA	9	0.46
(4,797)	1:8:A:GLU:HB3	1:10:A:CYS:HA	9	0.46
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	14	0.46
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	16	0.46
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	16	0.46
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	16	0.46
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	16	0.46
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	2	0.46
(1,1116)	1:9:A:LYS:HG2	1:10:A:CYS:H	2	0.46
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	2	0.46
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	9	0.46
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	9	0.46
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	2	0.46
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	2	0.46
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	2	0.46
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	2	0.46
(1,943)	1:8:A:GLU:HB2	1:10:A:CYS:HA	9	0.46
(1,943)	1:8:A:GLU:HB3	1:10:A:CYS:HA	9	0.46
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD2	15	0.46
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD2	15	0.46
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD3	15	0.46
(1,911)	1:15:A:ARG:HB3	1:15:A:ARG:HD2	15	0.46
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	15	0.46
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	15	0.46
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	15	0.46
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	8	0.46
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	8	0.46
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	8	0.46
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	8	0.46
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	8	0.46
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	8	0.46
(1,876)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	8	0.46
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	4	0.46
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	4	0.46
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	6	0.46
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	6	0.46
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	7	0.46
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	7	0.46
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	13	0.46
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	13	0.46
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	13	0.46
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	13	0.46
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	13	0.46
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	19	0.46
(1,275)	1:21:A:CYS:HB2	1:24:A:LYS:H	19	0.46
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	19	0.46
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	1	0.46
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	1	0.46
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	1	0.46
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	7	0.46
(4,860)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	4	0.45
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	9	0.45
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	9	0.45
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	4	0.45
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	4	0.45
(4,355)	1:11:A:THR:HG22	1:26:A:GLN:HE21	12	0.45
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	9	0.45
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	9	0.45
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	9	0.45
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	9	0.45
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	4	0.45
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	4	0.45
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	4	0.45
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD2	7	0.45
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD2	7	0.45
(1,911)	1:15:A:ARG:HB2	1:15:A:ARG:HD3	7	0.45
(1,911)	1:15:A:ARG:HB3	1:15:A:ARG:HD2	7	0.45
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	13	0.45
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	13	0.45
(1,671)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	13	0.45
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	17	0.45
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	20	0.45
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	20	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	7	0.45
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	7	0.45
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG3	7	0.45
(1,29)	1:17:A:GLU:H	1:20:A:GLN:HE22	6	0.45
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	12	0.44
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	12	0.44
(4,277)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	17	0.44
(4,269)	1:40:A:ASN:H	1:67:A:LYS:HD2	18	0.44
(4,269)	1:40:A:ASN:H	1:67:A:LYS:HD3	18	0.44
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	6	0.44
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	6	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	3	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	0.44
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	0.44
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	3	0.44
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	14	0.44
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	14	0.44
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	14	0.44
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	14	0.44
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	14	0.44
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	14	0.44
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	14	0.44
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	14	0.44
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	14	0.44
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	12	0.44
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	12	0.44
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	12	0.44
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	12	0.44
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	12	0.44
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	12	0.44
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	12	0.44
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	17	0.44
(1,747)	1:21:A:CYS:HB2	1:25:A:CYS:HA	17	0.44
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	17	0.44
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	15	0.44
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	15	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	15	0.44
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	15	0.44
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	17	0.44
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	17	0.44
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	17	0.44
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	17	0.44
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	16	0.44
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	16	0.44
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	16	0.44
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	13	0.44
(1,473)	1:40:A:ASN:HB3	1:40:A:ASN:HD21	5	0.44
(1,473)	1:40:A:ASN:HB2	1:40:A:ASN:HD21	5	0.44
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	10	0.44
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	10	0.44
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	12	0.44
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	12	0.44
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	17	0.44
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	17	0.44
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	17	0.44
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	17	0.44
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	17	0.44
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	17	0.44
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	20	0.43
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	20	0.43
(4,836)	1:31:A:CYS:H	1:37:A:LYS:HG2	3	0.43
(4,826)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	20	0.43
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD2	12	0.43
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD3	12	0.43
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	17	0.43
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	17	0.43
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	15	0.43
(1,1099)	1:28:A:GLY:HA2	1:29:A:GLU:H	15	0.43
(1,1099)	1:28:A:GLY:HA3	1:29:A:GLU:H	15	0.43
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	20	0.43
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	20	0.43
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	20	0.43
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	20	0.43
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	15	0.43
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	15	0.43
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	15	0.43
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	15	0.43
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	15	0.43
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	15	0.43
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	15	0.43
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	15	0.43
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	18	0.43
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	18	0.43
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	18	0.43
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	18	0.43
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	18	0.43
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	18	0.43
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	18	0.43
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	18	0.43
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	18	0.43
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	18	0.43
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	18	0.43
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	18	0.43
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	5	0.43
(1,892)	1:33:A:CYS:HB2	1:36:A:CYS:HA	5	0.43
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	5	0.43
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	1	0.43
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	1	0.43
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	1	0.43
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	1	0.43
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	13	0.43
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	13	0.43
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	13	0.43
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	13	0.43
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	13	0.43
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	13	0.43
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	20	0.43
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	20	0.43
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	20	0.43
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	8	0.43
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	8	0.43
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD3	8	0.43
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	15	0.43
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	11	0.43
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	11	0.43
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	5	0.43
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	5	0.43
(4,850)	1:37:A:LYS:HG2	1:38:A:THR:H	9	0.42
(4,850)	1:37:A:LYS:HG3	1:38:A:THR:H	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	20	0.42
(4,702)	1:38:A:THR:HG21	1:40:A:ASN:HB3	8	0.42
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	20	0.42
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	20	0.42
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	9	0.42
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	9	0.42
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	9	0.42
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	9	0.42
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	3	0.42
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	3	0.42
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	3	0.42
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	3	0.42
(1,757)	1:11:A:THR:HG21	1:26:A:GLN:HG3	10	0.42
(1,757)	1:11:A:THR:HG22	1:26:A:GLN:HG3	10	0.42
(1,757)	1:11:A:THR:HG23	1:26:A:GLN:HG3	10	0.42
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	7	0.42
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	7	0.42
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	7	0.42
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	7	0.42
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD3	2	0.42
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD2	2	0.42
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD3	2	0.42
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB3	7	0.42
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB2	7	0.42
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB2	7	0.42
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB3	7	0.42
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	13	0.42
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	18	0.42
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	14	0.42
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	14	0.42
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	14	0.42
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	17	0.42
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	17	0.42
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	17	0.42
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	19	0.42
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	19	0.42
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	19	0.42
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	18	0.42
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	18	0.42
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	18	0.42
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	18	0.42
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG3	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	3	0.41
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	3	0.41
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	9	0.41
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	12	0.41
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	17	0.41
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	17	0.41
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	17	0.41
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	17	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	12	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	12	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	12	0.41
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	12	0.41
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	3	0.41
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	3	0.41
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	3	0.41
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	3	0.41
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	7	0.41
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	7	0.41
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	10	0.41
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	10	0.41
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	11	0.41
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	11	0.41
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	11	0.41
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	11	0.41
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	5	0.41
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	5	0.41
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	5	0.41
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	5	0.41
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	5	0.41
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	5	0.41
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	9	0.41
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	9	0.41
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	9	0.41
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	9	0.41
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	9	0.41
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	7	0.41
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	7	0.41
(1,787)	1:19:A:CYS:HB3	1:35:A:ALA:HA	7	0.41
(1,787)	1:19:A:CYS:HB2	1:35:A:ALA:HA	7	0.41
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	17	0.41
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	13	0.41
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	13	0.41
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	13	0.41
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	1	0.41
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	9	0.41
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	9	0.41
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	12	0.41
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	12	0.41
(1,141)	1:60:A:CYS:HB3	1:61:A:GLY:H	18	0.41
(1,141)	1:60:A:CYS:HB2	1:61:A:GLY:H	18	0.41
(1,141)	1:60:A:CYS:HB3	1:61:A:GLY:H	18	0.41
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	15	0.41
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	15	0.41
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	15	0.41
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	14	0.41
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	14	0.41
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	14	0.41
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	14	0.41
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	14	0.41
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	14	0.41
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	15	0.4
(4,377)	1:29:A:GLU:HA	1:30:A:GLY:H	9	0.4
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	19	0.4
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	19	0.4
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	1	0.4
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	1	0.4
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	9	0.4
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	4	0.4
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	16	0.4
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	13	0.4
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	13	0.4
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	13	0.4
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	13	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	17	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	17	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	17	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	17	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	17	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	17	0.4
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	17	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	17	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	17	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	17	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	17	0.4
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	17	0.4
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	1	0.4
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	1	0.4
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	1	0.4
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	1	0.4
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	1	0.4
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	1	0.4
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	16	0.4
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	16	0.4
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	16	0.4
(1,704)	1:16:A:SER:HB2	1:20:A:GLN:HG2	19	0.4
(1,704)	1:16:A:SER:HB2	1:20:A:GLN:HG3	19	0.4
(1,704)	1:16:A:SER:HB3	1:20:A:GLN:HG2	19	0.4
(1,704)	1:16:A:SER:HB3	1:20:A:GLN:HG3	19	0.4
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	13	0.4
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	13	0.4
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	13	0.4
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	13	0.4
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	8	0.4
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	8	0.4
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	8	0.4
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	8	0.4
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	8	0.4
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	8	0.4
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	8	0.4
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	8	0.4
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	8	0.4
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	3	0.4
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	0.4
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	0.4
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.4
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	6	0.4
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.4
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	6	0.4
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	6	0.4
(1,409)	1:29:A:GLU:HA	1:30:A:GLY:H	9	0.4
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	9	0.4
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	9	0.4
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	1	0.4
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	4	0.4
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	4	0.4
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	16	0.4
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	16	0.4
(4,951)	1:38:A:THR:H	1:67:A:LYS:HB3	7	0.39
(4,910)	1:9:A:LYS:H	1:27:A:CYS:HB2	11	0.39
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	8	0.39
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	8	0.39
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	15	0.39
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	20	0.39
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	11	0.39
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	11	0.39
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	7	0.39
(4,138)	1:61:A:GLY:H	1:64:A:CYS:HB3	18	0.39
(4,114)	1:55:A:PRO:HB2	1:57:A:SER:H	15	0.39
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	7	0.39
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	8	0.39
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	8	0.39
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	8	0.39
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	2	0.39
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	2	0.39
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	2	0.39
