



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 03:45 PM UTC

PDB ID : 6QK6 / pdb_00006qk6
BMRB ID : 34356
Title : Solution Structure of the Cd-loaded form of a Metallothionein from Helix Pomatia
Authors : Zerbe, O.; Jurt, S.; Beil, A.
Deposited on : 2019-01-28

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

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

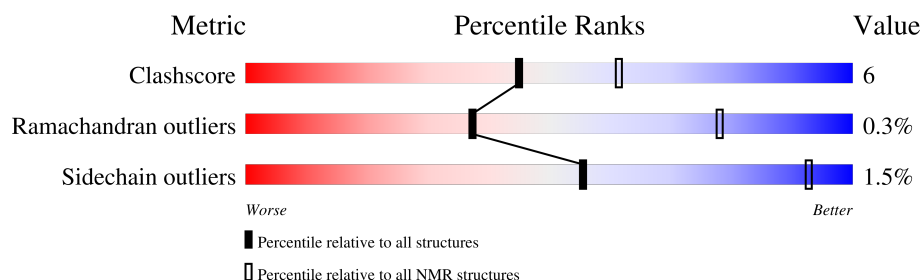
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	67	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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)	0.92	18

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

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

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

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

3 Entry composition

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
1	A	67	Total	C	H	N	O	S	0
			837	244	397	82	96	18	

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 CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

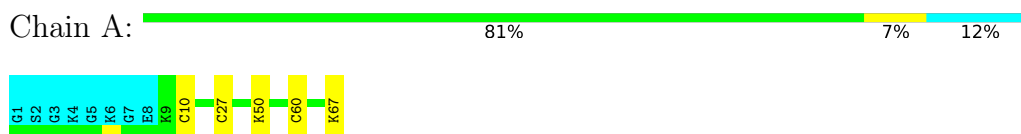
Mol	Chain	Residues	Atoms	
2	A	6	Total	Cd
			6	6