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	2	0.39
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	2	0.39
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	2	0.39
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	2	0.39
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	2	0.39
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	2	0.39
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	2	0.39
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	2	0.39
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	2	0.39
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	2	0.39
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB3	14	0.39
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB2	14	0.39
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB2	14	0.39
(1,596)	1:34:A:ALA:HA	1:37:A:LYS:HB3	14	0.39
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	13	0.39
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	15	0.39
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	15	0.39
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	7	0.39
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	7	0.39
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	20	0.39
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	20	0.39
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	20	0.39
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	7	0.39
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	7	0.39
(1,142)	1:61:A:GLY:H	1:64:A:CYS:HB2	18	0.39
(1,142)	1:61:A:GLY:H	1:64:A:CYS:HB3	18	0.39
(1,117)	1:55:A:PRO:HB2	1:57:A:SER:H	15	0.39
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	15	0.38
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	15	0.38
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD2	5	0.38
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	0.38
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	16	0.38
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	16	0.38
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	7	0.38
(4,650)	1:38:A:THR:H	1:67:A:LYS:HD2	4	0.38
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	11	0.38
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	11	0.38
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	1	0.38
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	19	0.38
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	19	0.38
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	9	0.38
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	9	0.38
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	9	0.38
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	10	0.38
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	10	0.38
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	10	0.38
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	15	0.38
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	15	0.38
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	15	0.38
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD2	5	0.38
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	0.38
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	0.38
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	11	0.38
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	11	0.38
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	16	0.38
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	16	0.38
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	16	0.38
(1,740)	1:38:A:THR:H	1:67:A:LYS:HD2	4	0.38
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	1	0.38
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	1	0.38
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	19	0.38
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	19	0.38
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG3	19	0.38
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	4	0.38
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	4	0.38
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	4	0.38
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	20	0.38
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	20	0.38
(1,410)	1:6:A:LYS:HE2	1:7:A:GLY:H	20	0.38
(1,410)	1:6:A:LYS:HE3	1:7:A:GLY:H	20	0.38
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	1	0.38
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	6	0.38
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	6	0.38
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	14	0.38
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	14	0.38
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	18	0.38
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	16	0.38
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	16	0.38
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	16	0.38
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	16	0.38
(4,174)	1:38:A:THR:H	1:67:A:LYS:HE2	6	0.37
(4,174)	1:38:A:THR:H	1:67:A:LYS:HE3	6	0.37
(4,139)	1:60:A:CYS:HB2	1:61:A:GLY:H	12	0.37
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	12	0.37
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	12	0.37
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	19	0.37
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	19	0.37
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	19	0.37
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	19	0.37
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA2	19	0.37
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA2	19	0.37
(1,955)	1:9:A:LYS:HG2	1:28:A:GLY:HA3	19	0.37
(1,955)	1:9:A:LYS:HG3	1:28:A:GLY:HA3	19	0.37
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	2	0.37
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	9	0.37
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	9	0.37
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	9	0.37
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	9	0.37
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	9	0.37
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	9	0.37
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	9	0.37
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	9	0.37
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	9	0.37
(1,487)	1:11:A:THR:H	1:26:A:GLN:H	13	0.37
(1,487)	1:11:A:THR:H	1:26:A:GLN:H	15	0.37
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	7	0.37
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	18	0.37
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	18	0.37
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	18	0.37
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	19	0.37
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	19	0.37
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	3	0.37
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	3	0.37
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	3	0.37
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	4	0.37
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	4	0.37
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	4	0.37
(1,144)	1:60:A:CYS:HB2	1:61:A:GLY:H	12	0.37
(4,959)	1:37:A:LYS:H	1:37:A:LYS:HE2	4	0.36
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	1	0.36
(4,844)	1:33:A:CYS:H	1:37:A:LYS:HE2	13	0.36
(4,844)	1:33:A:CYS:H	1:37:A:LYS:HE3	13	0.36
(4,656)	1:21:A:CYS:HB2	1:25:A:CYS:HA	8	0.36
(4,656)	1:21:A:CYS:HB3	1:25:A:CYS:HA	8	0.36
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	15	0.36
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	15	0.36
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	2	0.36
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	11	0.36
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	1	0.36
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE2	13	0.36
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE3	13	0.36
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE2	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE3	13	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	3	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	3	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	3	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	3	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	20	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	20	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	20	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	20	0.36
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	20	0.36
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	20	0.36
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD3	13	0.36
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD2	13	0.36
(1,602)	1:15:A:ARG:H	1:15:A:ARG:HD3	13	0.36
(1,460)	1:60:A:CYS:HB2	1:64:A:CYS:H	14	0.36
(1,460)	1:60:A:CYS:HB2	1:64:A:CYS:H	14	0.36
(1,460)	1:60:A:CYS:HB3	1:64:A:CYS:H	14	0.36
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	8	0.36
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	8	0.36
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	8	0.36
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	17	0.36
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	8	0.36
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	8	0.36
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	8	0.36
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	2	0.36
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	2	0.36
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	11	0.36
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	11	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	17	0.36
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	17	0.36
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	17	0.36
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	16	0.36
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	16	0.36
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB3	16	0.36
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	20	0.36
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	20	0.36
(4,941)	1:6:A:LYS:HG2	1:9:A:LYS:H	9	0.35
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	19	0.35
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	19	0.35
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	3	0.35
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	3	0.35
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	10	0.35
(4,829)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	10	0.35
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	10	0.35
(4,829)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	10	0.35
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	4	0.35
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	4	0.35
(4,585)	1:38:A:THR:HB	1:55:A:PRO:HB3	17	0.35
(4,324)	1:11:A:THR:HG21	1:27:A:CYS:H	10	0.35
(4,324)	1:11:A:THR:HG22	1:27:A:CYS:H	10	0.35
(4,324)	1:11:A:THR:HG23	1:27:A:CYS:H	10	0.35
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	2	0.35
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	2	0.35
(4,297)	1:62:A:SER:H	1:64:A:CYS:HB2	13	0.35
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	3	0.35
(4,139)	1:60:A:CYS:HB2	1:61:A:GLY:H	4	0.35
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	1	0.35
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	1	0.35
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	1	0.35
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	20	0.35
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	20	0.35
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	20	0.35
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	20	0.35
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	19	0.35
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	19	0.35
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	19	0.35
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	19	0.35
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	3	0.35
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	3	0.35
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	3	0.35
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	10	0.35
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE22	10	0.35
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	10	0.35
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE22	10	0.35
(1,986)	1:24:A:LYS:HE2	1:26:A:GLN:HE21	10	0.35
(1,986)	1:24:A:LYS:HE3	1:26:A:GLN:HE21	10	0.35
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	4	0.35
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	4	0.35
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	4	0.35
(1,854)	1:45:A:GLY:HA3	1:47:A:LYS:HG2	9	0.35
(1,854)	1:45:A:GLY:HA3	1:47:A:LYS:HG2	9	0.35
(1,854)	1:45:A:GLY:HA3	1:47:A:LYS:HG3	9	0.35
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	4	0.35
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	4	0.35
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	4	0.35
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	4	0.35
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	4	0.35
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	4	0.35
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	4	0.35
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	4	0.35
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	4	0.35
(1,651)	1:38:A:THR:HB	1:55:A:PRO:HB3	17	0.35
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	20	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	10	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	10	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	10	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	10	0.35
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	0.35
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	10	0.35
(1,487)	1:11:A:THR:H	1:26:A:GLN:H	20	0.35
(1,352)	1:11:A:THR:HG21	1:27:A:CYS:H	10	0.35
(1,352)	1:11:A:THR:HG22	1:27:A:CYS:H	10	0.35
(1,352)	1:11:A:THR:HG23	1:27:A:CYS:H	10	0.35
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	10	0.35
(1,322)	1:62:A:SER:H	1:64:A:CYS:HB2	13	0.35
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	13	0.35
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD2	13	0.35
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	13	0.35
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	3	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	3	0.35
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	10	0.35
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	10	0.35
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	10	0.35
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	6	0.35
(1,144)	1:60:A:CYS:HB2	1:61:A:GLY:H	4	0.35
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	4	0.35
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	4	0.35
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	4	0.35
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	18	0.34
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	18	0.34
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	11	0.34
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	11	0.34
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	10	0.34
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	20	0.34
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	20	0.34
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	18	0.34
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	18	0.34
(1,1071)	1:51:A:GLU:H	1:51:A:GLU:HG2	4	0.34
(1,1071)	1:51:A:GLU:H	1:51:A:GLU:HG3	4	0.34
(1,1071)	1:51:A:GLU:H	1:51:A:GLU:HG2	4	0.34
(1,1071)	1:51:A:GLU:H	1:51:A:GLU:HG3	4	0.34
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	11	0.34
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	11	0.34
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	11	0.34
(1,956)	1:9:A:LYS:HG2	1:29:A:GLU:H	1	0.34
(1,956)	1:9:A:LYS:HG3	1:29:A:GLU:H	1	0.34
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	16	0.34
(1,671)	1:66:A:CYS:HB2	1:67:A:LYS:HD3	16	0.34
(1,671)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	16	0.34
(1,411)	1:29:A:GLU:HG2	1:30:A:GLY:H	12	0.34
(1,411)	1:29:A:GLU:HG3	1:30:A:GLY:H	12	0.34
(1,411)	1:29:A:GLU:HG2	1:30:A:GLY:H	12	0.34
(1,411)	1:29:A:GLU:HG3	1:30:A:GLY:H	12	0.34
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	20	0.34
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	20	0.34
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	12	0.34
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD2	12	0.34
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	12	0.34
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	15	0.34
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	15	0.34
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	10	0.33
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD2	17	0.33
(4,841)	1:32:A:THR:HB	1:37:A:LYS:HD3	17	0.33
(4,789)	1:7:A:GLY:HA2	1:9:A:LYS:H	6	0.33
(4,789)	1:7:A:GLY:HA3	1:9:A:LYS:H	6	0.33
(4,767)	1:12:A:SER:HA	1:15:A:ARG:HD2	16	0.33
(4,649)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	8	0.33
(4,585)	1:38:A:THR:HB	1:55:A:PRO:HB3	8	0.33
(4,585)	1:38:A:THR:HB	1:55:A:PRO:HB3	9	0.33
(4,297)	1:62:A:SER:H	1:64:A:CYS:HB2	15	0.33
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	19	0.33
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	15	0.33
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	15	0.33
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	9	0.33
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	10	0.33
(1,1140)	1:39:A:CYS:H	1:55:A:PRO:HD2	14	0.33
(1,1140)	1:39:A:CYS:H	1:55:A:PRO:HD3	14	0.33
(1,1068)	1:50:A:LYS:HE2	1:51:A:GLU:H	14	0.33
(1,1068)	1:50:A:LYS:HE3	1:51:A:GLU:H	14	0.33
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	17	0.33
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	17	0.33
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD3	17	0.33
(1,1008)	1:32:A:THR:HB	1:37:A:LYS:HD2	17	0.33
(1,927)	1:7:A:GLY:HA2	1:9:A:LYS:H	6	0.33
(1,927)	1:7:A:GLY:HA3	1:9:A:LYS:H	6	0.33
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	16	0.33
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD2	16	0.33
(1,898)	1:12:A:SER:HA	1:15:A:ARG:HD3	16	0.33
(1,816)	1:39:A:CYS:H	1:55:A:PRO:HD2	14	0.33
(1,816)	1:39:A:CYS:H	1:55:A:PRO:HD3	14	0.33
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	18	0.33
(1,814)	1:60:A:CYS:HB2	1:64:A:CYS:H	18	0.33
(1,814)	1:60:A:CYS:HB3	1:64:A:CYS:H	18	0.33
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	17	0.33
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	17	0.33
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	17	0.33
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	17	0.33
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	17	0.33
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	17	0.33
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	5	0.33
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	5	0.33
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:9:A:LYS:HB3	1:29:A:GLU:H	14	0.33
(1,651)	1:38:A:THR:HB	1:55:A:PRO:HB3	8	0.33
(1,651)	1:38:A:THR:HB	1:55:A:PRO:HB3	9	0.33
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	3	0.33
(1,322)	1:62:A:SER:H	1:64:A:CYS:HB2	15	0.33
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	12	0.33
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	12	0.33
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	12	0.33
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	12	0.33
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	7	0.33
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	7	0.33
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	7	0.33
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	19	0.33
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	19	0.33
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	3	0.33
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	3	0.33
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	3	0.33
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	11	0.33
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	11	0.33
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	11	0.33
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	16	0.33
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	16	0.33
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	16	0.33
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	16	0.33
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	8	0.33
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	8	0.33
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	11	0.33
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	11	0.33
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD2	19	0.32
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD3	19	0.32
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	2	0.32
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	2	0.32
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	19	0.32
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	19	0.32
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	16	0.32
(4,656)	1:21:A:CYS:HB2	1:25:A:CYS:HA	17	0.32
(4,656)	1:21:A:CYS:HB3	1:25:A:CYS:HA	17	0.32
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	16	0.32
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	16	0.32
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	10	0.32
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	1	0.32
(4,132)	1:13:A:ALA:H	1:15:A:ARG:HB2	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,132)	1:13:A:ALA:H	1:15:A:ARG:HB3	14	0.32
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	4	0.32
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	4	0.32
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	4	0.32
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	12	0.32
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	12	0.32
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	12	0.32
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	1	0.32
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	1	0.32
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	1	0.32
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	1	0.32
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	16	0.32
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	16	0.32
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD2	19	0.32
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	19	0.32
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	19	0.32
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	2	0.32
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	2	0.32
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	2	0.32
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	19	0.32
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	19	0.32
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	19	0.32