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Cadmium-metallothionein

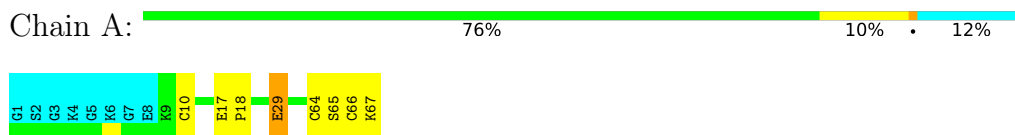


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

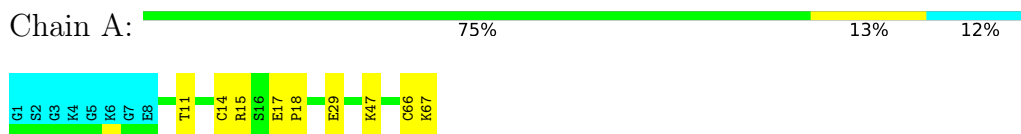
4.2.1 Score per residue for model 1

- Molecule 1: Cadmium-metallothionein



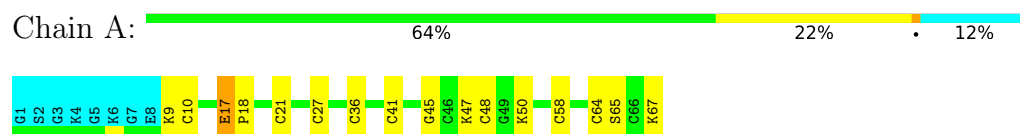
4.2.2 Score per residue for model 2

- Molecule 1: Cadmium-metallothionein



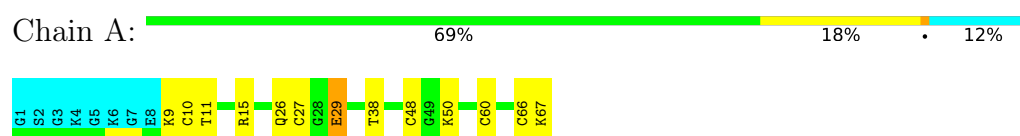
4.2.3 Score per residue for model 3

- Molecule 1: Cadmium-metallothionein



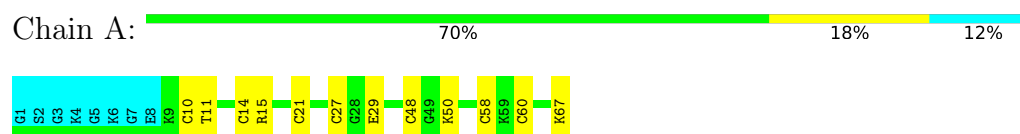
4.2.4 Score per residue for model 4

- Molecule 1: Cadmium-metallothionein



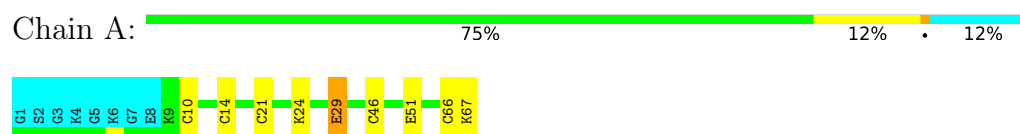
4.2.5 Score per residue for model 5

- Molecule 1: Cadmium-metallothionein



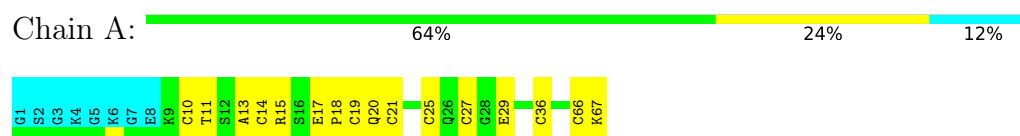
4.2.6 Score per residue for model 6

- Molecule 1: Cadmium-metallothionein



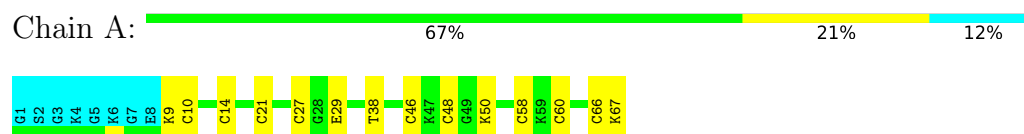
4.2.7 Score per residue for model 7

- Molecule 1: Cadmium-metallothionein



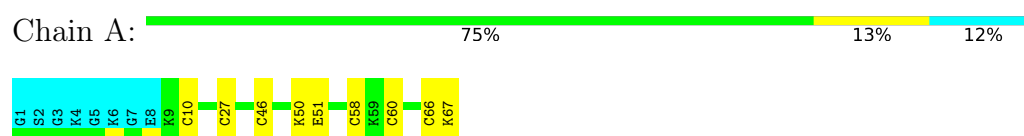
4.2.8 Score per residue for model 8

- Molecule 1: Cadmium-metallothionein



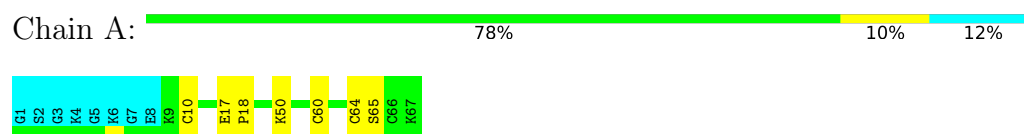
4.2.9 Score per residue for model 9

- Molecule 1: Cadmium-metallothionein



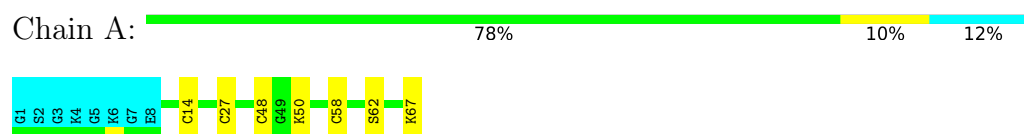
4.2.10 Score per residue for model 10

- Molecule 1: Cadmium-metallothionein



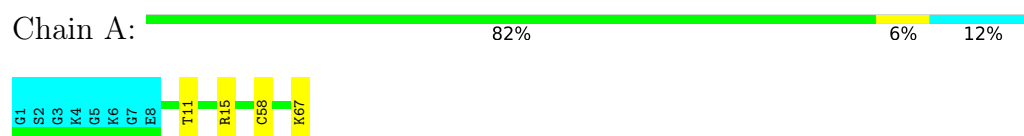
4.2.11 Score per residue for model 11

- Molecule 1: Cadmium-metallothionein



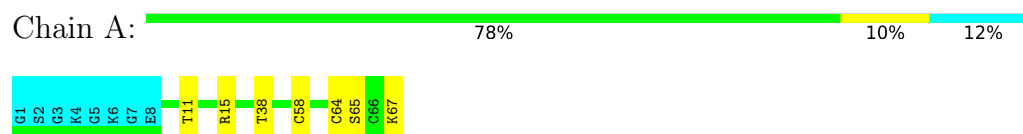
4.2.12 Score per residue for model 12

- Molecule 1: Cadmium-metallothionein



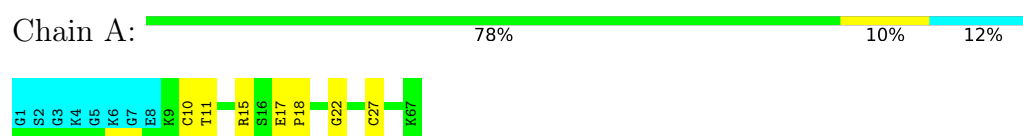
4.2.13 Score per residue for model 13

- Molecule 1: Cadmium-metallothionein



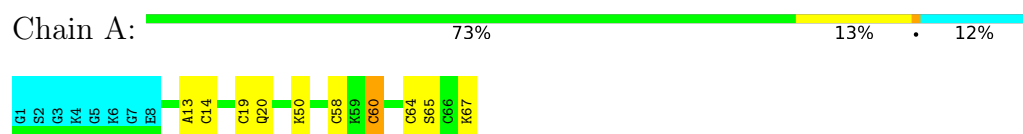
4.2.14 Score per residue for model 14

- Molecule 1: Cadmium-metallothionein



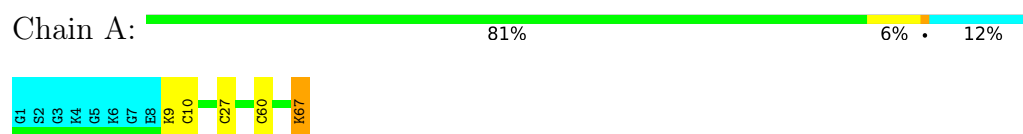
4.2.15 Score per residue for model 15

- Molecule 1: Cadmium-metallothionein



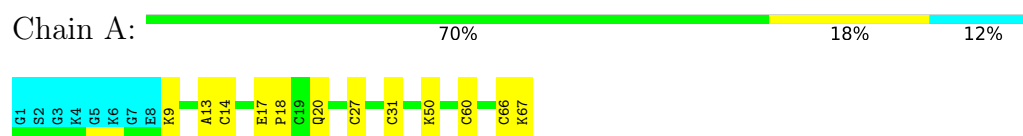
4.2.16 Score per residue for model 16

- Molecule 1: Cadmium-metallothionein



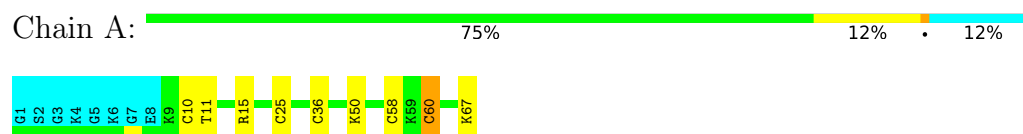
4.2.17 Score per residue for model 17

- Molecule 1: Cadmium-metallothionein



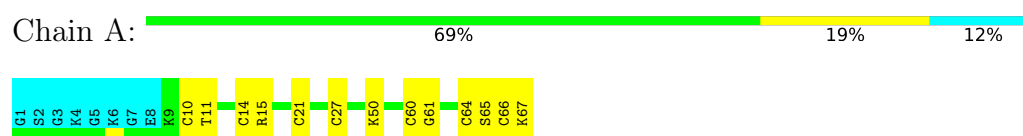
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Cadmium-metallothionein



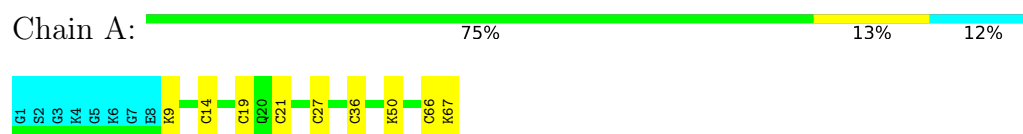
4.2.19 Score per residue for model 19

- Molecule 1: Cadmium-metallothionein



4.2.20 Score per residue for model 20

- Molecule 1: Cadmium-metallothionein



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	3.85

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	575
Number of shifts mapped to atoms	575
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 [i](#)

6.1 Standard geometry [i](#)

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	391	349	349	5±2
All	All	7940	6980	6980	94

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LYS:HG3	1:A:60:CYS:SG	0.70	2.26	10	9
1:A:66:CYS:SG	1:A:67:LYS:HE3	0.64	2.33	2	1
1:A:10:CYS:HA	1:A:27:CYS:SG	0.58	2.38	7	6
1:A:48:CYS:SG	1:A:50:LYS:HG2	0.57	2.39	5	5
1:A:61:GLY:O	1:A:67:LYS:HG3	0.57	2.00	19	1
1:A:11:THR:O	1:A:15:ARG:HG3	0.56	2.00	7	8
1:A:17:GLU:HA	1:A:18:PRO:C	0.53	2.29	14	7
1:A:66:CYS:SG	1:A:67:LYS:NZ	0.51	2.84	9	9
1:A:14:CYS:HB2	1:A:21:CYS:SG	0.50	2.45	5	3
1:A:58:CYS:SG	1:A:67:LYS:NZ	0.50	2.84	18	9
1:A:9:LYS:O	1:A:27:CYS:HA	0.50	2.07	4	6
1:A:25:CYS:SG	1:A:36:CYS:HB2	0.49	2.48	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:THR:O	1:A:67:LYS:HE3	0.47	2.10	4	1
1:A:21:CYS:HB2	1:A:36:CYS:HB3	0.45	1.89	20	3
1:A:29:GLU:CD	1:A:29:GLU:H	0.44	2.21	6	2
1:A:64:CYS:SG	1:A:65:SER:N	0.44	2.91	1	6
1:A:46:CYS:SG	1:A:51:GLU:N	0.43	2.90	6	2
1:A:11:THR:O	1:A:15:ARG:HG2	0.43	2.13	14	1
1:A:27:CYS:O	1:A:62:SER:HB2	0.43	2.14	11	1
1:A:60:CYS:O	1:A:67:LYS:HE3	0.43	2.12	16	1
1:A:11:THR:CG2	1:A:26:GLN:HB2	0.42	2.45	4	1
1:A:14:CYS:HA	1:A:19:CYS:SG	0.42	2.54	20	3
1:A:21:CYS:HA	1:A:24:LYS:O	0.42	2.15	6	1
1:A:13:ALA:HB1	1:A:20:GLN:C	0.42	2.40	17	2
1:A:29:GLU:H	1:A:29:GLU:CD	0.41	2.23	4	1
1:A:21:CYS:CB	1:A:36:CYS:HB3	0.41	2.46	7	1
1:A:41:CYS:SG	1:A:47:LYS:HB2	0.40	2.56	3	1
1:A:13:ALA:HB1	1:A:20:GLN:HB2	0.40	1.92	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/67 (87%)	52±2 (91±3%)	5±2 (9±3%)	0±0 (0±1%)	37	78
All	All	1160/1340 (87%)	1050 (91%)	107 (9%)	3 (0%)	37	78

All 3 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	45	GLY	1
1	A	46	CYS	1
1	A	22	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%)	48±1 (98±1%)	1±1 (2±1%)	55	93
All	All	980/1060 (92%)	965 (98%)	15 (2%)	55	93

All 7 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	29	GLU	7
1	A	38	THR	2
1	A	60	CYS	2
1	A	47	LYS	1
1	A	17	GLU	1
1	A	67	LYS	1
1	A	50	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 84% 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	575
Number of shifts mapped to atoms	575
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	67	-0.12 ± 0.30	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	56	0.51 ± 0.18	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	59	-0.67 ± 0.49	None needed (imprecise)

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	^1H	^{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 84%, i.e. 575 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	263/342 (77%)	137/143 (96%)	67/134 (50%)	59/65 (91%)
Sidechain	312/339 (92%)	209/214 (98%)	100/110 (91%)	3/15 (20%)
Overall	575/681 (84%)	346/357 (97%)	167/244 (68%)	62/80 (78%)

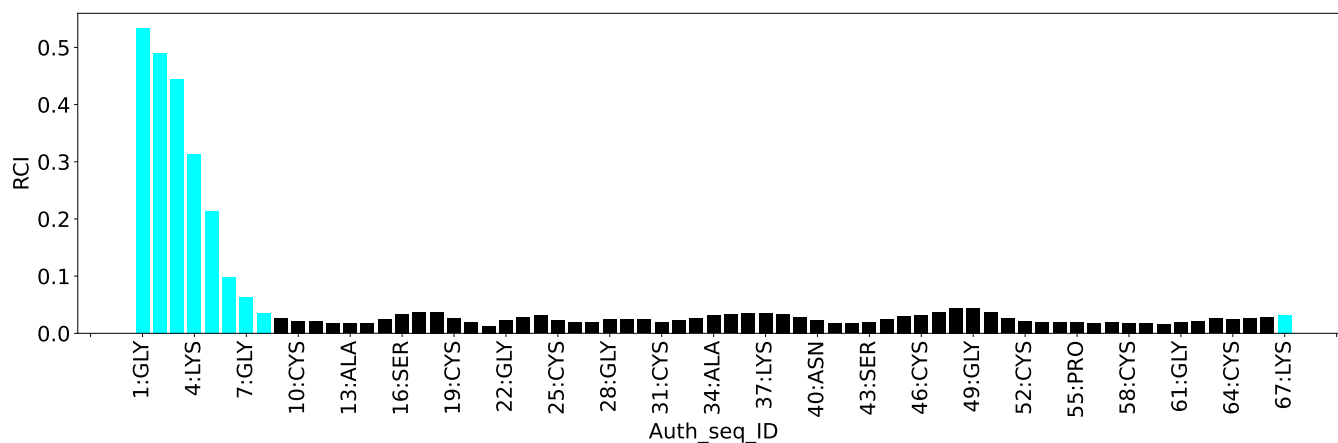
7.1.4 Statistically unusual chemical shifts [i](#)

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	2204
Intra-residue ($ i-j =0$)	452
Sequential ($ i-j =1$)	733
Medium range ($ i-j >1$ and $ i-j <5$)	430
Long range ($ i-j \geq 5$)	589
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	30.2
Number of long range restraints per residue ¹	8.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	27.9	0.2
0.2-0.5 (Medium)	34.4	0.5
>0.5 (Large)	313.6	15.5

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

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

9 Distance violation analysis ⓘ

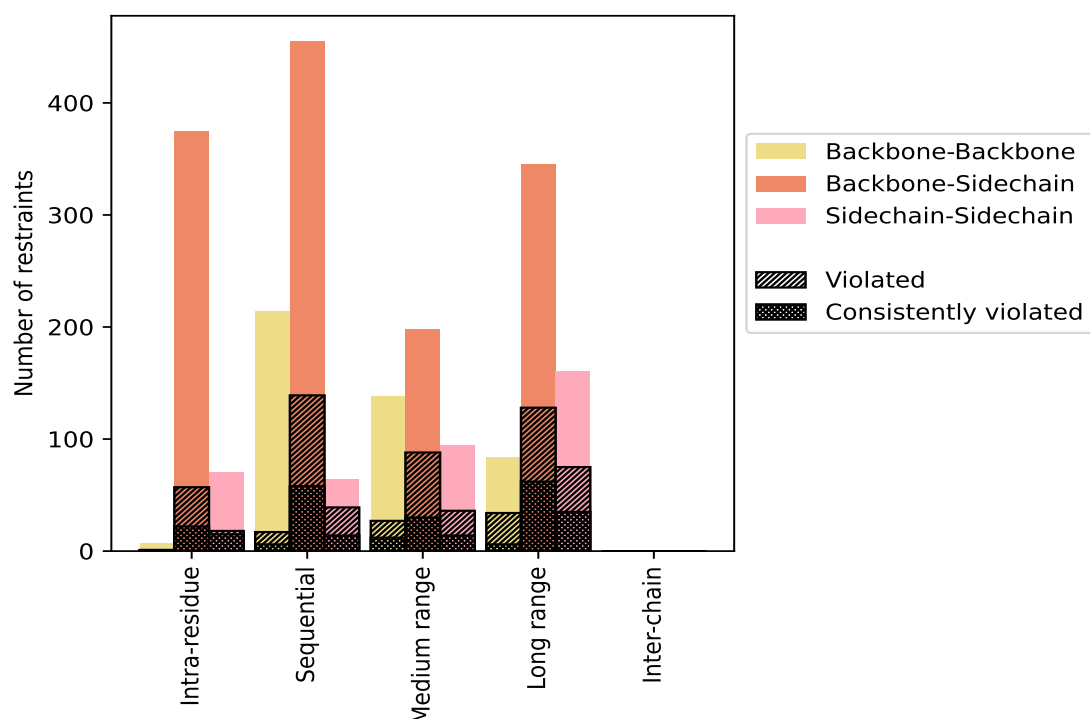
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	452	20.5	76	16.8	3.4	38	8.4	1.7
Backbone-Backbone	7	0.3	1	14.3	0.0	1	14.3	0.0
Backbone-Sidechain	375	17.0	57	15.2	2.6	22	5.9	1.0
Sidechain-Sidechain	70	3.2	18	25.7	0.8	15	21.4	0.7
Sequential ($i-j =1$)	733	33.3	195	26.6	8.8	78	10.6	3.5
Backbone-Backbone	214	9.7	17	7.9	0.8	6	2.8	0.3
Backbone-Sidechain	455	20.6	139	30.5	6.3	58	12.7	2.6
Sidechain-Sidechain	64	2.9	39	60.9	1.8	14	21.9	0.6
Medium range ($i-j >1$ & $i-j <5$)	430	19.5	151	35.1	6.9	56	13.0	2.5
Backbone-Backbone	138	6.3	27	19.6	1.2	12	8.7	0.5
Backbone-Sidechain	198	9.0	88	44.4	4.0	30	15.2	1.4
Sidechain-Sidechain	94	4.3	36	38.3	1.6	14	14.9	0.6
Long range ($i-j \geq 5$)	589	26.7	237	40.2	10.8	103	17.5	4.7
Backbone-Backbone	84	3.8	34	40.5	1.5	6	7.1	0.3
Backbone-Sidechain	345	15.7	128	37.1	5.8	62	18.0	2.8
Sidechain-Sidechain	160	7.3	75	46.9	3.4	35	21.9	1.6
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	2204	100.0	659	29.9	29.9	275	12.5	12.5
Backbone-Backbone	443	20.1	79	17.8	3.6	25	5.6	1.1
Backbone-Sidechain	1373	62.3	412	30.0	18.7	172	12.5	7.8
Sidechain-Sidechain	388	17.6	168	43.3	7.6	78	20.1	3.5