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	15	0.32
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	15	0.32
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	15	0.32
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	15	0.32
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	13	0.32
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	13	0.32
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	13	0.32
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	13	0.32
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	18	0.32
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	18	0.32
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	18	0.32
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	13	0.32
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	14	0.32
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	14	0.32
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	14	0.32
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	14	0.32
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	14	0.32
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	14	0.32
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	14	0.32
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	14	0.32
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	5	0.32
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	18	0.32
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	18	0.32
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	18	0.32
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	15	0.32
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	6	0.32
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	6	0.32
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	6	0.32
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	16	0.32
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	16	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	12	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	12	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	12	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	18	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	18	0.32
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	18	0.32
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	1	0.32
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	1	0.32
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	12	0.32
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	12	0.32
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	12	0.32
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	1	0.32
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	1	0.32
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	1	0.32
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	1	0.32
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	4	0.31
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	4	0.31
(4,814)	1:16:A:SER:HA	1:17:A:GLU:HG2	6	0.31
(4,814)	1:16:A:SER:HA	1:17:A:GLU:HG3	6	0.31
(4,585)	1:38:A:THR:HB	1:55:A:PRO:HB3	13	0.31
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD2	10	0.31
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD3	10	0.31
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	8	0.31
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	20	0.31
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	4	0.31
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	4	0.31
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG2	6	0.31
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG3	6	0.31
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG2	6	0.31
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG3	6	0.31
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	17	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	17	0.31
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	17	0.31
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	17	0.31
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	9	0.31
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	9	0.31
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	9	0.31
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	3	0.31
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	3	0.31
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	3	0.31
(1,651)	1:38:A:THR:HB	1:55:A:PRO:HB3	13	0.31
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	10	0.31
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	8	0.31
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	20	0.31
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	20	0.31
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	15	0.31
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	15	0.31
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	16	0.31
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG2	16	0.31
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	16	0.31
(4,907)	1:9:A:LYS:HE3	1:29:A:GLU:H	20	0.3
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD2	9	0.3
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD3	9	0.3
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	12	0.3
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	8	0.3
(4,646)	1:43:A:SER:H	1:54:A:GLY:HA3	15	0.3
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	10	0.3
(4,438)	1:39:A:CYS:H	1:40:A:ASN:HD21	5	0.3
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	20	0.3
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	20	0.3
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	5	0.3
(4,277)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	12	0.3
(4,206)	1:43:A:SER:H	1:54:A:GLY:HA3	15	0.3
(4,140)	1:61:A:GLY:H	1:64:A:CYS:H	18	0.3
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD2	9	0.3
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	9	0.3
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	9	0.3
(1,956)	1:9:A:LYS:HG2	1:29:A:GLU:H	9	0.3
(1,956)	1:9:A:LYS:HG3	1:29:A:GLU:H	9	0.3
(1,904)	1:38:A:THR:HA	1:55:A:PRO:HG3	14	0.3
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.3
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.3
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.3
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	6	0.3
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.3
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	0.3
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	6	0.3
(1,871)	1:50:A:LYS:HG3	1:52:A:CYS:H	5	0.3
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	15	0.3
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	15	0.3
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	15	0.3
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	15	0.3
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	15	0.3
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	15	0.3
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	15	0.3
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	15	0.3
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	15	0.3
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	13	0.3
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	13	0.3
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	13	0.3
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	13	0.3
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	6	0.3
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	6	0.3
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	6	0.3
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	6	0.3
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	6	0.3
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	6	0.3
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	6	0.3
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	6	0.3
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	6	0.3
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	10	0.3
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	3	0.3
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	3	0.3
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	3	0.3
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	3	0.3
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	9	0.3
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	9	0.3
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	9	0.3
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	9	0.3
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	0.3
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	0.3
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	13	0.3
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	13	0.3
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	13	0.3
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	0.3
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	13	0.3
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD22	3	0.3
(1,302)	1:39:A:CYS:H	1:40:A:ASN:HD21	3	0.3
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	12	0.3
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	12	0.3
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	13	0.3
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	13	0.3
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	17	0.3
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	17	0.3
(1,145)	1:61:A:GLY:H	1:64:A:CYS:H	18	0.3
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	9	0.29
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	9	0.29
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB3	14	0.29
(4,646)	1:43:A:SER:H	1:54:A:GLY:HA3	16	0.29
(4,405)	1:11:A:THR:HG21	1:26:A:GLN:HE22	11	0.29
(4,206)	1:43:A:SER:H	1:54:A:GLY:HA3	16	0.29
(4,174)	1:38:A:THR:H	1:67:A:LYS:HE2	8	0.29
(4,174)	1:38:A:THR:H	1:67:A:LYS:HE3	8	0.29
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	14	0.29
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	14	0.29
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB2	14	0.29
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	14	0.29
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB2	14	0.29
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	14	0.29
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	14	0.29
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	14	0.29
(1,1145)	1:14:A:CYS:HA	1:19:A:CYS:HB3	19	0.29
(1,1145)	1:14:A:CYS:HA	1:19:A:CYS:HB2	19	0.29
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	3	0.29
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	3	0.29
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	3	0.29
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	3	0.29
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	9	0.29
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	9	0.29
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	13	0.29
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	13	0.29
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE2	13	0.29
(1,849)	1:32:A:THR:H	1:37:A:LYS:HE3	13	0.29
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	16	0.29
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	16	0.29
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	16	0.29
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	16	0.29
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	16	0.29
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	18	0.29
(1,641)	1:17:A:GLU:HA	1:17:A:GLU:HG3	8	0.29
(1,641)	1:17:A:GLU:HA	1:17:A:GLU:HG2	8	0.29
(1,641)	1:17:A:GLU:HA	1:17:A:GLU:HG3	8	0.29
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	5	0.29
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.29
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.29
(1,554)	1:46:A:CYS:HA	1:47:A:LYS:HG3	4	0.29
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	6	0.29
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	6	0.29
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	6	0.29
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	16	0.29
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	16	0.29
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	16	0.29
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	3	0.29
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	3	0.29
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	3	0.29
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	3	0.29
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	3	0.29
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	3	0.29
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	15	0.29
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	15	0.29
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	15	0.29
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	15	0.29
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	15	0.29
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	15	0.29
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	15	0.29
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	15	0.29
(4,951)	1:38:A:THR:H	1:67:A:LYS:HB3	6	0.28
(4,946)	1:39:A:CYS:H	1:67:A:LYS:HE2	5	0.28
(4,946)	1:39:A:CYS:H	1:67:A:LYS:HE3	5	0.28
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	20	0.28
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	7	0.28
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	7	0.28
(4,807)	1:15:A:ARG:HD3	1:16:A:SER:H	8	0.28
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	7	0.28
(4,477)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	8	0.28
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	5	0.28
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	5	0.28
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	8	0.28
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	8	0.28
(4,343)	1:63:A:SER:H	1:64:A:CYS:HB2	18	0.28
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD2	11	0.28
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD3	11	0.28
(4,257)	1:21:A:CYS:HB3	1:24:A:LYS:H	17	0.28
(4,203)	1:42:A:THR:HB	1:43:A:SER:H	8	0.28
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	9	0.28
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	9	0.28
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	6	0.28
(1,1158)	1:39:A:CYS:H	1:67:A:LYS:HE2	5	0.28
(1,1158)	1:39:A:CYS:H	1:67:A:LYS:HE3	5	0.28
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	8	0.28
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	8	0.28
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	8	0.28
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	20	0.28
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	12	0.28
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	12	0.28
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	12	0.28
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	12	0.28
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	12	0.28
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	12	0.28
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	7	0.28
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	7	0.28
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	7	0.28
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	13	0.28
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	13	0.28
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	13	0.28
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	13	0.28
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	13	0.28
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	13	0.28
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	13	0.28
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	13	0.28
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	13	0.28
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	13	0.28
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	13	0.28
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	13	0.28
(1,707)	1:16:A:SER:HB2	1:20:A:GLN:H	19	0.28
(1,707)	1:16:A:SER:HB3	1:20:A:GLN:H	19	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	15	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	15	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	15	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	15	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	15	0.28
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	15	0.28
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	15	0.28
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	15	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	19	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	19	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	19	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	19	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	19	0.28
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	19	0.28
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	19	0.28
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	19	0.28
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	19	0.28
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	6	0.28
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	7	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	8	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG2	8	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	8	0.28
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	8	0.28
(1,520)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	8	0.28
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	5	0.28
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	5	0.28
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	5	0.28
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	14	0.28
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	15	0.28
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	15	0.28
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE3	15	0.28
(1,373)	1:63:A:SER:H	1:64:A:CYS:HB2	18	0.28
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	17	0.28
(1,275)	1:21:A:CYS:HB2	1:24:A:LYS:H	17	0.28
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	17	0.28
(1,214)	1:42:A:THR:HB	1:43:A:SER:H	8	0.28
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	2	0.28
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG2	2	0.28
(1,59)	1:9:A:LYS:H	1:9:A:LYS:HG3	2	0.28
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	7	0.28
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	7	0.28
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	7	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	7	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	7	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	7	0.28
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	7	0.28
(4,951)	1:38:A:THR:H	1:67:A:LYS:HB3	15	0.27
(4,944)	1:31:A:CYS:HA	1:37:A:LYS:HG3	2	0.27
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	13	0.27
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	13	0.27
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD2	1	0.27
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD3	1	0.27
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	15	0.27
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	15	0.27
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	20	0.27
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	20	0.27
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	3	0.27
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	17	0.27
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	15	0.27
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	1	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	1	0.27
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB2	1	0.27
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	1	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB2	1	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	1	0.27
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	1	0.27
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	1	0.27
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	18	0.27
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	18	0.27
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	18	0.27
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	1	0.27
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	1	0.27
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	1	0.27
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	1	0.27
(1,1099)	1:28:A:GLY:HA2	1:29:A:GLU:H	17	0.27
(1,1099)	1:28:A:GLY:HA3	1:29:A:GLU:H	17	0.27
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	13	0.27
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	13	0.27
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	13	0.27
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	13	0.27
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD2	1	0.27
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	1	0.27
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	15	0.27
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	15	0.27
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	15	0.27
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	20	0.27
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	20	0.27
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	20	0.27
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	5	0.27
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	5	0.27
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	5	0.27
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	5	0.27
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	11	0.27
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	11	0.27
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	11	0.27
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	11	0.27
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	5	0.27
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	5	0.27
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	5	0.27
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	5	0.27
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	5	0.27
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	5	0.27
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG21	12	0.27
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG22	12	0.27
(1,807)	1:40:A:ASN:HB2	1:42:A:THR:HG23	12	0.27
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG21	12	0.27
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG22	12	0.27
(1,807)	1:40:A:ASN:HB3	1:42:A:THR:HG23	12	0.27
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	18	0.27
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	18	0.27
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD3	18	0.27
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	1	0.27
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	1	0.27
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	1	0.27
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	1	0.27
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	3	0.27