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	47	101	77	144	0	369	3.53	14.51	2.31	3.81
2	48	116	81	146	0	391	3.37	12.85	2.33	3.71
3	50	115	72	145	0	382	3.45	14.06	2.36	3.84
4	49	115	73	136	0	373	3.48	13.31	2.29	3.86
5	47	114	78	144	0	383	3.4	14.51	2.34	3.87
6	47	111	85	138	0	381	3.39	12.95	2.28	3.76
7	50	113	80	139	0	382	3.47	12.13	2.29	3.82
8	51	108	84	144	0	387	3.48	14.42	2.37	3.87
9	49	105	75	130	0	359	3.67	13.38	2.26	4.0
10	47	112	79	138	0	376	3.49	14.75	2.31	3.82

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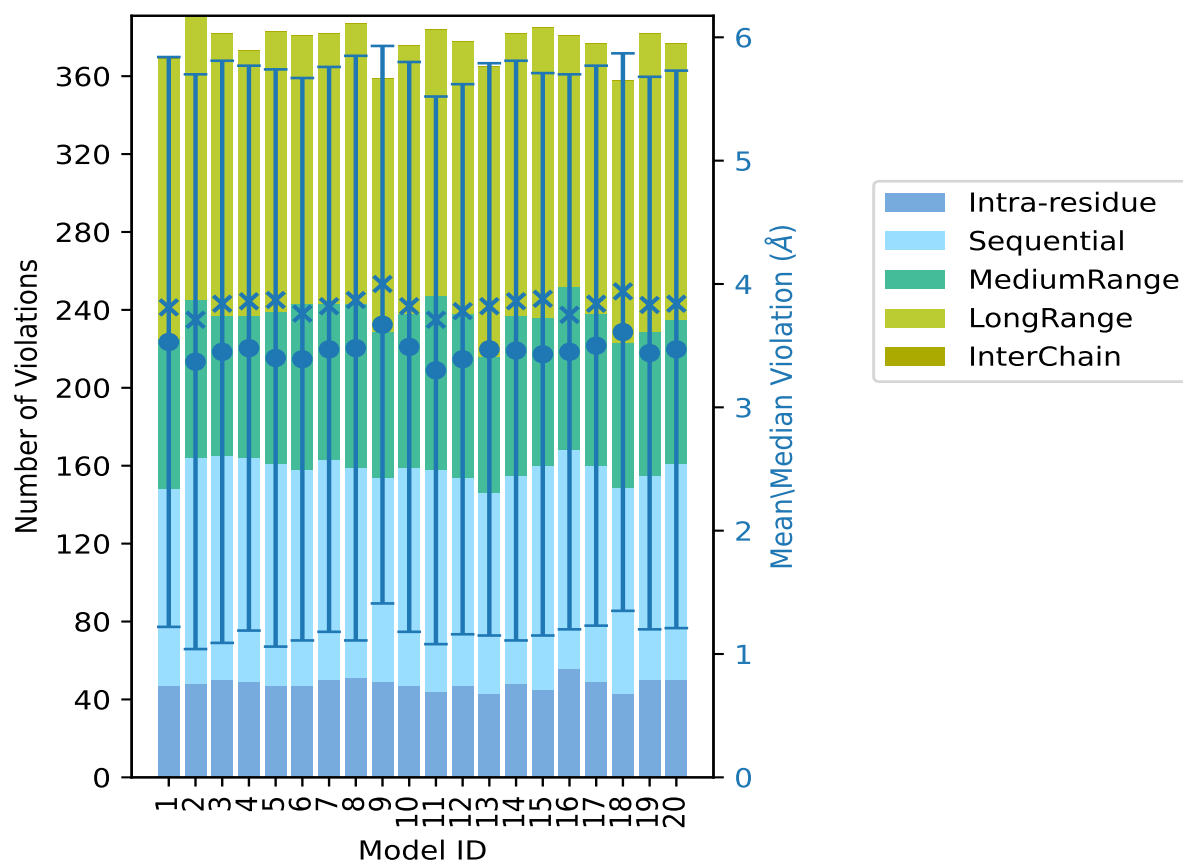
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	44	114	89	137	0	384	3.3	12.76	2.22	3.71
12	47	107	84	140	0	378	3.39	12.81	2.23	3.78
13	43	103	70	149	0	365	3.47	15.5	2.32	3.82
14	48	107	82	145	0	382	3.46	13.42	2.35	3.86
15	45	115	76	149	0	385	3.43	13.63	2.28	3.88
16	56	112	84	129	0	381	3.45	12.29	2.25	3.75
17	49	111	78	139	0	377	3.5	13.45	2.27	3.84
18	43	106	74	135	0	358	3.61	13.5	2.26	3.94
19	50	105	74	153	0	382	3.44	13.56	2.24	3.83
20	50	111	74	142	0	377	3.47	13.1	2.26	3.84

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

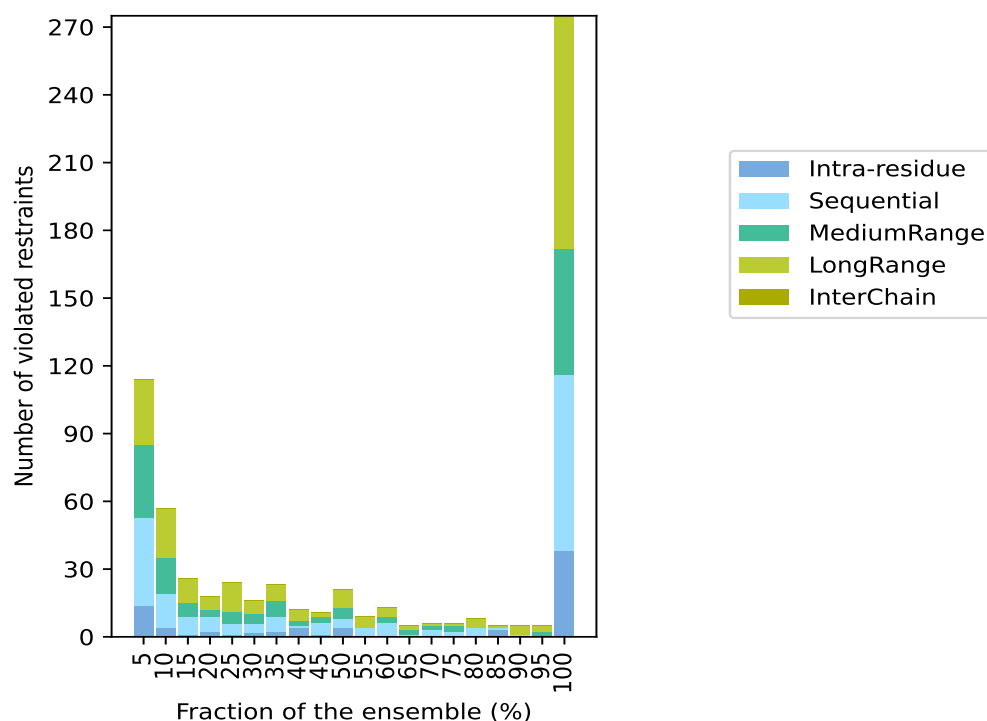
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1545(IR:376, SQ:538, MR:279, LR:352, IC:0) restraints are 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	%
14	39	32	29	0	114	1	5.0
4	15	16	22	0	57	2	10.0
1	8	6	11	0	26	3	15.0
2	7	3	6	0	18	4	20.0
1	5	5	13	0	24	5	25.0
2	4	4	6	0	16	6	30.0
2	7	7	7	0	23	7	35.0
4	1	2	5	0	12	8	40.0
1	5	3	2	0	11	9	45.0
4	4	5	8	0	21	10	50.0
0	4	0	5	0	9	11	55.0
0	6	3	4	0	13	12	60.0
0	1	2	2	0	5	13	65.0
0	3	2	1	0	6	14	70.0
0	2	3	1	0	6	15	75.0
0	4	0	4	0	8	16	80.0
3	1	0	1	0	5	17	85.0
0	1	0	4	0	5	18	90.0
0	0	2	3	0	5	19	95.0
38	78	56	103	0	275	20	100.0

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

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

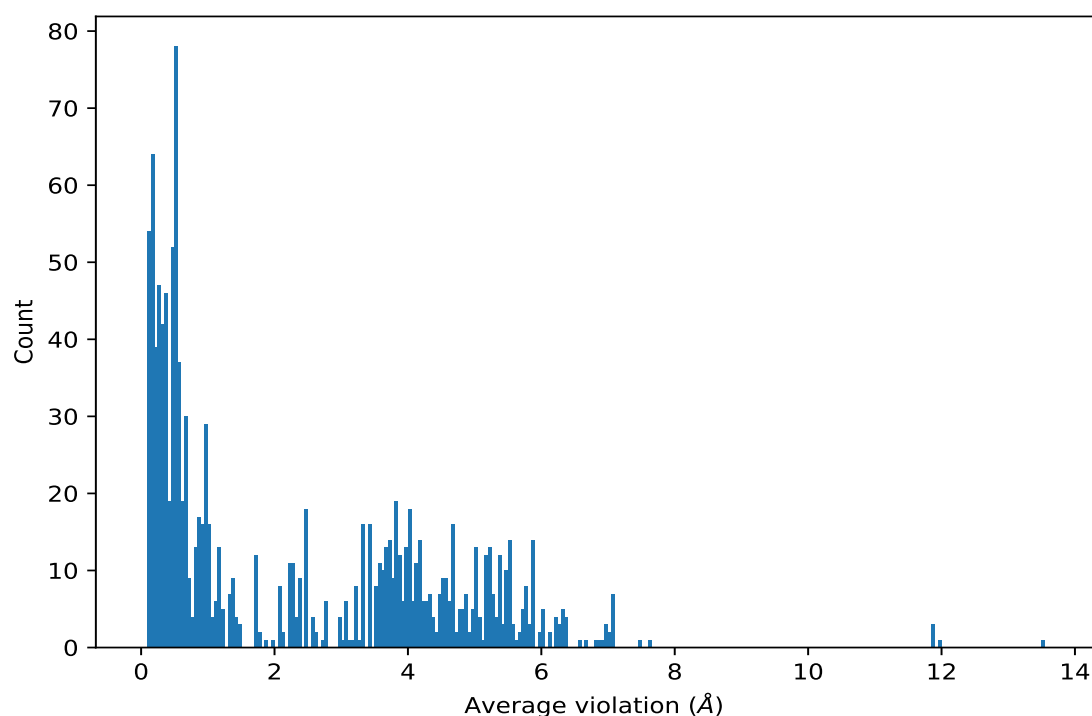
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	20	13.54	0.84	13.43
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	20	11.95	0.93	11.72
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	20	11.88	0.86	11.68
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	20	11.88	0.86	11.68
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	20	11.88	0.86	11.68
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	20	7.62	1.06	7.82
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	20	7.46	0.38	7.42
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	20	7.06	0.55	6.98
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	20	7.06	0.55	6.98
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	20	7.06	0.55	6.98
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	20	7.05	1.15	7.38
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	20	7.05	1.15	7.38
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	20	7.05	1.15	7.38
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	20	7.05	0.84	7.09
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	20	7.02	1.11	6.91
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	20	7.0	0.2	6.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	20	6.97	0.3	7.05
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	20	6.97	1.48	7.04
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	20	6.96	0.58	6.94
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	20	6.92	0.51	6.94
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	6.88	1.23	6.94
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	20	6.8	1.5	7.2
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	20	6.66	0.72	6.68
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	20	6.59	0.63	6.72
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	20	6.37	1.38	6.4
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	20	6.36	1.14	6.49
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	20	6.36	1.14	6.49
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	20	6.35	0.2	6.4
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	20	6.34	0.21	6.38
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	20	6.31	0.36	6.42
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	20	6.31	0.36	6.42
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	20	6.31	0.36	6.42
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	20	6.31	0.59	6.45
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	20	6.29	0.94	6.46
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	6.29	0.94	6.46
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	20	6.29	0.92	6.14
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	20	6.24	0.37	6.16
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	20	6.23	0.65	6.57
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	20	6.2	1.43	6.39
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	20	6.2	1.43	6.39
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	6.13	0.23	6.16
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	6.12	1.28	6.41
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	20	6.02	0.6	6.07
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	20	6.01	0.48	6.09
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	20	6.01	0.48	6.09
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	20	6.01	0.48	6.09
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	20	6.0	0.95	6.14
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	20	5.99	0.52	6.24
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	20	5.97	0.26	5.91
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	20	5.88	0.86	6.16
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	20	5.88	1.05	5.74
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	20	5.86	0.33	5.73