(1,411)	1:29:A:GLU:HG2	1:30:A:GLY:H	2	0.27
(1,411)	1:29:A:GLU:HG3	1:30:A:GLY:H	2	0.27
(1,411)	1:29:A:GLU:HG2	1:30:A:GLY:H	2	0.27
(1,411)	1:29:A:GLU:HG3	1:30:A:GLY:H	2	0.27
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	8	0.27
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	17	0.27
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	17	0.27
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	16	0.27
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	16	0.27
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	4	0.27
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	4	0.27
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	4	0.27
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	14	0.27
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	14	0.27
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	14	0.27
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	14	0.27
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	12	0.26
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	12	0.26
(4,850)	1:37:A:LYS:HG2	1:38:A:THR:H	1	0.26
(4,850)	1:37:A:LYS:HG3	1:38:A:THR:H	1	0.26
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD2	18	0.26
(4,837)	1:31:A:CYS:H	1:37:A:LYS:HD3	18	0.26
(4,814)	1:16:A:SER:HA	1:17:A:GLU:HG2	17	0.26
(4,814)	1:16:A:SER:HA	1:17:A:GLU:HG3	17	0.26
(4,789)	1:7:A:GLY:HA2	1:9:A:LYS:H	17	0.26
(4,789)	1:7:A:GLY:HA3	1:9:A:LYS:H	17	0.26
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG21	17	0.26
(4,649)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	15	0.26
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	4	0.26
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	5	0.26
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	1	0.26
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	1	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	5	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	5	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	5	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	17	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	17	0.26
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	17	0.26
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	16	0.26
(1,1116)	1:9:A:LYS:HG2	1:10:A:CYS:H	16	0.26
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	16	0.26
(1,1099)	1:28:A:GLY:HA2	1:29:A:GLU:H	9	0.26
(1,1099)	1:28:A:GLY:HA3	1:29:A:GLU:H	9	0.26
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	12	0.26
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	12	0.26
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	1	0.26
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	1	0.26
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	1	0.26
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD2	18	0.26
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	18	0.26
(1,1001)	1:31:A:CYS:H	1:37:A:LYS:HD3	18	0.26
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG2	17	0.26
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG3	17	0.26
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG2	17	0.26
(1,969)	1:16:A:SER:HA	1:17:A:GLU:HG3	17	0.26
(1,927)	1:7:A:GLY:HA2	1:9:A:LYS:H	17	0.26
(1,927)	1:7:A:GLY:HA3	1:9:A:LYS:H	17	0.26
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	15	0.26
(1,892)	1:33:A:CYS:HB2	1:36:A:CYS:HA	15	0.26
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	15	0.26
(1,858)	1:11:A:THR:HG21	1:14:A:CYS:HB2	7	0.26
(1,858)	1:11:A:THR:HG22	1:14:A:CYS:HB2	7	0.26
(1,858)	1:11:A:THR:HG23	1:14:A:CYS:HB2	7	0.26
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB2	20	0.26
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB2	20	0.26
(1,844)	1:12:A:SER:HA	1:15:A:ARG:HB3	20	0.26
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	3	0.26
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	3	0.26
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	3	0.26
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	8	0.26
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	8	0.26
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	8	0.26
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	4	0.26
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	4	0.26
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD3	4	0.26
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	15	0.26
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	15	0.26
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	15	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	20	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	20	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	20	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	20	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	20	0.26
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	20	0.26
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	20	0.26
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	20	0.26
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	20	0.26
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	4	0.26
(1,528)	1:21:A:CYS:H	1:36:A:CYS:HB2	1	0.26
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	11	0.26
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	11	0.26
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	11	0.26
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	5	0.26
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	15	0.26
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	15	0.26
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	15	0.26
(1,198)	1:20:A:GLN:H	1:20:A:GLN:HE22	3	0.26
(1,198)	1:20:A:GLN:H	1:20:A:GLN:HE21	3	0.26
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	14	0.26
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	14	0.26
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	14	0.26
(1,40)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	14	0.26
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	16	0.25
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	16	0.25
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	7	0.25
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	7	0.25
(4,850)	1:37:A:LYS:HG2	1:38:A:THR:H	4	0.25
(4,850)	1:37:A:LYS:HG3	1:38:A:THR:H	4	0.25
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG21	7	0.25
(4,646)	1:43:A:SER:H	1:54:A:GLY:HA3	17	0.25
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	2	0.25
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	13	0.25
(4,459)	1:62:A:SER:HA	1:67:A:LYS:HG3	13	0.25
(4,405)	1:11:A:THR:HG22	1:26:A:GLN:HE22	17	0.25
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	18	0.25
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	18	0.25
(4,303)	1:37:A:LYS:HG3	1:62:A:SER:H	9	0.25
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	3	0.25
(4,220)	1:42:A:THR:H	1:54:A:GLY:HA2	13	0.25
(4,206)	1:43:A:SER:H	1:54:A:GLY:HA3	17	0.25
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	16	0.25
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	16	0.25
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	7	0.25
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	7	0.25
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	7	0.25
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	7	0.25
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	4	0.25
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	4	0.25
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	4	0.25
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	4	0.25
(1,1004)	1:32:A:THR:HA	1:37:A:LYS:HG2	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:32:A:THR:HA	1:37:A:LYS:HG3	8	0.25
(1,924)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	14	0.25
(1,924)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	14	0.25
(1,924)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	14	0.25
(1,924)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	14	0.25
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	9	0.25
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	9	0.25
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	9	0.25
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	9	0.25
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	9	0.25
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	9	0.25
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	9	0.25
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	9	0.25
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	17	0.25
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	17	0.25
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	1	0.25
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	2	0.25
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	13	0.25
(1,581)	1:42:A:THR:HB	1:43:A:SER:HB2	8	0.25
(1,581)	1:42:A:THR:HB	1:43:A:SER:HB3	8	0.25
(1,581)	1:42:A:THR:HB	1:43:A:SER:HB2	8	0.25
(1,581)	1:42:A:THR:HB	1:43:A:SER:HB3	8	0.25
(1,503)	1:62:A:SER:HA	1:67:A:LYS:HG3	13	0.25
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	8	0.25
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	8	0.25
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	8	0.25
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	1	0.25
(1,378)	1:21:A:CYS:HB2	1:25:A:CYS:H	1	0.25
(1,378)	1:21:A:CYS:HB3	1:25:A:CYS:H	1	0.25
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB2	8	0.25
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB2	8	0.25
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB3	8	0.25
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB3	8	0.25
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	6	0.25
(1,275)	1:21:A:CYS:HB2	1:24:A:LYS:H	6	0.25
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	6	0.25
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	3	0.25
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA2	13	0.25
(1,231)	1:42:A:THR:H	1:54:A:GLY:HA3	13	0.25
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	1	0.25
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	1	0.25
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	1	0.25
(1,184)	1:38:A:THR:H	1:67:A:LYS:HD3	2	0.25
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	20	0.25
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	20	0.25
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	20	0.25
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	20	0.25
(1,26)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	14	0.25
(1,26)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	14	0.25
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	2	0.25
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	2	0.25
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	12	0.25
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	12	0.25
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	12	0.25
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	12	0.25
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	11	0.24
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	1	0.24
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	1	0.24
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.24
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.24
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	1	0.24
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	6	0.24
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	3	0.24
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	8	0.24
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	8	0.24
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD2	20	0.24
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD3	20	0.24
(4,289)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	0.24
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	4	0.24
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	11	0.24
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	1	0.24
(4,103)	1:31:A:CYS:H	1:32:A:THR:HG21	8	0.24
(4,103)	1:31:A:CYS:H	1:32:A:THR:HG22	8	0.24
(4,103)	1:31:A:CYS:H	1:32:A:THR:HG23	8	0.24
(4,25)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	14	0.24
(4,25)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	16	0.24
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	12	0.24
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	12	0.24
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	12	0.24
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	12	0.24
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	11	0.24
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	15	0.24
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	15	0.24
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	15	0.24
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	1	0.24
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	1	0.24
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.24
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.24
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.24
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.24
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	16	0.24
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	16	0.24
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	6	0.24
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	6	0.24
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	6	0.24
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	6	0.24
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	6	0.24
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	6	0.24
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	6	0.24
(1,991)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	6	0.24
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	6	0.24
(1,991)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	6	0.24
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	5	0.24
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	5	0.24
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	5	0.24
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	5	0.24
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	5	0.24
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	5	0.24
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	5	0.24
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	5	0.24
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	5	0.24
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	5	0.24
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	5	0.24
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	5	0.24
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB1	4	0.24
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB2	4	0.24
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB3	4	0.24
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB1	4	0.24
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB2	4	0.24
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB3	4	0.24
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB1	4	0.24
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB2	4	0.24
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB3	4	0.24
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB1	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB2	4	0.24
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB3	4	0.24
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	8	0.24
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	8	0.24
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	8	0.24
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	8	0.24
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	1	0.24
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	1	0.24
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	1	0.24
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB2	1	0.24
(1,822)	1:28:A:GLY:HA3	1:29:A:GLU:HB3	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB2	1	0.24
(1,822)	1:28:A:GLY:HA2	1:29:A:GLU:HB3	1	0.24
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	11	0.24
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	12	0.24
(1,747)	1:21:A:CYS:HB2	1:25:A:CYS:HA	12	0.24
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	12	0.24
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	10	0.24
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	10	0.24
(1,738)	1:64:A:CYS:HB2	1:67:A:LYS:HD3	10	0.24
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	1	0.24
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	6	0.24
(1,643)	1:50:A:LYS:HB2	1:58:A:CYS:HA	10	0.24
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	10	0.24
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	10	0.24
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	10	0.24
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	11	0.24
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	14	0.24
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	3	0.24
(1,485)	1:21:A:CYS:HB3	1:26:A:GLN:H	11	0.24
(1,485)	1:21:A:CYS:HB2	1:26:A:GLN:H	11	0.24
(1,485)	1:21:A:CYS:HB3	1:26:A:GLN:H	11	0.24
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	4	0.24
(1,329)	1:62:A:SER:H	1:67:A:LYS:HG2	7	0.24
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	19	0.24
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	19	0.24
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE2	20	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:6:A:LYS:H	1:6:A:LYS:HE3	20	0.24
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	11	0.24
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	20	0.24
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	20	0.24
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	20	0.24
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	20	0.24
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	1	0.24
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	17	0.24
(1,106)	1:31:A:CYS:H	1:32:A:THR:HG21	8	0.24
(1,106)	1:31:A:CYS:H	1:32:A:THR:HG22	8	0.24
(1,106)	1:31:A:CYS:H	1:32:A:THR:HG23	8	0.24
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	12	0.24
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	12	0.24
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	12	0.24
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	12	0.24
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	11	0.24
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB2	11	0.24
(1,104)	1:31:A:CYS:H	1:33:A:CYS:HB3	11	0.24
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	3	0.24
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	3	0.24
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	3	0.24
(1,56)	1:9:A:LYS:H	1:10:A:CYS:HB2	8	0.24
(1,56)	1:9:A:LYS:H	1:10:A:CYS:HB2	8	0.24
(1,56)	1:9:A:LYS:H	1:10:A:CYS:HB3	8	0.24
(1,26)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	16	0.24
(1,26)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	16	0.24
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	13	0.24
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	13	0.24
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	20	0.24
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	20	0.24
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	20	0.24
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	20	0.24
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	13	0.23
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	14	0.23
(4,646)	1:43:A:SER:H	1:54:A:GLY:HA2	1	0.23
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	17	0.23
(4,518)	1:9:A:LYS:H	1:9:A:LYS:HD2	14	0.23
(4,400)	1:18:A:PRO:HG2	1:19:A:CYS:H	18	0.23
(4,377)	1:29:A:GLU:HA	1:30:A:GLY:H	12	0.23
(4,343)	1:63:A:SER:H	1:64:A:CYS:HB2	16	0.23
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	12	0.23
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	14	0.23
(4,206)	1:43:A:SER:H	1:54:A:GLY:HA2	1	0.23
(4,22)	1:17:A:GLU:H	1:20:A:GLN:HE21	1	0.23
(4,22)	1:17:A:GLU:H	1:20:A:GLN:HE22	1	0.23
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	3	0.23
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	8	0.23
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	15	0.23
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	15	0.23
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	15	0.23
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	16	0.23
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	16	0.23
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	16	0.23
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	13	0.23
(1,1034)	1:39:A:CYS:HB2	1:67:A:LYS:HD3	4	0.23
(1,1034)	1:39:A:CYS:HB3	1:67:A:LYS:HD3	4	0.23
(1,1034)	1:39:A:CYS:HB2	1:67:A:LYS:HD3	4	0.23
(1,1034)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	4	0.23
(1,1034)	1:39:A:CYS:HB2	1:67:A:LYS:HD3	4	0.23
(1,1034)	1:39:A:CYS:HB3	1:67:A:LYS:HD2	4	0.23
(1,1034)	1:39:A:CYS:HB3	1:67:A:LYS:HD3	4	0.23
(1,1034)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	4	0.23
(1,1034)	1:39:A:CYS:HB2	1:67:A:LYS:HD3	4	0.23
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD2	5	0.23
(1,932)	1:8:A:GLU:H	1:9:A:LYS:HD3	5	0.23
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	14	0.23
(1,915)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	14	0.23
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	14	0.23
(1,915)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	14	0.23
(1,858)	1:11:A:THR:HG21	1:14:A:CYS:HB2	15	0.23
(1,858)	1:11:A:THR:HG22	1:14:A:CYS:HB2	15	0.23
(1,858)	1:11:A:THR:HG23	1:14:A:CYS:HB2	15	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	4	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	4	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	4	0.23
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	4	0.23
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	15	0.23
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	15	0.23
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	15	0.23
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	20	0.23
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	20	0.23
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	20	0.23
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	1	0.23
(1,691)	1:16:A:SER:HB3	1:20:A:GLN:HB2	1	0.23
(1,691)	1:16:A:SER:HB2	1:20:A:GLN:HB2	1	0.23
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	13	0.23
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	13	0.23
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	13	0.23
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	13	0.23
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	13	0.23
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	13	0.23
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	13	0.23
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	13	0.23
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	13	0.23
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	17	0.23