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	20	5.86	0.33	5.73
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	20	5.86	0.33	5.73
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	5.86	1.52	5.98
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	5.86	1.52	5.98
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	20	5.85	0.58	5.74
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	20	5.83	0.59	5.78
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	20	5.81	0.54	5.68
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	20	5.81	0.54	5.68
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	20	5.79	0.72	5.82
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	20	5.79	0.72	5.82
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	20	5.79	0.72	5.82
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	20	5.77	1.13	5.57
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	20	5.76	0.39	5.78
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	20	5.75	0.25	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	20	5.75	0.25	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	20	5.75	0.25	5.82
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	20	5.72	0.21	5.72
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	20	5.72	0.21	5.72
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	20	5.72	0.21	5.72
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	20	5.7	0.82	5.58
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	20	5.7	0.82	5.58
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	20	5.65	0.29	5.68
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	20	5.65	0.29	5.68
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	20	5.6	0.18	5.6
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	20	5.57	0.33	5.54
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	20	5.55	1.19	5.74
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	20	5.55	0.14	5.54
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	5.52	0.16	5.57
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	20	5.52	0.16	5.57
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	20	5.51	0.47	5.44
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	20	5.51	0.47	5.44
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	20	5.49	0.2	5.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	20	5.49	0.2	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	20	5.49	0.2	5.54
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	20	5.49	0.72	5.74
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	20	5.48	0.13	5.44
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	20	5.48	0.15	5.45
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	20	5.48	0.52	5.53
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	20	5.48	0.52	5.53
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	5.46	0.45	5.68
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	20	5.46	0.12	5.49
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	20	5.43	0.85	5.8
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	20	5.42	0.24	5.38
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	20	5.4	0.13	5.38
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	20	5.38	0.33	5.2
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	20	5.37	0.32	5.3
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	20	5.37	0.32	5.3
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	20	5.35	0.05	5.36
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	20	5.35	0.05	5.36
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	20	5.35	0.05	5.36
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	20	5.35	0.05	5.36
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	20	5.35	0.05	5.36
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	20	5.35	0.05	5.36
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	20	5.35	0.41	5.38
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	20	5.35	0.41	5.38
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	20	5.35	0.41	5.38
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	20	5.34	0.22	5.32
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	20	5.34	1.46	5.44
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	20	5.32	0.49	5.26
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	20	5.3	0.76	5.46
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	20	5.28	0.63	5.22
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	20	5.28	0.63	5.22
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	20	5.28	0.63	5.22
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	20	5.28	0.63	5.22
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	20	5.28	0.82	5.16
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	20	5.27	0.3	5.29
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	20	5.27	0.3	5.29
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.24	0.47	5.13
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.24	0.47	5.13
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	20	5.24	0.47	5.13
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	20	5.23	0.4	5.23
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	20	5.22	0.71	5.48
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	5.21	1.2	5.52
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	5.21	1.2	5.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	5.21	1.2	5.52
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	5.21	1.2	5.52
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	20	5.21	0.2	5.12
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	20	5.2	0.2	5.22
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	20	5.2	0.2	5.22
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	20	5.2	0.2	5.22
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	20	5.18	0.52	5.2
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	20	5.18	0.52	5.2
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	20	5.18	0.52	5.2
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	20	5.18	0.52	5.2
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	20	5.18	0.55	5.26
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	20	5.18	0.55	5.26
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	20	5.17	0.71	4.97
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	20	5.17	0.71	4.97
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	20	5.17	0.71	4.97
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	20	5.17	0.71	4.97
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	20	5.16	0.17	5.18
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	20	5.16	0.52	5.28
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	20	5.11	0.18	5.06
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	20	5.09	0.33	5.18
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	20	5.09	0.85	4.84
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	20	5.07	0.05	5.08
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	20	5.06	0.34	5.15
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	20	5.03	0.92	4.74
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	20	5.03	0.92	4.74
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	20	5.03	0.25	5.08
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	20	5.03	0.25	5.08
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	20	5.03	0.25	5.08
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	20	5.03	0.31	5.0
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	20	5.03	0.31	5.0
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.0	0.51	4.97
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	20	5.0	0.51	4.97
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.0	0.51	4.97
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	20	5.0	0.51	4.97
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	20	5.0	0.12	5.01
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	20	5.0	0.24	4.94
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	20	4.99	0.27	5.09
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	20	4.99	0.83	4.99
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	4.99	0.83	4.99
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	20	4.98	0.24	5.11
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	20	4.98	0.32	4.88
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	20	4.94	0.28	4.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	20	4.94	0.37	4.96
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	20	4.89	0.66	4.82
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	20	4.89	0.66	4.82
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	20	4.87	0.22	4.86
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	20	4.85	0.11	4.82
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	20	4.85	0.11	4.82
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	20	4.85	0.11	4.82
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	20	4.85	0.29	4.84
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	20	4.84	0.19	4.85
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	20	4.81	0.59	4.92
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	20	4.81	0.59	4.92
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	20	4.81	0.59	4.92
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	4.8	0.55	4.86
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	20	4.76	0.14	4.73
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	20	4.76	0.14	4.73
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	20	4.76	0.14	4.73
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	20	4.76	0.14	4.73
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	20	4.75	0.24	4.7
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	20	4.74	0.2	4.78
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	20	4.73	0.72	5.04
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	20	4.69	0.4	4.62
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	20	4.69	0.4	4.62
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	20	4.69	0.12	4.7
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	4.69	0.79	4.68
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	20	4.69	0.79	4.68
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	4.69	0.79	4.68
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	20	4.69	0.17	4.72
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	20	4.69	0.17	4.72
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	20	4.69	0.17	4.72
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	20	4.69	0.17	4.69
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	20	4.67	0.18	4.64
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	20	4.67	0.18	4.64
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	20	4.67	0.18	4.64
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	20	4.66	0.12	4.65
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	20	4.66	0.12	4.65
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	20	4.65	0.16	4.67
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	20	4.64	0.42	4.74
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	20	4.63	0.46	4.53
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	20	4.6	0.63	4.32
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	20	4.6	0.83	4.75
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	20	4.6	0.83	4.75
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	20	4.6	0.83	4.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	20	4.58	0.99	4.53
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	20	4.58	0.99	4.53
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	20	4.58	0.99	4.53
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	20	4.58	0.99	4.53
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	20	4.57	0.09	4.58
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	4.55	0.95	4.35
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	20	4.55	0.95	4.35
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	4.55	0.95	4.35
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	20	4.55	0.95	4.35
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	20	4.54	0.96	4.72
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	20	4.53	1.36	4.89
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	20	4.53	1.36	4.89
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	20	4.53	1.36	4.89
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	20	4.53	0.66	4.64
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	20	4.51	0.47	4.68
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	20	4.51	0.47	4.68
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	20	4.51	0.29	4.37
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	4.51	0.19	4.56
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	20	4.49	0.27	4.42
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	20	4.48	0.54	4.63
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	20	4.48	0.54	4.63
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	20	4.48	0.54	4.63
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	20	4.47	0.13	4.46
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	20	4.46	0.16	4.41
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	20	4.46	0.16	4.41
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	20	4.44	0.27	4.47
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	20	4.43	1.0	4.33
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	20	4.37	1.1	4.07
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	20	4.37	1.1	4.07
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	20	4.37	1.1	4.07
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	20	4.36	0.09	4.38
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	20	4.34	0.04	4.35
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	20	4.34	0.23	4.44
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	20	4.31	0.08	4.31
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	20	4.3	0.18	4.24
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	20	4.3	0.18	4.24
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	20	4.3	0.15	4.28
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	20	4.3	0.15	4.28
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	20	4.29	0.88	4.0
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	20	4.29	0.88	4.0
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	20	4.29	0.88	4.0
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	20	4.29	0.88	4.0

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	20	4.27	0.95	4.38
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	20	4.25	0.4	4.31
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	20	4.23	0.14	4.26
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	20	4.22	0.14	4.22
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	20	4.22	0.14	4.22
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	20	4.22	0.14	4.22
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	20	4.2	0.37	4.33
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	20	4.2	1.08	4.47
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	20	4.19	0.02	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	20	4.19	0.02	4.2
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	20	4.19	0.17	4.22
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	4.19	0.17	4.22
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	20	4.18	0.49	4.08
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	20	4.18	0.49	4.08
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	20	4.18	0.49	4.08
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	20	4.16	0.34	4.04
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	20	4.16	0.34	4.04
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	20	4.16	0.07	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	20	4.16	0.07	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	20	4.16	0.07	4.19
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	20	4.15	0.35	4.2
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	20	4.15	0.16	4.1
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	20	4.14	0.76	3.8
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	20	4.14	0.76	3.8
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	20	4.14	0.76	3.8
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	20	4.14	0.76	3.8
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	20	4.13	0.18	4.1
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	20	4.13	0.18	4.1
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	20	4.11	0.2	4.13
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	4.11	0.94	3.7
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	20	4.11	0.94	3.7
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	4.11	0.94	3.7
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	20	4.11	0.26	4.08
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	20	4.09	0.35	4.15
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	20	4.06	0.15	4.1
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	20	4.05	0.96	4.14
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	20	4.05	0.96	4.14
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	20	4.05	0.96	4.14
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	20	4.05	0.96	4.14
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	20	4.04	1.03	3.7
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	20	4.04	1.03	3.7
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	20	4.04	1.03	3.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	20	4.04	0.73	4.06
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	20	4.02	0.06	4.02
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	20	4.02	0.06	4.02
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	20	4.02	0.06	4.02
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	20	4.02	0.16	4.02
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	20	4.02	0.16	4.02
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	20	4.01	0.52	3.98
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	20	4.01	0.52	3.98
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	20	4.01	0.52	3.98
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	20	4.01	0.52	3.98
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	20	4.01	0.52	3.98
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	20	4.01	0.52	3.98
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	20	4.0	0.19	4.0
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	20	4.0	0.19	4.0
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	20	4.0	0.19	4.0
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	20	3.99	0.63	4.26
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	20	3.99	0.63	4.26
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	20	3.99	0.27	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	20	3.99	0.27	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	20	3.99	0.27	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	20	3.99	0.27	4.1
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	20	3.99	0.45	3.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	20	3.99	0.45	3.87
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	20	3.98	0.1	3.95
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	20	3.96	0.12	3.97
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	20	3.96	0.12	3.97
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	20	3.96	0.12	3.97
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	20	3.96	0.12	3.97
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	3.94	0.87	3.53
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	3.94	0.87	3.53
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	3.94	0.87	3.53
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	20	3.94	0.11	3.98
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	20	3.92	0.31	3.95
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	20	3.92	0.31	3.95
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	20	3.88	0.08	3.9
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	20	3.88	0.08	3.9
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	20	3.88	0.08	3.9
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	20	3.87	0.44	3.85
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	3.87	0.62	3.6
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	20	3.87	0.62	3.6
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	3.87	0.62	3.6
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	20	3.86	0.63	3.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	20	3.86	0.63	3.8
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.85	0.14	3.83
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	20	3.85	0.14	3.83
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.85	0.14	3.83
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	20	3.84	0.18	3.82
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	20	3.84	0.18	3.82
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	20	3.84	0.18	3.82
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	20	3.83	1.12	4.14
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	20	3.83	1.12	4.14
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	3.83	0.27	3.88
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	3.83	0.27	3.88
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	3.83	0.27	3.88
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	3.83	0.27	3.88
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	3.83	0.27	3.88
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	3.83	0.27	3.88
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.81	0.08	3.8
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.81	0.08	3.8
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.81	0.08	3.8
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	20	3.81	0.08	3.8
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.81	0.08	3.8
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.81	0.08	3.8
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.81	0.08	3.8
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	20	3.81	0.66	3.53
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	20	3.79	0.48	3.66
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	20	3.79	0.48	3.66
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	3.79	0.48	3.66
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	20	3.77	0.47	3.68
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	20	3.75	0.27	3.68
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	3.75	0.23	3.84
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	3.75	0.23	3.84
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	3.75	0.23	3.84
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	3.75	0.23	3.84
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.74	0.07	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	20	3.74	0.07	3.74
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	20	3.71	1.01	3.57
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	20	3.71	1.01	3.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	20	3.71	1.01	3.57
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	20	3.71	1.01	3.57
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	20	3.7	0.05	3.7
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	20	3.7	0.41	3.62
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	20	3.69	1.05	3.49
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	20	3.69	0.41	3.8
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	20	3.69	0.41	3.8
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	20	3.69	0.18	3.73
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	20	3.69	0.18	3.73
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	20	3.66	0.16	3.65
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	20	3.66	0.16	3.65
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	20	3.62	0.12	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	20	3.62	0.12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	20	3.62	0.12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.62	0.12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	20	3.62	0.12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.62	0.12	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	20	3.6	0.02	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	20	3.6	0.02	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	20	3.6	0.02	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	20	3.6	0.02	3.6
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	20	3.59	0.87	3.23
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	20	3.59	0.12	3.54
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	20	3.59	0.12	3.54
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	20	3.58	0.47	3.68
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	20	3.58	0.47	3.68
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	20	3.58	0.47	3.68
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	20	3.58	0.47	3.68
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	20	3.56	0.04	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	20	3.56	0.04	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	20	3.56	0.04	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	20	3.56	0.04	3.56
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	20	3.54	0.84	3.42
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	20	3.54	0.84	3.42
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	3.54	0.84	3.42
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	20	3.54	0.84	3.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	20	3.54	0.84	3.42
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	20	3.54	0.84	3.42
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	20	3.54	0.84	3.42
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	20	3.54	0.84	3.42
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	20	3.44	0.36	3.48
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	20	3.44	0.36	3.48
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	20	3.44	0.84	3.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	20	3.44	0.84	3.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	20	3.44	0.84	3.43
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	20	3.44	0.05	3.45
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	20	3.43	0.4	3.39
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	20	3.43	0.4	3.39
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	20	3.41	0.08	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	20	3.41	0.08	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	20	3.41	0.08	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	20	3.41	0.08	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	20	3.41	0.08	3.44
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	20	3.41	0.08	3.44
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	20	3.4	0.56	3.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	20	3.4	0.56	3.71
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	20	3.33	0.07	3.34
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	20	3.33	0.07	3.34
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	20	3.32	0.22	3.38
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	20	3.32	0.22	3.38
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	20	3.32	0.59	3.59
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	20	3.32	0.59	3.59
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	20	3.25	0.5	3.32
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	20	3.21	0.87	3.04
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	20	3.21	0.87	3.04
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	20	3.21	0.87	3.04
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	20	3.21	0.87	3.04
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	20	3.21	0.65	3.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	20	3.21	0.65	3.51
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	20	3.21	0.65	3.51
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	20	3.21	0.65	3.51
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	20	3.16	0.13	3.16
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	20	3.11	0.52	3.43
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	20	3.09	0.37	3.11
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	20	3.09	0.37	3.11
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	20	3.09	0.37	3.11
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	20	3.07	0.77	3.08
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	20	3.07	0.77	3.08
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	20	3.07	0.77	3.08
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	20	3.03	0.06	3.04
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	20	2.95	0.4	3.01
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	20	2.95	0.4	3.01
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	20	2.95	0.4	3.01
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	20	2.95	0.4	3.01
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	20	2.79	0.3	2.72
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	20	2.77	0.24	2.78
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	20	2.75	0.25	2.87
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	20	2.75	0.48	2.78
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	20	2.75	0.48	2.78
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	20	2.75	0.48	2.78
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	20	2.72	0.27	2.56
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	20	2.62	0.33	2.45
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	20	2.62	0.33	2.45
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	20	2.58	0.36	2.48
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	20	2.58	0.36	2.48
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	2.56	0.28	2.44
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	2.56	0.28	2.44
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	20	2.49	0.25	2.41
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	20	2.49	0.25	2.41
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	20	2.49	0.17	2.42
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	20	2.49	0.17	2.42
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	20	2.49	0.04	2.47
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	20	2.48	0.17	2.42
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	20	2.48	0.17	2.42
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	20	2.48	0.04	2.47
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	2.48	0.8	2.06
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	2.48	0.8	2.06
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	2.48	0.8	2.06
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	2.48	0.8	2.06
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.46	0.29	2.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.46	0.29	2.46
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.45	0.15	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	20	2.45	0.15	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	20	2.45	0.15	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	20	2.45	0.15	2.49
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	20	2.36	0.03	2.36
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	20	2.36	0.03	2.36
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	20	2.36	0.3	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.36	0.3	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.36	0.3	2.3
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	20	2.35	0.21	2.32
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	20	2.35	0.21	2.32
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	20	2.35	0.21	2.32
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	20	2.35	0.21	2.32
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	20	2.33	0.18	2.34
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	20	2.33	0.18	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	20	2.33	0.18	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	20	2.33	0.18	2.34
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	2.28	0.25	2.17
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	2.28	0.25	2.17
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	2.28	0.25	2.17
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	2.28	0.25	2.17
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	20	2.26	0.21	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	20	2.26	0.21	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	20	2.26	0.21	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	20	2.26	0.21	2.18
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	20	2.25	0.05	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	20	2.25	0.05	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	20	2.25	0.05	2.27
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	20	2.24	0.22	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	20	2.24	0.22	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	20	2.24	0.22	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	20	2.24	0.22	2.14
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	20	2.23	0.08	2.26
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	20	2.23	0.08	2.26
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	20	2.23	0.08	2.26
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	20	2.21	0.24	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.21	0.24	2.13
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	20	2.21	0.24	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.21	0.24	2.13
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	20	2.12	0.14	2.12
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	20	2.12	0.14	2.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	20	2.09	0.21	1.98
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	20	2.09	0.21	1.98
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	20	1.99	0.09	2.0
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	20	1.88	0.62	1.98
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	20	1.04	0.04	1.04
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	20	1.04	0.04	1.04
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	20	1.04	0.04	1.04
(1,736)	1:11:A:THR:HG21	1:62:A:SER:HB2	20	1.04	0.04	1.04
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	20	0.96	0.26	1.0
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	20	0.96	0.26	1.0
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	20	0.96	0.26	1.0
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	20	0.96	0.26	1.0
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	20	0.82	0.27	0.84
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	20	0.57	0.18	0.6
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	20	0.57	0.18	0.6
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	20	0.44	0.16	0.42
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	19	1.04	0.46	1.15
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	19	1.04	0.46	1.15
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	19	1.04	0.46	1.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	19	0.97	0.7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	19	0.97	0.7	0.75
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	19	0.49	0.21	0.47
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	19	0.49	0.18	0.49
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	19	0.49	0.18	0.49
(1,443)	1:6:A:LYS:H	1:10:A:CYS:HB2	19	0.49	0.18	0.49
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB3	19	0.49	0.18	0.49
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	19	0.48	0.18	0.53
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	19	0.48	0.18	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	18	1.74	0.68	2.04
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG23	18	1.74	0.68	2.04
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG22	18	1.74	0.68	2.04
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG21	18	1.74	0.68	2.04
(1,884)	1:32:A:THR:HG23	1:37:A:LYS:HE2	18	1.74	0.68	2.04
(1,884)	1:32:A:THR:HG22	1:37:A:LYS:HE2	18	1.74	0.68	2.04
(1,884)	1:32:A:THR:HG21	1:37:A:LYS:HE3	18	1.74	0.68	2.04
(1,884)	1:32:A:THR:HG21	1:37:A:LYS:HE2	18	1.74	0.68	2.04
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	18	1.4	0.59	1.39
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	18	1.4	0.59	1.39
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	18	1.4	0.59	1.39
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	18	0.94	0.61	0.84
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	18	0.94	0.61	0.84
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	18	0.94	0.61	0.84
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	18	0.94	0.61	0.84
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	18	0.15	0.03	0.15
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	18	0.15	0.03	0.15
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	17	0.92	0.35	0.88
(1,896)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	17	0.92	0.35	0.88
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	17	0.89	0.16	0.89
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	17	0.89	0.16	0.89
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	17	0.89	0.16	0.89
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	17	0.51	0.31	0.62
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.51	0.31	0.62
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	17	0.35	0.08	0.33
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	17	0.35	0.08	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	17	0.35	0.08	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	17	0.35	0.08	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	17	0.35	0.08	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	17	0.35	0.08	0.33
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	16	1.47	1.04	1.46
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	16	1.11	0.31	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	16	1.11	0.31	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	16	1.11	0.31	1.07
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	16	1.11	0.31	1.07
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	16	1.11	0.31	1.07
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	16	0.78	0.3	0.81
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	16	0.69	0.33	0.62
(1,897)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	16	0.69	0.33	0.62
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	16	0.61	0.18	0.66
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	16	0.61	0.18	0.66
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	16	0.61	0.18	0.66