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	8	0.23
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	8	0.23
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	8	0.23
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	8	0.23
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	5	0.23
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	5	0.23
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	5	0.23
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	11	0.23
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	11	0.23
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	11	0.23
(1,566)	1:9:A:LYS:H	1:9:A:LYS:HD2	14	0.23
(1,566)	1:9:A:LYS:H	1:9:A:LYS:HD3	14	0.23
(1,566)	1:9:A:LYS:H	1:9:A:LYS:HD2	14	0.23
(1,566)	1:9:A:LYS:H	1:9:A:LYS:HD3	14	0.23
(1,433)	1:18:A:PRO:HG2	1:19:A:CYS:H	18	0.23
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	11	0.23
(1,409)	1:29:A:GLU:HA	1:30:A:GLY:H	12	0.23
(1,390)	1:64:A:CYS:HB2	1:67:A:LYS:H	17	0.23
(1,373)	1:63:A:SER:H	1:64:A:CYS:HB2	16	0.23
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	12	0.23
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	20	0.23
(1,275)	1:21:A:CYS:HB2	1:24:A:LYS:H	20	0.23
(1,275)	1:21:A:CYS:HB3	1:24:A:LYS:H	20	0.23
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	13	0.23
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	13	0.23
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	13	0.23
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	1	0.23
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	1	0.23
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	19	0.23
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	19	0.23
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	19	0.23
(1,180)	1:38:A:THR:H	1:67:A:LYS:HA	15	0.23
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	8	0.23
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	8	0.23
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	8	0.23
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	8	0.23
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	3	0.23
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	8	0.23
(4,944)	1:37:A:LYS:HG3	1:62:A:SER:HA	15	0.22
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	17	0.22
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	17	0.22
(4,815)	1:16:A:SER:HB2	1:17:A:GLU:H	10	0.22
(4,815)	1:16:A:SER:HB3	1:17:A:GLU:H	10	0.22
(4,797)	1:8:A:GLU:HB2	1:10:A:CYS:HA	4	0.22
(4,797)	1:8:A:GLU:HB3	1:10:A:CYS:HA	4	0.22
(4,797)	1:8:A:GLU:HB2	1:10:A:CYS:HA	19	0.22
(4,797)	1:8:A:GLU:HB3	1:10:A:CYS:HA	19	0.22
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	19	0.22
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG22	12	0.22
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	9	0.22
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	11	0.22
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	16	0.22
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	7	0.22
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	17	0.22
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	17	0.22
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	17	0.22
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	8	0.22
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	10	0.22
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	10	0.22
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB2	10	0.22
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	10	0.22
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB2	10	0.22
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	10	0.22
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	10	0.22
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	10	0.22
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	5	0.22
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	5	0.22
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	17	0.22
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	17	0.22
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	17	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	17	0.22
(1,970)	1:16:A:SER:HB2	1:17:A:GLU:H	10	0.22
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	10	0.22
(1,970)	1:16:A:SER:HB3	1:17:A:GLU:H	10	0.22
(1,943)	1:8:A:GLU:HB2	1:10:A:CYS:HA	4	0.22
(1,943)	1:8:A:GLU:HB3	1:10:A:CYS:HA	4	0.22
(1,943)	1:8:A:GLU:HB2	1:10:A:CYS:HA	19	0.22
(1,943)	1:8:A:GLU:HB3	1:10:A:CYS:HA	19	0.22
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD2	10	0.22
(1,928)	1:7:A:GLY:HA2	1:9:A:LYS:HD3	10	0.22
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD2	10	0.22
(1,928)	1:7:A:GLY:HA3	1:9:A:LYS:HD3	10	0.22
(1,924)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	4	0.22
(1,924)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	4	0.22
(1,924)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	4	0.22
(1,924)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	4	0.22
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	12	0.22
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	12	0.22
(1,834)	1:21:A:CYS:HB2	1:36:A:CYS:HA	12	0.22
(1,834)	1:21:A:CYS:HB3	1:36:A:CYS:HA	12	0.22
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	19	0.22
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	19	0.22
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	19	0.22
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	9	0.22
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	11	0.22
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	16	0.22
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	0.22
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	7	0.22
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	0.22
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	7	0.22
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	7	0.22
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	6	0.22
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	14	0.22
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	14	0.22
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE3	14	0.22
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	4	0.22
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	4	0.22
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	17	0.22
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	8	0.22
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	8	0.22
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB2	8	0.22
(1,266)	1:32:A:THR:H	1:37:A:LYS:HB3	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	10	0.22
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	10	0.22
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	10	0.22
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	8	0.22
(1,198)	1:20:A:GLN:H	1:20:A:GLN:HE22	19	0.22
(1,198)	1:20:A:GLN:H	1:20:A:GLN:HE21	19	0.22
(1,2)	1:28:A:GLY:HA3	1:29:A:GLU:H	11	0.22
(1,2)	1:28:A:GLY:HA2	1:29:A:GLU:H	11	0.22
(1,2)	1:28:A:GLY:HA2	1:29:A:GLU:H	11	0.22
(1,2)	1:28:A:GLY:HA3	1:29:A:GLU:H	11	0.22
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB2	16	0.21
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB3	16	0.21
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB2	16	0.21
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB3	16	0.21
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	15	0.21
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	17	0.21
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	17	0.21
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	13	0.21
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	13	0.21
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	19	0.21
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	3	0.21
(4,377)	1:29:A:GLU:HA	1:30:A:GLY:H	2	0.21
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD2	2	0.21
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD3	2	0.21
(4,300)	1:62:A:SER:H	1:67:A:LYS:HB3	8	0.21
(4,282)	1:8:A:GLU:HA	1:10:A:CYS:H	5	0.21
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	1	0.21
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	16	0.21
(4,149)	1:54:A:GLY:H	1:56:A:ASP:H	14	0.21
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	13	0.21
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB2	16	0.21
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB3	16	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	16	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	16	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	16	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	16	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	16	0.21
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	16	0.21
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	12	0.21
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	12	0.21
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB2	12	0.21
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB2	12	0.21
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	12	0.21
(1,1150)	1:12:A:SER:HB2	1:15:A:ARG:HB3	12	0.21
(1,1150)	1:12:A:SER:HB3	1:15:A:ARG:HB3	12	0.21
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	10	0.21
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	10	0.21
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	10	0.21
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	10	0.21
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	15	0.21
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	17	0.21
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	17	0.21
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	13	0.21
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	13	0.21
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	13	0.21
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	13	0.21
(1,856)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	3	0.21
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	9	0.21
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	9	0.21
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	7	0.21
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	7	0.21
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	7	0.21
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	7	0.21
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	7	0.21
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	7	0.21
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	7	0.21
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	7	0.21
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	7	0.21
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	0.21
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	10	0.21
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	0.21
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	10	0.21
(1,423)	1:21:A:CYS:HB2	1:22:A:GLY:H	16	0.21
(1,423)	1:21:A:CYS:HB3	1:22:A:GLY:H	16	0.21
(1,423)	1:21:A:CYS:HB2	1:22:A:GLY:H	16	0.21
(1,423)	1:21:A:CYS:HB3	1:22:A:GLY:H	16	0.21
(1,423)	1:21:A:CYS:HB3	1:22:A:GLY:H	16	0.21
(1,423)	1:21:A:CYS:HB2	1:22:A:GLY:H	16	0.21
(1,409)	1:29:A:GLU:HA	1:30:A:GLY:H	2	0.21
(1,326)	1:62:A:SER:H	1:67:A:LYS:HB3	8	0.21
(1,304)	1:8:A:GLU:HA	1:10:A:CYS:H	5	0.21
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB2	4	0.21
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB3	4	0.21
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	1	0.21
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	16	0.21
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	1	0.21
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	1	0.21
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	1	0.21
(1,156)	1:54:A:GLY:H	1:56:A:ASP:H	14	0.21
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	10	0.21
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	10	0.21
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	10	0.21
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	10	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	10	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	10	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	10	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	17	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	17	0.21
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	17	0.21
(1,91)	1:10:A:CYS:HA	1:14:A:CYS:H	17	0.21
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	13	0.21
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB2	13	0.2
(4,945)	1:37:A:LYS:HG2	1:62:A:SER:HB3	13	0.2
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB2	13	0.2
(4,945)	1:37:A:LYS:HG3	1:62:A:SER:HB3	13	0.2
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	12	0.2
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	12	0.2
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG21	15	0.2
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	15	0.2
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG21	7	0.2
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG22	7	0.2
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG23	7	0.2
(4,445)	1:14:A:CYS:H	1:26:A:GLN:H	13	0.2
(4,443)	1:21:A:CYS:HB2	1:26:A:GLN:H	12	0.2
(4,443)	1:21:A:CYS:HB3	1:26:A:GLN:H	12	0.2
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	19	0.2
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	19	0.2
(4,332)	1:33:A:CYS:H	1:36:A:CYS:H	17	0.2
(4,297)	1:62:A:SER:H	1:64:A:CYS:HB2	17	0.2
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	16	0.2
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	20	0.2
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	20	0.2
(4,172)	1:37:A:LYS:HA	1:38:A:THR:H	6	0.2
(4,114)	1:55:A:PRO:HB2	1:57:A:SER:H	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	12	0.2
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB2	13	0.2
(1,1157)	1:37:A:LYS:HG2	1:62:A:SER:HB3	13	0.2
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	13	0.2
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	13	0.2
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	13	0.2
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	13	0.2
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB2	13	0.2
(1,1157)	1:37:A:LYS:HG3	1:62:A:SER:HB3	13	0.2
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	6	0.2
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	6	0.2
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	6	0.2
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	20	0.2
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	20	0.2
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	20	0.2
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	20	0.2
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	8	0.2
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	8	0.2
(1,1110)	1:16:A:SER:HB3	1:20:A:GLN:H	8	0.2
(1,1110)	1:16:A:SER:HB2	1:20:A:GLN:H	8	0.2
(1,1099)	1:28:A:GLY:HA2	1:29:A:GLU:H	5	0.2
(1,1099)	1:28:A:GLY:HA3	1:29:A:GLU:H	5	0.2
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	12	0.2
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	12	0.2
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	12	0.2
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	12	0.2
(1,980)	1:24:A:LYS:HB2	1:26:A:GLN:HE21	1	0.2
(1,980)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	1	0.2
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	4	0.2
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	4	0.2
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	4	0.2
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	4	0.2
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	4	0.2
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	4	0.2
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	9	0.2
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	9	0.2
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	9	0.2
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	9	0.2
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	9	0.2
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	9	0.2
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	9	0.2
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	9	0.2
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	9	0.2
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	9	0.2
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	9	0.2
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	10	0.2
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	10	0.2
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	10	0.2
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	10	0.2
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	19	0.2
(1,747)	1:21:A:CYS:HB2	1:25:A:CYS:HA	19	0.2
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	19	0.2
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	8	0.2
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	8	0.2
(1,692)	1:16:A:SER:HB3	1:20:A:GLN:H	8	0.2
(1,692)	1:16:A:SER:HB2	1:20:A:GLN:H	8	0.2
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	15	0.2
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	10	0.2
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	10	0.2
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	10	0.2
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	17	0.2
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	17	0.2
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	17	0.2
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG21	7	0.2
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG22	7	0.2
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG23	7	0.2
(1,487)	1:11:A:THR:H	1:26:A:GLN:H	5	0.2
(1,460)	1:60:A:CYS:HB2	1:64:A:CYS:H	6	0.2
(1,460)	1:60:A:CYS:HB2	1:64:A:CYS:H	6	0.2
(1,460)	1:60:A:CYS:HB3	1:64:A:CYS:H	6	0.2
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	11	0.2
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	11	0.2
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	11	0.2
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	4	0.2
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	4	0.2
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	4	0.2
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	7	0.2
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	7	0.2
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	7	0.2
(1,360)	1:33:A:CYS:H	1:36:A:CYS:H	17	0.2
(1,322)	1:62:A:SER:H	1:64:A:CYS:HB2	17	0.2
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	5	0.2
(1,179)	1:37:A:LYS:HA	1:38:A:THR:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:55:A:PRO:HB2	1:57:A:SER:H	16	0.2
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	20	0.2
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	20	0.2
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	20	0.2
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	20	0.2
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	12	0.2
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	2	0.19
(4,910)	1:9:A:LYS:H	1:9:A:LYS:HE3	5	0.19
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	15	0.19
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	15	0.19
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	6	0.19
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD3	6	0.19
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD2	13	0.19
(4,845)	1:33:A:CYS:HA	1:37:A:LYS:HD3	13	0.19
(4,789)	1:7:A:GLY:HA2	1:9:A:LYS:H	10	0.19
(4,789)	1:7:A:GLY:HA3	1:9:A:LYS:H	10	0.19
(4,682)	1:13:A:ALA:HB3	1:26:A:GLN:HG2	10	0.19
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	8	0.19
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	20	0.19
(4,468)	1:11:A:THR:HG21	1:26:A:GLN:HB3	10	0.19
(4,468)	1:11:A:THR:HG22	1:26:A:GLN:HB3	10	0.19
(4,468)	1:11:A:THR:HG23	1:26:A:GLN:HB3	10	0.19
(4,405)	1:11:A:THR:HG22	1:26:A:GLN:HE22	12	0.19
(4,377)	1:29:A:GLU:HA	1:30:A:GLY:H	16	0.19
(4,343)	1:63:A:SER:H	1:64:A:CYS:HB2	12	0.19
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE2	17	0.19
(4,299)	1:62:A:SER:H	1:67:A:LYS:HE3	17	0.19
(4,287)	1:9:A:LYS:H	1:10:A:CYS:H	8	0.19
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	13	0.19
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	18	0.19
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	6	0.19
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	9	0.19
(1,1181)	1:11:A:THR:H	1:27:A:CYS:HB2	18	0.19
(1,1181)	1:11:A:THR:H	1:27:A:CYS:HB3	18	0.19
(1,1181)	1:11:A:THR:H	1:27:A:CYS:HB2	18	0.19
(1,1181)	1:11:A:THR:H	1:27:A:CYS:HB3	18	0.19
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	19	0.19
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	19	0.19
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	19	0.19
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	6	0.19
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	6	0.19
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	6	0.19
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	2	0.19
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	15	0.19
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	15	0.19
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	13	0.19
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	13	0.19
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD3	13	0.19
(1,1012)	1:33:A:CYS:HA	1:37:A:LYS:HD2	13	0.19
(1,927)	1:7:A:GLY:HA2	1:9:A:LYS:H	10	0.19
(1,927)	1:7:A:GLY:HA3	1:9:A:LYS:H	10	0.19
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG21	7	0.19
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG22	7	0.19
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG23	7	0.19
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG21	7	0.19
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG22	7	0.19
(1,878)	1:30:A:GLY:HA2	1:32:A:THR:HG23	7	0.19
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG21	7	0.19
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG22	7	0.19
(1,878)	1:30:A:GLY:HA3	1:32:A:THR:HG23	7	0.19
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	14	0.19
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	14	0.19
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE2	14	0.19
(1,835)	1:32:A:THR:HA	1:37:A:LYS:HE3	14	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	1	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	1	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	1	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	1	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	17	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	17	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	17	0.19
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	17	0.19
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD3	8	0.19
(1,800)	1:54:A:GLY:HA2	1:55:A:PRO:HD2	8	0.19
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD2	8	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	1	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	1	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	1	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	1	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	1	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	1	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	1	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	1	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	2	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	2	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	2	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	2	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	2	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	2	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	2	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	2	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	2	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	12	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	12	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	12	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	12	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	12	0.19
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	12	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	12	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	12	0.19
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	12	0.19
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	8	0.19
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	20	0.19
(1,572)	1:9:A:LYS:HB2	1:27:A:CYS:HA	1	0.19
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	16	0.19
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	16	0.19
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	16	0.19
(1,409)	1:29:A:GLU:HA	1:30:A:GLY:H	16	0.19
(1,373)	1:63:A:SER:H	1:64:A:CYS:HB2	12	0.19
(1,312)	1:9:A:LYS:H	1:10:A:CYS:H	8	0.19
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	2	0.19
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	2	0.19
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	2	0.19
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	12	0.19
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	12	0.19
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	18	0.19
(1,141)	1:60:A:CYS:HB3	1:61:A:GLY:H	16	0.19
(1,141)	1:60:A:CYS:HB2	1:61:A:GLY:H	16	0.19
(1,141)	1:60:A:CYS:HB3	1:61:A:GLY:H	16	0.19
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	19	0.19
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	6	0.19
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	6	0.19
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	6	0.19
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:20:A:GLN:H	1:20:A:GLN:HE21	19	0.19
(1,43)	1:20:A:GLN:H	1:20:A:GLN:HE22	19	0.19
(1,43)	1:20:A:GLN:H	1:20:A:GLN:HE21	19	0.19
(1,43)	1:20:A:GLN:H	1:20:A:GLN:HE22	19	0.19
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	10	0.19
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	10	0.19
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	18	0.19
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	18	0.19
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	18	0.19
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	18	0.19
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	6	0.19
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	9	0.19
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	4	0.18
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG3	17	0.18
(4,925)	1:11:A:THR:HG21	1:28:A:GLY:H	9	0.18
(4,925)	1:11:A:THR:HG22	1:28:A:GLY:H	9	0.18
(4,925)	1:11:A:THR:HG23	1:28:A:GLY:H	9	0.18
(4,892)	1:56:A:ASP:HB2	1:57:A:SER:H	14	0.18
(4,892)	1:56:A:ASP:HB3	1:57:A:SER:H	14	0.18
(4,872)	1:42:A:THR:H	1:44:A:ASP:HB2	15	0.18
(4,872)	1:42:A:THR:H	1:44:A:ASP:HB3	15	0.18
(4,818)	1:17:A:GLU:HB2	1:18:A:PRO:HA	17	0.18
(4,818)	1:17:A:GLU:HB3	1:18:A:PRO:HA	17	0.18
(4,808)	1:11:A:THR:HB	1:12:A:SER:HB2	1	0.18
(4,808)	1:11:A:THR:HB	1:12:A:SER:HB3	1	0.18
(4,797)	1:8:A:GLU:HB2	1:10:A:CYS:HA	7	0.18
(4,797)	1:8:A:GLU:HB3	1:10:A:CYS:HA	7	0.18
(4,634)	1:10:A:CYS:HA	1:27:A:CYS:HB2	18	0.18
(4,634)	1:10:A:CYS:HA	1:27:A:CYS:HB3	18	0.18
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	6	0.18
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	6	0.18
(4,320)	1:21:A:CYS:HA	1:27:A:CYS:H	12	0.18
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	16	0.18
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	3	0.18
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	3	0.18
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	12	0.18
(4,128)	1:13:A:ALA:H	1:21:A:CYS:HA	9	0.18
(4,105)	1:29:A:GLU:H	1:31:A:CYS:H	18	0.18
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	5	0.18
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	4	0.18
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	7	0.18
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	7	0.18
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	20	0.18
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	20	0.18
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	20	0.18
(1,1125)	1:11:A:THR:HG21	1:28:A:GLY:H	9	0.18
(1,1125)	1:11:A:THR:HG22	1:28:A:GLY:H	9	0.18
(1,1125)	1:11:A:THR:HG23	1:28:A:GLY:H	9	0.18
(1,1082)	1:56:A:ASP:HB2	1:57:A:SER:H	14	0.18
(1,1082)	1:56:A:ASP:HB3	1:57:A:SER:H	14	0.18
(1,1048)	1:42:A:THR:H	1:44:A:ASP:HB2	15	0.18
(1,1048)	1:42:A:THR:H	1:44:A:ASP:HB3	15	0.18
(1,1048)	1:42:A:THR:H	1:44:A:ASP:HB3	15	0.18
(1,980)	1:24:A:LYS:HB2	1:26:A:GLN:HE21	12	0.18
(1,980)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	12	0.18
(1,973)	1:17:A:GLU:HB2	1:18:A:PRO:HA	17	0.18
(1,973)	1:17:A:GLU:HB3	1:18:A:PRO:HA	17	0.18
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	10	0.18
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	10	0.18
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	10	0.18
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	10	0.18
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	10	0.18
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	10	0.18
(1,962)	1:11:A:THR:HB	1:12:A:SER:HB2	1	0.18
(1,962)	1:11:A:THR:HB	1:12:A:SER:HB3	1	0.18
(1,943)	1:8:A:GLU:HB2	1:10:A:CYS:HA	7	0.18
(1,943)	1:8:A:GLU:HB3	1:10:A:CYS:HA	7	0.18
(1,888)	1:33:A:CYS:HB3	1:34:A:ALA:H	3	0.18
(1,871)	1:50:A:LYS:HG3	1:52:A:CYS:H	14	0.18
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	6	0.18
(1,747)	1:21:A:CYS:HB2	1:25:A:CYS:HA	6	0.18
(1,747)	1:21:A:CYS:HB3	1:25:A:CYS:HA	6	0.18
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	12	0.18
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	12	0.18
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD3	12	0.18
(1,740)	1:38:A:THR:H	1:67:A:LYS:HD2	16	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	13	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	13	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	13	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	15	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	15	0.18
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	15	0.18
(1,438)	1:11:A:THR:HG21	1:26:A:GLN:HE22	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:11:A:THR:HG22	1:26:A:GLN:HE22	1	0.18
(1,438)	1:11:A:THR:HG23	1:26:A:GLN:HE22	1	0.18
(1,347)	1:21:A:CYS:HA	1:27:A:CYS:H	12	0.18
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	16	0.18
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB2	9	0.18
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB2	9	0.18
(1,265)	1:32:A:THR:H	1:33:A:CYS:HB3	9	0.18
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	12	0.18
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	2	0.18
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	2	0.18
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	2	0.18
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	2	0.18
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	3	0.18
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	3	0.18
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	3	0.18
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	8	0.18
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	8	0.18
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	8	0.18
(1,180)	1:38:A:THR:H	1:67:A:LYS:HA	2	0.18
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	2	0.18
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	2	0.18
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	2	0.18
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	12	0.18
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	12	0.18
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	12	0.18
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	2	0.18
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB2	2	0.18
(1,135)	1:13:A:ALA:H	1:15:A:ARG:HB3	2	0.18
(1,131)	1:13:A:ALA:H	1:21:A:CYS:HA	9	0.18
(1,108)	1:29:A:GLU:H	1:31:A:CYS:H	18	0.18
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	13	0.18
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	13	0.18
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	13	0.18
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	12	0.18
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	12	0.18
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	5	0.18
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	19	0.17
(4,925)	1:11:A:THR:HG21	1:28:A:GLY:H	12	0.17
(4,925)	1:11:A:THR:HG22	1:28:A:GLY:H	12	0.17
(4,925)	1:11:A:THR:HG23	1:28:A:GLY:H	12	0.17
(4,903)	1:66:A:CYS:H	1:67:A:LYS:HE2	8	0.17
(4,903)	1:66:A:CYS:H	1:67:A:LYS:HE3	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,851)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.17
(4,851)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.17
(4,844)	1:33:A:CYS:H	1:37:A:LYS:HE2	16	0.17
(4,844)	1:33:A:CYS:H	1:37:A:LYS:HE3	16	0.17
(4,818)	1:17:A:GLU:HB2	1:18:A:PRO:HA	6	0.17
(4,818)	1:17:A:GLU:HB3	1:18:A:PRO:HA	6	0.17
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	13	0.17
(4,797)	1:8:A:GLU:HB2	1:10:A:CYS:HA	15	0.17
(4,797)	1:8:A:GLU:HB3	1:10:A:CYS:HA	15	0.17
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	12	0.17
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	14	0.17
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	19	0.17
(4,547)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	8	0.17
(4,477)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	2	0.17
(4,445)	1:14:A:CYS:H	1:26:A:GLN:H	20	0.17
(4,400)	1:18:A:PRO:HG2	1:19:A:CYS:H	15	0.17
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	2	0.17
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	2	0.17
(4,270)	1:40:A:ASN:H	1:67:A:LYS:HG2	13	0.17
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	2	0.17
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	13	0.17
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	20	0.17
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	8	0.17
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	8	0.17
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	13	0.17
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	16	0.17
(4,185)	1:20:A:GLN:H	1:35:A:ALA:HB1	7	0.17
(4,185)	1:20:A:GLN:H	1:35:A:ALA:HB2	7	0.17
(4,185)	1:20:A:GLN:H	1:35:A:ALA:HB3	7	0.17
(4,172)	1:37:A:LYS:HA	1:38:A:THR:H	15	0.17
(4,105)	1:29:A:GLU:H	1:31:A:CYS:H	13	0.17
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	4	0.17
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	17	0.17
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	4	0.17
(4,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	4	0.17
(1,1167)	1:38:A:THR:H	1:67:A:LYS:HB3	2	0.17
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	19	0.17
(1,1125)	1:11:A:THR:HG21	1:28:A:GLY:H	12	0.17
(1,1125)	1:11:A:THR:HG22	1:28:A:GLY:H	12	0.17
(1,1125)	1:11:A:THR:HG23	1:28:A:GLY:H	12	0.17
(1,1094)	1:66:A:CYS:H	1:67:A:LYS:HE2	8	0.17
(1,1094)	1:66:A:CYS:H	1:67:A:LYS:HE3	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.17
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.17
(1,1020)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.17
(1,1020)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.17
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE2	16	0.17
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE3	16	0.17
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE2	16	0.17
(1,1011)	1:33:A:CYS:H	1:37:A:LYS:HE3	16	0.17
(1,973)	1:17:A:GLU:HB2	1:18:A:PRO:HA	6	0.17
(1,973)	1:17:A:GLU:HB3	1:18:A:PRO:HA	6	0.17
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	7	0.17
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	7	0.17
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	7	0.17
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	7	0.17
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	7	0.17
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	7	0.17
(1,943)	1:8:A:GLU:HB2	1:10:A:CYS:HA	15	0.17
(1,943)	1:8:A:GLU:HB3	1:10:A:CYS:HA	15	0.17
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	1	0.17
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	1	0.17
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	1	0.17
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	1	0.17
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	1	0.17
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	1	0.17
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	1	0.17
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	1	0.17
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	1	0.17
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	1	0.17
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	1	0.17
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	1	0.17
(1,858)	1:11:A:THR:HG21	1:14:A:CYS:HB2	5	0.17
(1,858)	1:11:A:THR:HG22	1:14:A:CYS:HB2	5	0.17
(1,858)	1:11:A:THR:HG23	1:14:A:CYS:HB2	5	0.17
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	2	0.17
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	2	0.17
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	2	0.17
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	11	0.17
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	11	0.17
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	19	0.17
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	19	0.17
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	10	0.17
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	10	0.17
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	10	0.17
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	10	0.17
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	10	0.17
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	10	0.17
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	10	0.17
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	10	0.17
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	12	0.17
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	14	0.17
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	19	0.17
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	2	0.17
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	2	0.17
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	2	0.17
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	2	0.17
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG2	2	0.17
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	2	0.17
(1,520)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	2	0.17
(1,520)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	2	0.17
(1,433)	1:18:A:PRO:HG2	1:19:A:CYS:H	15	0.17
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	9	0.17
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB2	17	0.17
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB2	17	0.17
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB3	17	0.17
(1,357)	1:33:A:CYS:H	1:37:A:LYS:HB3	17	0.17
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	5	0.17
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB2	5	0.17
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	5	0.17
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	19	0.17
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	19	0.17
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	19	0.17
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	19	0.17
(1,289)	1:40:A:ASN:H	1:67:A:LYS:HG2	13	0.17
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	2	0.17
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	13	0.17
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	20	0.17
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	13	0.17
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	16	0.17
(1,196)	1:20:A:GLN:H	1:35:A:ALA:HB1	7	0.17
(1,196)	1:20:A:GLN:H	1:35:A:ALA:HB2	7	0.17
(1,196)	1:20:A:GLN:H	1:35:A:ALA:HB3	7	0.17
(1,179)	1:37:A:LYS:HA	1:38:A:THR:H	15	0.17
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	11	0.17
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	11	0.17
(1,150)	1:52:A:CYS:HB2	1:56:A:ASP:H	13	0.17
(1,124)	1:15:A:ARG:HB3	1:16:A:SER:H	14	0.17
(1,124)	1:15:A:ARG:HB2	1:16:A:SER:H	14	0.17
(1,124)	1:15:A:ARG:HB2	1:16:A:SER:H	14	0.17
(1,124)	1:15:A:ARG:HB3	1:16:A:SER:H	14	0.17
(1,124)	1:15:A:ARG:HB2	1:16:A:SER:H	14	0.17
(1,124)	1:15:A:ARG:HB3	1:16:A:SER:H	14	0.17
(1,108)	1:29:A:GLU:H	1:31:A:CYS:H	13	0.17
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	9	0.17
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	9	0.17
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	16	0.17
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	16	0.17
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	16	0.17
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	16	0.17
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	4	0.17
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	17	0.17
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	16	0.17
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB2	16	0.17
(1,6)	1:29:A:GLU:H	1:29:A:GLU:HB3	16	0.17
(4,925)	1:11:A:THR:HG21	1:28:A:GLY:H	2	0.16
(4,925)	1:11:A:THR:HG22	1:28:A:GLY:H	2	0.16
(4,925)	1:11:A:THR:HG23	1:28:A:GLY:H	2	0.16
(4,925)	1:11:A:THR:HG21	1:28:A:GLY:H	19	0.16
(4,925)	1:11:A:THR:HG22	1:28:A:GLY:H	19	0.16
(4,925)	1:11:A:THR:HG23	1:28:A:GLY:H	19	0.16
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	11	0.16
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	20	0.16
(4,702)	1:40:A:ASN:HB3	1:42:A:THR:HG22	4	0.16
(4,650)	1:39:A:CYS:H	1:67:A:LYS:HD3	16	0.16
(4,547)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	5	0.16
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	6	0.16
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	8	0.16
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	8	0.16
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	8	0.16
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG21	20	0.16
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG22	20	0.16
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG23	20	0.16
(4,318)	1:25:A:CYS:HA	1:27:A:CYS:H	10	0.16
(4,305)	1:35:A:ALA:HA	1:37:A:LYS:H	20	0.16
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	1	0.16
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	9	0.16
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	15	0.16
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	15	0.16
(4,139)	1:60:A:CYS:HB2	1:61:A:GLY:H	6	0.16
(4,128)	1:13:A:ALA:H	1:21:A:CYS:HA	4	0.16
(1,1125)	1:11:A:THR:HG21	1:28:A:GLY:H	2	0.16
(1,1125)	1:11:A:THR:HG22	1:28:A:GLY:H	2	0.16
(1,1125)	1:11:A:THR:HG23	1:28:A:GLY:H	2	0.16
(1,1125)	1:11:A:THR:HG21	1:28:A:GLY:H	19	0.16
(1,1125)	1:11:A:THR:HG22	1:28:A:GLY:H	19	0.16
(1,1125)	1:11:A:THR:HG23	1:28:A:GLY:H	19	0.16
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	11	0.16
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	11	0.16
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	11	0.16
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	11	0.16
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	11	0.16
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	11	0.16
(1,879)	1:33:A:CYS:HB3	1:37:A:LYS:HB2	17	0.16
(1,879)	1:33:A:CYS:HB3	1:37:A:LYS:HB2	17	0.16
(1,879)	1:33:A:CYS:HB3	1:37:A:LYS:HB3	17	0.16
(1,879)	1:33:A:CYS:HB3	1:37:A:LYS:HB3	17	0.16
(1,879)	1:33:A:CYS:HB2	1:37:A:LYS:HB3	17	0.16
(1,879)	1:33:A:CYS:HB3	1:37:A:LYS:HB3	17	0.16
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	19	0.16
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	19	0.16
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	19	0.16
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	19	0.16
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	20	0.16
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	20	0.16
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	20	0.16
(1,568)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	2	0.16
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	6	0.16
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	8	0.16
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	8	0.16
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	8	0.16
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG21	20	0.16
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG22	20	0.16
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG23	20	0.16
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	18	0.16
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	18	0.16
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:25:A:CYS:HA	1:27:A:CYS:H	10	0.16
(1,332)	1:35:A:ALA:HA	1:37:A:LYS:H	20	0.16
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	1	0.16
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	9	0.16
(1,270)	1:39:A:CYS:H	1:55:A:PRO:HA	17	0.16
(1,144)	1:60:A:CYS:HB2	1:61:A:GLY:H	6	0.16
(1,131)	1:13:A:ALA:H	1:21:A:CYS:HA	4	0.16
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	1	0.16
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	1	0.16
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	1	0.16
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	18	0.16
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	18	0.16
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	18	0.16
(1,42)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	18	0.16
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	18	0.16
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	18	0.16
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	18	0.16
(1,42)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	18	0.16
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	8	0.15
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	5	0.15
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	17	0.15
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	10	0.15
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	10	0.15
(4,792)	1:8:A:GLU:H	1:9:A:LYS:HB2	19	0.15
(4,737)	1:14:A:CYS:HB2	1:15:A:ARG:HB2	2	0.15
(4,639)	1:60:A:CYS:H	1:67:A:LYS:HE2	12	0.15
(4,484)	1:25:A:CYS:H	1:36:A:CYS:HB2	18	0.15
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	12	0.15
(4,405)	1:11:A:THR:HG21	1:26:A:GLN:HE21	19	0.15
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB1	6	0.15
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB2	6	0.15
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB3	6	0.15
(4,380)	1:6:A:LYS:HB2	1:7:A:GLY:H	16	0.15
(4,305)	1:35:A:ALA:HA	1:37:A:LYS:H	17	0.15
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	8	0.15
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	6	0.15
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	4	0.15
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	13	0.15
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	14	0.15
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	14	0.15
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	15	0.15
(4,172)	1:37:A:LYS:HA	1:38:A:THR:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,169)	1:46:A:CYS:H	1:47:A:LYS:HG2	3	0.15
(4,169)	1:46:A:CYS:H	1:47:A:LYS:HG3	3	0.15
(4,140)	1:61:A:GLY:H	1:64:A:CYS:H	16	0.15
(4,139)	1:60:A:CYS:HB2	1:61:A:GLY:H	5	0.15
(4,121)	1:15:A:ARG:HB3	1:16:A:SER:H	14	0.15
(4,114)	1:55:A:PRO:HB2	1:57:A:SER:H	12	0.15
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	11	0.15
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	8	0.15
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	3	0.15
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB2	3	0.15
(1,1146)	1:14:A:CYS:HA	1:15:A:ARG:HB3	3	0.15
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	5	0.15
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	17	0.15
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	7	0.15
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	7	0.15
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	7	0.15
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	7	0.15
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	10	0.15
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	10	0.15
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	0.15
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	0.15
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	0.15
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	0.15
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	0.15
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	16	0.15
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	0.15
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	0.15
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	0.15
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	16	0.15
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	19	0.15
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	19	0.15
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	19	0.15
(1,871)	1:50:A:LYS:HG3	1:52:A:CYS:H	16	0.15
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	11	0.15
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	11	0.15
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	11	0.15
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD3	10	0.15
(1,800)	1:54:A:GLY:HA2	1:55:A:PRO:HD2	10	0.15
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD2	10	0.15
(1,790)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	16	0.15
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	13	0.15
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,744)	1:67:A:LYS:HB3	1:67:A:LYS:HD3	13	0.15
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA3	14	0.15
(1,734)	1:43:A:SER:H	1:54:A:GLY:HA2	14	0.15
(1,724)	1:60:A:CYS:H	1:67:A:LYS:HE2	12	0.15
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	12	0.15
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	12	0.15
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	12	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	12	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	12	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	12	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	15	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	15	0.15
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	15	0.15
(1,530)	1:25:A:CYS:H	1:36:A:CYS:HB2	18	0.15
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	12	0.15
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB1	6	0.15
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB2	6	0.15
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB3	6	0.15
(1,413)	1:6:A:LYS:HB2	1:7:A:GLY:H	16	0.15
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.15
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.15
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE3	17	0.15
(1,390)	1:64:A:CYS:HB2	1:67:A:LYS:H	14	0.15
(1,386)	1:11:A:THR:HG21	1:26:A:GLN:HE21	17	0.15
(1,386)	1:11:A:THR:HG22	1:26:A:GLN:HE21	17	0.15
(1,386)	1:11:A:THR:HG23	1:26:A:GLN:HE21	17	0.15
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	9	0.15
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	9	0.15
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	9	0.15
(1,332)	1:35:A:ALA:HA	1:37:A:LYS:H	17	0.15
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	4	0.15
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	13	0.15
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	14	0.15
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	14	0.15
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	6	0.15
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	9	0.15
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	9	0.15
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	9	0.15
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	15	0.15
(1,179)	1:37:A:LYS:HA	1:38:A:THR:H	4	0.15
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	15	0.15
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	15	0.15
(1,145)	1:61:A:GLY:H	1:64:A:CYS:H	16	0.15
(1,144)	1:60:A:CYS:HB2	1:61:A:GLY:H	5	0.15
(1,117)	1:55:A:PRO:HB2	1:57:A:SER:H	12	0.15
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	2	0.15
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	2	0.15
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	2	0.15
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	17	0.15
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	17	0.15
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB3	17	0.15
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	5	0.15
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	5	0.15
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE22	16	0.15
(1,25)	1:19:A:CYS:HA	1:20:A:GLN:HE21	16	0.15
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	11	0.15
(4,943)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.14
(4,943)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.14
(4,932)	1:42:A:THR:HG21	1:47:A:LYS:H	6	0.14
(4,932)	1:42:A:THR:HG22	1:47:A:LYS:H	6	0.14
(4,932)	1:42:A:THR:HG23	1:47:A:LYS:H	6	0.14
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	10	0.14
(4,903)	1:66:A:CYS:H	1:67:A:LYS:HE2	7	0.14
(4,903)	1:66:A:CYS:H	1:67:A:LYS:HE3	7	0.14
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	19	0.14
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	19	0.14
(4,842)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.14
(4,842)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.14
(4,656)	1:21:A:CYS:HB2	1:25:A:CYS:HA	12	0.14
(4,656)	1:21:A:CYS:HB3	1:25:A:CYS:HA	12	0.14
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	5	0.14
(4,589)	1:20:A:GLN:HG3	1:21:A:CYS:H	18	0.14
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD2	17	0.14
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD3	17	0.14
(4,540)	1:34:A:ALA:HA	1:37:A:LYS:H	15	0.14
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG21	6	0.14
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG22	6	0.14
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG23	6	0.14
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	15	0.14
(4,450)	1:47:A:LYS:H	1:49:A:GLY:HA2	5	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	9	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	9	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	18	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	18	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	18	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	20	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	20	0.14
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	20	0.14
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB1	20	0.14
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB2	20	0.14
(4,401)	1:19:A:CYS:H	1:35:A:ALA:HB3	20	0.14
(4,380)	1:6:A:LYS:HB3	1:7:A:GLY:H	9	0.14
(4,305)	1:35:A:ALA:HA	1:37:A:LYS:H	13	0.14
(4,300)	1:62:A:SER:H	1:67:A:LYS:HB3	10	0.14
(4,288)	1:10:A:CYS:H	1:28:A:GLY:H	15	0.14
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	8	0.14
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	16	0.14
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	17	0.14
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	20	0.14
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	7	0.14
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	7	0.14
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	12	0.14
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	12	0.14
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	14	0.14
(4,190)	1:45:A:GLY:H	1:47:A:LYS:HG2	10	0.14
(4,190)	1:45:A:GLY:H	1:47:A:LYS:HG3	10	0.14
(4,172)	1:37:A:LYS:HA	1:38:A:THR:H	20	0.14
(4,128)	1:13:A:ALA:H	1:21:A:CYS:HA	7	0.14
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	2	0.14
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	20	0.14
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	20	0.14
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	20	0.14
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE2	20	0.14
(1,1177)	1:37:A:LYS:H	1:37:A:LYS:HE3	20	0.14
(1,1151)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.14
(1,1151)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.14
(1,1151)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.14
(1,1151)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.14
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	17	0.14
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	17	0.14
(1,1143)	1:29:A:GLU:HB2	1:31:A:CYS:H	17	0.14
(1,1143)	1:29:A:GLU:HB3	1:31:A:CYS:H	17	0.14
(1,1139)	1:42:A:THR:HG21	1:47:A:LYS:H	6	0.14
(1,1139)	1:42:A:THR:HG22	1:47:A:LYS:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:42:A:THR:HG23	1:47:A:LYS:H	6	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	4	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	4	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	4	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	4	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	9	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	9	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	9	0.14
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	9	0.14
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	10	0.14
(1,1094)	1:66:A:CYS:H	1:67:A:LYS:HE2	7	0.14
(1,1094)	1:66:A:CYS:H	1:67:A:LYS:HE3	7	0.14
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	19	0.14
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	19	0.14
(1,1009)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.14
(1,1009)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.14
(1,1009)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.14
(1,1009)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.14
(1,984)	1:24:A:LYS:HB3	1:26:A:GLN:HE21	19	0.14
(1,984)	1:24:A:LYS:HB3	1:26:A:GLN:HE22	19	0.14
(1,984)	1:24:A:LYS:HB3	1:26:A:GLN:HE21	19	0.14
(1,984)	1:24:A:LYS:HB2	1:26:A:GLN:HE21	19	0.14
(1,984)	1:24:A:LYS:HB2	1:26:A:GLN:HE22	19	0.14
(1,984)	1:24:A:LYS:HB3	1:26:A:GLN:HE21	19	0.14
(1,984)	1:24:A:LYS:HB3	1:26:A:GLN:HE22	19	0.14
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	1	0.14
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	1	0.14
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	1	0.14
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	1	0.14
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	1	0.14
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	1	0.14
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	8	0.14
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	8	0.14
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	8	0.14
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	8	0.14
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	8	0.14
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	8	0.14
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	8	0.14
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	8	0.14
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	8	0.14
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	8	0.14
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	8	0.14
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD3	11	0.14
(1,800)	1:54:A:GLY:HA2	1:55:A:PRO:HD2	11	0.14
(1,800)	1:54:A:GLY:HA3	1:55:A:PRO:HD2	11	0.14
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	1	0.14
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE2	1	0.14
(1,767)	1:60:A:CYS:H	1:67:A:LYS:HE3	1	0.14
(1,732)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	14	0.14
(1,732)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	14	0.14
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	5	0.14
(1,657)	1:20:A:GLN:HG3	1:21:A:CYS:H	18	0.14
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	15	0.14
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	15	0.14
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	15	0.14
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	15	0.14
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	16	0.14
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	16	0.14
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	16	0.14
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	16	0.14
(1,597)	1:34:A:ALA:HA	1:37:A:LYS:H	15	0.14
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	7	0.14
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	7	0.14
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	7	0.14
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	14	0.14
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	14	0.14
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	14	0.14
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG21	6	0.14
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG22	6	0.14
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG23	6	0.14
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	15	0.14
(1,493)	1:47:A:LYS:H	1:49:A:GLY:HA2	5	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	9	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	9	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	9	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	18	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	18	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	18	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	20	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	20	0.14
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	20	0.14
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB1	20	0.14
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB2	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:19:A:CYS:H	1:35:A:ALA:HB3	20	0.14
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	2	0.14
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	2	0.14
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	2	0.14
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	6	0.14
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	6	0.14
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	6	0.14
(1,332)	1:35:A:ALA:HA	1:37:A:LYS:H	13	0.14
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	3	0.14
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD2	3	0.14
(1,328)	1:62:A:SER:H	1:67:A:LYS:HD3	3	0.14
(1,326)	1:62:A:SER:H	1:67:A:LYS:HB3	10	0.14
(1,313)	1:10:A:CYS:H	1:28:A:GLY:H	15	0.14
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	17	0.14
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	20	0.14
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	19	0.14
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB2	19	0.14
(1,257)	1:41:A:CYS:H	1:48:A:CYS:HB3	19	0.14
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	14	0.14
(1,179)	1:37:A:LYS:HA	1:38:A:THR:H	20	0.14
(1,131)	1:13:A:ALA:H	1:21:A:CYS:HA	7	0.14
(1,115)	1:55:A:PRO:HB3	1:57:A:SER:H	3	0.14
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	17	0.14
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	17	0.14
(1,105)	1:29:A:GLU:HB2	1:31:A:CYS:H	17	0.14
(1,105)	1:29:A:GLU:HB3	1:31:A:CYS:H	17	0.14
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	7	0.14
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB2	7	0.14
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	7	0.14
(1,15)	1:35:A:ALA:H	1:37:A:LYS:HB3	7	0.14
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	2	0.14
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	20	0.14
(4,950)	1:14:A:CYS:H	1:26:A:GLN:HB3	15	0.13
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	8	0.13
(4,932)	1:42:A:THR:HG21	1:47:A:LYS:H	3	0.13
(4,932)	1:42:A:THR:HG22	1:47:A:LYS:H	3	0.13
(4,932)	1:42:A:THR:HG23	1:47:A:LYS:H	3	0.13
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	20	0.13
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	12	0.13
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD3	12	0.13
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	20	0.13
(4,876)	1:49:A:GLY:HA2	1:50:A:LYS:HD3	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,808)	1:11:A:THR:HB	1:12:A:SER:HB2	18	0.13
(4,808)	1:11:A:THR:HB	1:12:A:SER:HB3	18	0.13
(4,720)	1:21:A:CYS:HB2	1:25:A:CYS:H	19	0.13
(4,539)	1:34:A:ALA:HA	1:37:A:LYS:HB2	7	0.13
(4,539)	1:34:A:ALA:HA	1:37:A:LYS:HB3	7	0.13
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	12	0.13
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	12	0.13
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	12	0.13
(4,438)	1:39:A:CYS:H	1:40:A:ASN:HD21	9	0.13
(4,402)	1:19:A:CYS:H	1:21:A:CYS:H	3	0.13
(4,392)	1:22:A:GLY:H	1:24:A:LYS:H	15	0.13
(4,387)	1:21:A:CYS:HB2	1:22:A:GLY:H	16	0.13
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	4	0.13
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	4	0.13
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	1	0.13
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	1	0.13
(4,338)	1:9:A:LYS:HB2	1:28:A:GLY:H	11	0.13
(4,298)	1:62:A:SER:H	1:64:A:CYS:HB3	2	0.13
(4,285)	1:9:A:LYS:HB2	1:10:A:CYS:H	5	0.13
(4,280)	1:39:A:CYS:H	1:40:A:ASN:HD21	9	0.13
(4,270)	1:40:A:ASN:H	1:67:A:LYS:HG2	18	0.13
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	15	0.13
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	18	0.13
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	18	0.13
(4,241)	1:41:A:CYS:H	1:54:A:GLY:HA2	5	0.13
(4,202)	1:58:A:CYS:H	1:60:A:CYS:H	17	0.13
(4,188)	1:14:A:CYS:HA	1:20:A:GLN:H	5	0.13
(4,145)	1:55:A:PRO:HG2	1:56:A:ASP:H	14	0.13
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	18	0.13
(1,1164)	1:14:A:CYS:H	1:26:A:GLN:HB3	15	0.13
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	8	0.13
(1,1139)	1:42:A:THR:HG21	1:47:A:LYS:H	3	0.13
(1,1139)	1:42:A:THR:HG22	1:47:A:LYS:H	3	0.13
(1,1139)	1:42:A:THR:HG23	1:47:A:LYS:H	3	0.13
(1,1136)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	10	0.13
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	10	0.13
(1,1116)	1:9:A:LYS:HG2	1:10:A:CYS:H	10	0.13
(1,1116)	1:9:A:LYS:HG3	1:10:A:CYS:H	10	0.13
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	20	0.13
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG2	20	0.13
(1,998)	1:31:A:CYS:H	1:37:A:LYS:HG3	20	0.13
(1,962)	1:11:A:THR:HB	1:12:A:SER:HB2	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,962)	1:11:A:THR:HB	1:12:A:SER:HB3	18	0.13
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	0.13
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	0.13
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	0.13
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	0.13
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	0.13
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	8	0.13
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	0.13
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	0.13
(1,959)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	0.13
(1,959)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	8	0.13
(1,871)	1:50:A:LYS:HG3	1:52:A:CYS:H	9	0.13
(1,833)	1:21:A:CYS:HB2	1:25:A:CYS:H	19	0.13
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	18	0.13
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	18	0.13
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	18	0.13
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG21	18	0.13
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG22	18	0.13
(1,678)	1:43:A:SER:HB2	1:53:A:THR:HG23	18	0.13
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG21	18	0.13
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG22	18	0.13
(1,678)	1:43:A:SER:HB3	1:53:A:THR:HG23	18	0.13
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	4	0.13
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	4	0.13
(1,639)	1:56:A:ASP:HB2	1:57:A:SER:HA	4	0.13
(1,639)	1:56:A:ASP:HB3	1:57:A:SER:HA	4	0.13
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	13	0.13
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD2	13	0.13
(1,601)	1:12:A:SER:HA	1:15:A:ARG:HD3	13	0.13
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	4	0.13
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	4	0.13
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	4	0.13
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	14	0.13
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	14	0.13
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	14	0.13
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	12	0.13
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	12	0.13
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	12	0.13
(1,477)	1:38:A:THR:H	1:40:A:ASN:HD21	10	0.13
(1,435)	1:19:A:CYS:H	1:21:A:CYS:H	3	0.13
(1,427)	1:22:A:GLY:H	1:24:A:LYS:H	15	0.13
(1,324)	1:62:A:SER:H	1:64:A:CYS:HB3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,309)	1:9:A:LYS:HB2	1:10:A:CYS:H	5	0.13
(1,289)	1:40:A:ASN:H	1:67:A:LYS:HG2	18	0.13
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	16	0.13
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD2	16	0.13
(1,288)	1:40:A:ASN:H	1:67:A:LYS:HD3	16	0.13
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	15	0.13
(1,252)	1:41:A:CYS:H	1:54:A:GLY:HA2	5	0.13
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA2	18	0.13
(1,217)	1:43:A:SER:H	1:54:A:GLY:HA3	18	0.13
(1,213)	1:58:A:CYS:H	1:60:A:CYS:H	17	0.13
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	11	0.13
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG2	11	0.13
(1,201)	1:45:A:GLY:H	1:47:A:LYS:HG3	11	0.13
(1,199)	1:14:A:CYS:HA	1:20:A:GLN:H	5	0.13
(1,152)	1:55:A:PRO:HG2	1:56:A:ASP:H	14	0.13
(1,91)	1:10:A:CYS:HA	1:14:A:CYS:H	1	0.13
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	4	0.13
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	4	0.13
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE21	4	0.13
(1,23)	1:17:A:GLU:H	1:20:A:GLN:HE22	4	0.13
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	18	0.13
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	6	0.12
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	5	0.12
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	7	0.12
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	9	0.12
(4,914)	1:43:A:SER:HA	1:45:A:GLY:H	7	0.12
(4,914)	1:43:A:SER:HA	1:45:A:GLY:H	12	0.12
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG2	9	0.12
(4,825)	1:24:A:LYS:HA	1:26:A:GLN:HG3	9	0.12
(4,806)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	0.12
(4,806)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	0.12
(4,806)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	0.12
(4,806)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	0.12
(4,805)	1:9:A:LYS:HG3	1:29:A:GLU:H	5	0.12
(4,628)	1:55:A:PRO:HB3	1:58:A:CYS:H	15	0.12
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.12
(4,545)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	0.12
(4,511)	1:41:A:CYS:H	1:46:A:CYS:HA	15	0.12
(4,457)	1:21:A:CYS:H	1:36:A:CYS:H	14	0.12
(4,450)	1:47:A:LYS:H	1:49:A:GLY:HA2	18	0.12
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	3	0.12
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	3	0.12
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	16	0.12
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	16	0.12
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	16	0.12
(4,445)	1:14:A:CYS:H	1:26:A:GLN:H	5	0.12
(4,420)	1:64:A:CYS:H	1:64:A:CYS:HB2	14	0.12
(4,343)	1:63:A:SER:H	1:64:A:CYS:HB2	4	0.12
(4,332)	1:33:A:CYS:H	1:36:A:CYS:H	18	0.12
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD2	8	0.12
(4,302)	1:62:A:SER:H	1:67:A:LYS:HD3	8	0.12
(4,298)	1:62:A:SER:H	1:67:A:LYS:HE3	13	0.12
(4,297)	1:62:A:SER:H	1:64:A:CYS:HB2	10	0.12
(4,285)	1:9:A:LYS:HB2	1:10:A:CYS:H	14	0.12
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	9	0.12
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	15	0.12
(4,204)	1:43:A:SER:H	1:53:A:THR:HB	7	0.12
(4,140)	1:61:A:GLY:H	1:64:A:CYS:H	4	0.12
(4,138)	1:61:A:GLY:H	1:64:A:CYS:HB3	16	0.12
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB2	17	0.12
(4,101)	1:31:A:CYS:H	1:33:A:CYS:HB3	17	0.12
(4,74)	1:14:A:CYS:HB2	1:15:A:ARG:H	5	0.12
(4,74)	1:14:A:CYS:HB2	1:15:A:ARG:H	13	0.12
(4,22)	1:17:A:GLU:H	1:20:A:GLN:HE21	14	0.12
(4,22)	1:17:A:GLU:H	1:20:A:GLN:HE22	14	0.12
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	15	0.12
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	19	0.12
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	6	0.12
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	19	0.12
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	19	0.12
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA2	19	0.12
(1,1128)	1:9:A:LYS:HB3	1:28:A:GLY:HA3	19	0.12
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	5	0.12
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	7	0.12
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	9	0.12
(1,1111)	1:43:A:SER:HA	1:45:A:GLY:H	7	0.12
(1,1111)	1:43:A:SER:HA	1:45:A:GLY:H	12	0.12
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE2	7	0.12
(1,1104)	1:9:A:LYS:H	1:9:A:LYS:HE3	7	0.12
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG2	9	0.12
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	9	0.12
(1,979)	1:24:A:LYS:HA	1:26:A:GLN:HG3	9	0.12
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE22	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	2	0.12
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE22	2	0.12
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	2	0.12
(1,971)	1:16:A:SER:HB2	1:20:A:GLN:HE21	2	0.12
(1,971)	1:16:A:SER:HB3	1:20:A:GLN:HE21	2	0.12
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	17	0.12
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	17	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	4	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	4	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB3	4	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	9	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	9	0.12
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB3	9	0.12
(1,888)	1:33:A:CYS:HB3	1:34:A:ALA:H	12	0.12
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	5	0.12
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB2	5	0.12
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	5	0.12
(1,819)	1:36:A:CYS:HA	1:37:A:LYS:HB3	5	0.12
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	8	0.12
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE2	8	0.12
(1,768)	1:67:A:LYS:H	1:67:A:LYS:HE3	8	0.12
(1,742)	1:64:A:CYS:H	1:67:A:LYS:HD2	11	0.12
(1,742)	1:64:A:CYS:H	1:67:A:LYS:HD2	11	0.12
(1,742)	1:64:A:CYS:H	1:67:A:LYS:HD3	11	0.12
(1,709)	1:55:A:PRO:HB3	1:58:A:CYS:H	15	0.12
(1,700)	1:62:A:SER:HB2	1:64:A:CYS:H	18	0.12
(1,700)	1:62:A:SER:HB3	1:64:A:CYS:H	18	0.12
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	12	0.12
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	1	0.12
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB2	1	0.12
(1,589)	1:23:A:SER:HA	1:24:A:LYS:HB3	1	0.12
(1,558)	1:41:A:CYS:H	1:46:A:CYS:HA	15	0.12
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	5	0.12
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG2	5	0.12
(1,534)	1:15:A:ARG:HA	1:15:A:ARG:HG3	5	0.12
(1,501)	1:21:A:CYS:H	1:36:A:CYS:H	14	0.12
(1,493)	1:47:A:LYS:H	1:49:A:GLY:HA2	18	0.12
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	3	0.12
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	3	0.12
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	3	0.12
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	16	0.12
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	16	0.12
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	8	0.12
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	8	0.12
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE3	8	0.12
(1,373)	1:63:A:SER:H	1:64:A:CYS:HB2	4	0.12
(1,360)	1:33:A:CYS:H	1:36:A:CYS:H	18	0.12
(1,322)	1:62:A:SER:H	1:64:A:CYS:HB2	10	0.12
(1,309)	1:9:A:LYS:HB2	1:10:A:CYS:H	14	0.12
(1,298)	1:40:A:ASN:HD22	1:67:A:LYS:HB3	11	0.12
(1,298)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	11	0.12
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	9	0.12
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	15	0.12
(1,215)	1:43:A:SER:H	1:53:A:THR:HB	7	0.12
(1,145)	1:61:A:GLY:H	1:64:A:CYS:H	4	0.12
(1,142)	1:61:A:GLY:H	1:64:A:CYS:HB2	16	0.12
(1,142)	1:61:A:GLY:H	1:64:A:CYS:HB3	16	0.12
(1,91)	1:10:A:CYS:HA	1:14:A:CYS:H	19	0.12
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	9	0.12
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	9	0.12
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG3	9	0.12
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	14	0.12
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG2	14	0.12
(1,61)	1:9:A:LYS:H	1:9:A:LYS:HG3	14	0.12
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	8	0.12
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB2	8	0.12
(1,49)	1:59:A:LYS:H	1:60:A:CYS:HB3	8	0.12
(1,37)	1:20:A:GLN:HA	1:20:A:GLN:HE21	19	0.12
(1,37)	1:20:A:GLN:HA	1:20:A:GLN:HE22	19	0.12
(1,37)	1:20:A:GLN:HA	1:20:A:GLN:HE21	19	0.12
(1,37)	1:20:A:GLN:HA	1:20:A:GLN:HE22	19	0.12
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	15	0.12
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	19	0.12
(4,941)	1:5:A:GLY:H	1:6:A:LYS:HG3	15	0.11
(4,935)	1:21:A:CYS:H	1:36:A:CYS:HA	10	0.11
(4,932)	1:42:A:THR:HG21	1:47:A:LYS:H	5	0.11
(4,932)	1:42:A:THR:HG22	1:47:A:LYS:H	5	0.11
(4,932)	1:42:A:THR:HG23	1:47:A:LYS:H	5	0.11
(4,916)	1:45:A:GLY:H	1:46:A:CYS:H	19	0.11
(4,852)	1:37:A:LYS:HE2	1:38:A:THR:H	14	0.11
(4,852)	1:37:A:LYS:HE3	1:38:A:THR:H	14	0.11
(4,850)	1:37:A:LYS:HG2	1:38:A:THR:H	12	0.11
(4,850)	1:37:A:LYS:HG3	1:38:A:THR:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,830)	1:25:A:CYS:H	1:26:A:GLN:HG2	16	0.11
(4,830)	1:25:A:CYS:H	1:26:A:GLN:HG3	16	0.11
(4,826)	1:24:A:LYS:HB2	1:26:A:GLN:HE21	6	0.11
(4,803)	1:9:A:LYS:HG3	1:28:A:GLY:H	5	0.11
(4,750)	1:50:A:LYS:HG3	1:51:A:GLU:H	9	0.11
(4,731)	1:32:A:THR:H	1:37:A:LYS:HE2	2	0.11
(4,731)	1:32:A:THR:H	1:37:A:LYS:HE3	2	0.11
(4,656)	1:21:A:CYS:HB2	1:25:A:CYS:HA	19	0.11
(4,656)	1:21:A:CYS:HB3	1:25:A:CYS:HA	19	0.11
(4,645)	1:53:A:THR:HG21	1:54:A:GLY:HA3	14	0.11
(4,645)	1:53:A:THR:HG22	1:54:A:GLY:HA3	14	0.11
(4,645)	1:53:A:THR:HG23	1:54:A:GLY:HA3	14	0.11
(4,628)	1:55:A:PRO:HB3	1:58:A:CYS:H	19	0.11
(4,581)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	0.11
(4,511)	1:41:A:CYS:H	1:46:A:CYS:HA	6	0.11
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	19	0.11
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	19	0.11
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	19	0.11
(4,392)	1:22:A:GLY:H	1:24:A:LYS:H	10	0.11
(4,392)	1:22:A:GLY:H	1:24:A:LYS:H	13	0.11
(4,378)	1:6:A:LYS:HE2	1:7:A:GLY:H	1	0.11
(4,378)	1:6:A:LYS:HE3	1:7:A:GLY:H	1	0.11
(4,347)	1:21:A:CYS:HB2	1:25:A:CYS:H	11	0.11
(4,347)	1:21:A:CYS:HB3	1:25:A:CYS:H	11	0.11
(4,332)	1:33:A:CYS:H	1:36:A:CYS:H	10	0.11
(4,332)	1:33:A:CYS:H	1:36:A:CYS:H	20	0.11
(4,288)	1:10:A:CYS:H	1:28:A:GLY:H	6	0.11
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	7	0.11
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	8	0.11
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	19	0.11
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	2	0.11
(4,262)	1:24:A:LYS:H	1:26:A:GLN:H	4	0.11
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	6	0.11
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	6	0.11
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	7	0.11
(4,239)	1:34:A:ALA:H	1:36:A:CYS:H	10	0.11
(4,190)	1:45:A:GLY:H	1:47:A:LYS:HG2	12	0.11
(4,190)	1:45:A:GLY:H	1:47:A:LYS:HG3	12	0.11
(4,179)	1:20:A:GLN:H	1:21:A:CYS:HA	9	0.11
(4,156)	1:11:A:THR:H	1:14:A:CYS:HA	18	0.11
(4,128)	1:13:A:ALA:H	1:21:A:CYS:HA	16	0.11
(4,119)	1:16:A:SER:H	1:20:A:GLN:HG2	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,91)	1:14:A:CYS:H	1:21:A:CYS:HA	4	0.11
(4,74)	1:14:A:CYS:HB2	1:15:A:ARG:H	2	0.11
(4,69)	1:13:A:ALA:HB1	1:21:A:CYS:H	19	0.11
(4,69)	1:13:A:ALA:HB2	1:21:A:CYS:H	19	0.11
(4,69)	1:13:A:ALA:HB3	1:21:A:CYS:H	19	0.11
(4,69)	1:13:A:ALA:HB1	1:21:A:CYS:H	20	0.11
(4,69)	1:13:A:ALA:HB2	1:21:A:CYS:H	20	0.11
(4,69)	1:13:A:ALA:HB3	1:21:A:CYS:H	20	0.11
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	16	0.11
(1,1142)	1:21:A:CYS:H	1:36:A:CYS:HA	10	0.11
(1,1139)	1:42:A:THR:HG21	1:47:A:LYS:H	5	0.11
(1,1139)	1:42:A:THR:HG22	1:47:A:LYS:H	5	0.11
(1,1139)	1:42:A:THR:HG23	1:47:A:LYS:H	5	0.11
(1,1113)	1:45:A:GLY:H	1:46:A:CYS:H	19	0.11
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	14	0.11
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	14	0.11
(1,1021)	1:37:A:LYS:HE2	1:38:A:THR:H	14	0.11
(1,1021)	1:37:A:LYS:HE3	1:38:A:THR:H	14	0.11
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	12	0.11
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	12	0.11
(1,1019)	1:37:A:LYS:HG2	1:38:A:THR:H	12	0.11
(1,1019)	1:37:A:LYS:HG3	1:38:A:THR:H	12	0.11
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG2	16	0.11
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG3	16	0.11
(1,987)	1:25:A:CYS:H	1:26:A:GLN:HG3	16	0.11
(1,952)	1:9:A:LYS:HG2	1:28:A:GLY:H	17	0.11
(1,952)	1:9:A:LYS:HG3	1:28:A:GLY:H	17	0.11
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	3	0.11
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	3	0.11
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	3	0.11
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	3	0.11
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB3	3	0.11
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	3	0.11
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB3	3	0.11
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	3	0.11
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB3	3	0.11
(1,910)	1:13:A:ALA:HB1	1:16:A:SER:HB2	3	0.11
(1,910)	1:13:A:ALA:HB2	1:16:A:SER:HB2	3	0.11
(1,910)	1:13:A:ALA:HB3	1:16:A:SER:HB2	3	0.11
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	5	0.11
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB2	5	0.11
(1,901)	1:19:A:CYS:HA	1:19:A:CYS:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	17	0.11
(1,892)	1:33:A:CYS:HB2	1:36:A:CYS:HA	17	0.11
(1,892)	1:33:A:CYS:HB3	1:36:A:CYS:HA	17	0.11
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	0.11
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	20	0.11
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	0.11
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	0.11
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	20	0.11
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	20	0.11
(1,877)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	0.11
(1,877)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	20	0.11
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB1	9	0.11
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB2	9	0.11
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB3	9	0.11
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB1	9	0.11
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB2	9	0.11
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB3	9	0.11
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB1	9	0.11
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB2	9	0.11
(1,866)	1:19:A:CYS:HB2	1:35:A:ALA:HB3	9	0.11
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB1	9	0.11
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB2	9	0.11
(1,866)	1:19:A:CYS:HB3	1:35:A:ALA:HB3	9	0.11
(1,858)	1:11:A:THR:HG21	1:14:A:CYS:HB2	2	0.11
(1,858)	1:11:A:THR:HG22	1:14:A:CYS:HB2	2	0.11
(1,858)	1:11:A:THR:HG23	1:14:A:CYS:HB2	2	0.11
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	4	0.11
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB2	4	0.11
(1,806)	1:25:A:CYS:H	1:36:A:CYS:HB3	4	0.11
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	13	0.11
(1,802)	1:15:A:ARG:HB2	1:16:A:SER:HA	13	0.11
(1,802)	1:15:A:ARG:HB3	1:16:A:SER:HA	13	0.11
(1,733)	1:53:A:THR:HG21	1:54:A:GLY:HA3	14	0.11
(1,733)	1:53:A:THR:HG22	1:54:A:GLY:HA3	14	0.11
(1,733)	1:53:A:THR:HG23	1:54:A:GLY:HA3	14	0.11
(1,709)	1:55:A:PRO:HB3	1:58:A:CYS:H	19	0.11
(1,660)	1:10:A:CYS:HB3	1:15:A:ARG:HA	20	0.11
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	0.11
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	10	0.11
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	0.11
(1,646)	1:58:A:CYS:HA	1:59:A:LYS:HD3	10	0.11
(1,643)	1:50:A:LYS:HB2	1:58:A:CYS:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,563)	1:47:A:LYS:HA	1:47:A:LYS:HD2	19	0.11
(1,563)	1:47:A:LYS:HA	1:47:A:LYS:HD3	19	0.11
(1,563)	1:47:A:LYS:HA	1:47:A:LYS:HD2	19	0.11
(1,563)	1:47:A:LYS:HA	1:47:A:LYS:HD3	19	0.11
(1,558)	1:41:A:CYS:H	1:46:A:CYS:HA	6	0.11
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	11	0.11
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	11	0.11
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	11	0.11
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	11	0.11
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA3	11	0.11
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	11	0.11
(1,533)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	11	0.11
(1,533)	1:29:A:GLU:HB3	1:30:A:GLY:HA2	11	0.11
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	19	0.11
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	19	0.11
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	19	0.11
(1,427)	1:22:A:GLY:H	1:24:A:LYS:H	10	0.11
(1,427)	1:22:A:GLY:H	1:24:A:LYS:H	13	0.11
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.11
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.11
(1,393)	1:67:A:LYS:H	1:67:A:LYS:HE3	7	0.11
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	14	0.11
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB2	14	0.11
(1,380)	1:25:A:CYS:H	1:26:A:GLN:HB3	14	0.11
(1,360)	1:33:A:CYS:H	1:36:A:CYS:H	10	0.11
(1,360)	1:33:A:CYS:H	1:36:A:CYS:H	20	0.11
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	3	0.11
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB2	3	0.11
(1,348)	1:27:A:CYS:H	1:27:A:CYS:HB3	3	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	4	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	4	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	4	0.11
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	4	0.11
(1,313)	1:10:A:CYS:H	1:28:A:GLY:H	6	0.11
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	7	0.11
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	8	0.11
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	19	0.11
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	2	0.11
(1,281)	1:24:A:LYS:H	1:26:A:GLN:H	4	0.11
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	4	0.11
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	7	0.11
(1,249)	1:34:A:ALA:H	1:36:A:CYS:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	9	0.11
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	9	0.11
(1,207)	1:52:A:CYS:HB3	1:58:A:CYS:H	9	0.11
(1,207)	1:52:A:CYS:HB2	1:58:A:CYS:H	9	0.11
(1,190)	1:20:A:GLN:H	1:21:A:CYS:HA	9	0.11
(1,180)	1:38:A:THR:H	1:67:A:LYS:HA	4	0.11
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	10	0.11
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG2	10	0.11
(1,176)	1:46:A:CYS:H	1:47:A:LYS:HG3	10	0.11
(1,164)	1:11:A:THR:H	1:14:A:CYS:HA	18	0.11
(1,131)	1:13:A:ALA:H	1:21:A:CYS:HA	16	0.11
(1,123)	1:16:A:SER:H	1:20:A:GLN:HG2	19	0.11
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	16	0.11
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB2	16	0.11
(1,103)	1:31:A:CYS:H	1:31:A:CYS:HB3	16	0.11
(1,93)	1:14:A:CYS:H	1:21:A:CYS:HA	4	0.11
(1,72)	1:13:A:ALA:HB1	1:21:A:CYS:H	19	0.11
(1,72)	1:13:A:ALA:HB2	1:21:A:CYS:H	19	0.11
(1,72)	1:13:A:ALA:HB3	1:21:A:CYS:H	19	0.11
(1,72)	1:13:A:ALA:HB1	1:21:A:CYS:H	20	0.11
(1,72)	1:13:A:ALA:HB2	1:21:A:CYS:H	20	0.11
(1,72)	1:13:A:ALA:HB3	1:21:A:CYS:H	20	0.11
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	16	0.11
(4,925)	1:11:A:THR:HG21	1:28:A:GLY:H	18	0.1
(4,925)	1:11:A:THR:HG22	1:28:A:GLY:H	18	0.1
(4,925)	1:11:A:THR:HG23	1:28:A:GLY:H	18	0.1
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE2	13	0.1
(4,898)	1:64:A:CYS:H	1:67:A:LYS:HE3	13	0.1
(4,822)	1:23:A:SER:HA	1:24:A:LYS:HG2	6	0.1
(4,822)	1:23:A:SER:HA	1:24:A:LYS:HG3	6	0.1
(4,807)	1:11:A:THR:H	1:15:A:ARG:HD2	6	0.1
(4,781)	1:52:A:CYS:HA	1:54:A:GLY:H	5	0.1
(4,720)	1:21:A:CYS:HB2	1:25:A:CYS:H	17	0.1
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG21	14	0.1
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG22	14	0.1
(4,460)	1:31:A:CYS:HA	1:32:A:THR:HG23	14	0.1
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG21	6	0.1
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG22	6	0.1
(4,448)	1:48:A:CYS:H	1:53:A:THR:HG23	6	0.1
(4,420)	1:64:A:CYS:H	1:64:A:CYS:HB2	13	0.1
(4,392)	1:22:A:GLY:H	1:24:A:LYS:H	19	0.1
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG21	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG22	8	0.1
(4,382)	1:30:A:GLY:H	1:32:A:THR:HG23	8	0.1
(4,305)	1:35:A:ALA:HA	1:37:A:LYS:H	1	0.1
(4,305)	1:35:A:ALA:HA	1:37:A:LYS:H	16	0.1
(4,277)	1:40:A:ASN:HD21	1:67:A:LYS:HB3	18	0.1
(4,267)	1:40:A:ASN:H	1:48:A:CYS:HB3	10	0.1
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB2	16	0.1
(4,243)	1:41:A:CYS:H	1:48:A:CYS:HB3	16	0.1
(4,169)	1:46:A:CYS:H	1:47:A:LYS:HG2	16	0.1
(4,169)	1:46:A:CYS:H	1:47:A:LYS:HG3	16	0.1
(4,140)	1:61:A:GLY:H	1:64:A:CYS:H	19	0.1
(4,105)	1:29:A:GLU:H	1:31:A:CYS:H	3	0.1
(4,105)	1:29:A:GLU:H	1:31:A:CYS:H	10	0.1
(4,91)	1:14:A:CYS:H	1:21:A:CYS:HA	9	0.1
(4,74)	1:14:A:CYS:HB2	1:15:A:ARG:H	4	0.1
(4,69)	1:13:A:ALA:HB1	1:21:A:CYS:H	8	0.1
(4,69)	1:13:A:ALA:HB2	1:21:A:CYS:H	8	0.1
(4,69)	1:13:A:ALA:HB3	1:21:A:CYS:H	8	0.1
(4,9)	1:35:A:ALA:H	1:37:A:LYS:HA	10	0.1
(1,1125)	1:11:A:THR:HG21	1:28:A:GLY:H	18	0.1
(1,1125)	1:11:A:THR:HG22	1:28:A:GLY:H	18	0.1
(1,1125)	1:11:A:THR:HG23	1:28:A:GLY:H	18	0.1
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE2	13	0.1
(1,1088)	1:64:A:CYS:H	1:67:A:LYS:HE3	13	0.1
(1,976)	1:23:A:SER:HA	1:24:A:LYS:HG2	6	0.1
(1,976)	1:23:A:SER:HA	1:24:A:LYS:HG3	6	0.1
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD2	16	0.1
(1,960)	1:11:A:THR:H	1:15:A:ARG:HD3	16	0.1
(1,914)	1:52:A:CYS:HA	1:54:A:GLY:H	5	0.1
(1,912)	1:15:A:ARG:HA	1:15:A:ARG:HB3	8	0.1
(1,912)	1:15:A:ARG:HA	1:15:A:ARG:HB2	8	0.1
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	7	0.1
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB2	7	0.1
(1,887)	1:32:A:THR:HA	1:33:A:CYS:HB3	7	0.1
(1,833)	1:21:A:CYS:HB2	1:25:A:CYS:H	17	0.1
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG21	14	0.1
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG22	14	0.1
(1,504)	1:31:A:CYS:HA	1:32:A:THR:HG23	14	0.1
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG21	6	0.1
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG22	6	0.1
(1,491)	1:48:A:CYS:H	1:53:A:THR:HG23	6	0.1
(1,427)	1:22:A:GLY:H	1:24:A:LYS:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG21	8	0.1
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG22	8	0.1
(1,418)	1:30:A:GLY:H	1:32:A:THR:HG23	8	0.1
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	9	0.1
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG2	9	0.1
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	9	0.1
(1,341)	1:47:A:LYS:H	1:47:A:LYS:HG3	9	0.1
(1,332)	1:35:A:ALA:HA	1:37:A:LYS:H	1	0.1
(1,332)	1:35:A:ALA:HA	1:37:A:LYS:H	16	0.1
(1,286)	1:40:A:ASN:H	1:48:A:CYS:HB3	10	0.1
(1,272)	1:21:A:CYS:HA	1:24:A:LYS:H	14	0.1
(1,145)	1:61:A:GLY:H	1:64:A:CYS:H	19	0.1
(1,108)	1:29:A:GLU:H	1:31:A:CYS:H	3	0.1
(1,108)	1:29:A:GLU:H	1:31:A:CYS:H	10	0.1
(1,93)	1:14:A:CYS:H	1:21:A:CYS:HA	9	0.1
(1,84)	1:64:A:CYS:HA	1:66:A:CYS:H	15	0.1
(1,72)	1:13:A:ALA:HB1	1:21:A:CYS:H	8	0.1
(1,72)	1:13:A:ALA:HB2	1:21:A:CYS:H	8	0.1
(1,72)	1:13:A:ALA:HB3	1:21:A:CYS:H	8	0.1
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	3	0.1
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	3	0.1
(1,12)	1:19:A:CYS:HB2	1:35:A:ALA:H	3	0.1
(1,12)	1:19:A:CYS:HB3	1:35:A:ALA:H	3	0.1
(1,9)	1:35:A:ALA:H	1:37:A:LYS:HA	10	0.1

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found