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	16	0.55	0.2	0.57
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	16	0.55	0.2	0.57
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	16	0.52	0.33	0.48
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	16	0.52	0.33	0.48
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	16	0.52	0.33	0.48
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	16	0.52	0.33	0.48
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	16	0.52	0.17	0.57
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB2	16	0.52	0.17	0.57
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	15	1.42	0.75	1.33
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	15	0.63	0.4	0.63
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	15	0.58	0.27	0.58
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	15	0.58	0.27	0.58
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	15	0.58	0.27	0.58
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	15	0.55	0.19	0.57
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	15	0.55	0.19	0.57
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG2	15	0.55	0.19	0.57
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB1	15	0.55	0.19	0.57
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	15	0.39	0.26	0.3
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	15	0.24	0.06	0.25
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	14	1.72	1.6	1.25
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	14	1.72	1.6	1.25
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	14	1.72	1.6	1.25
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	14	1.72	1.6	1.25
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	14	1.47	0.98	1.53
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	14	1.47	0.98	1.53
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	14	1.3	1.02	1.2
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	14	1.3	1.02	1.2
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	14	1.3	1.02	1.2
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	14	1.3	1.02	1.2
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	14	0.9	0.25	0.84
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	14	0.9	0.25	0.84
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	14	0.23	0.08	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	14	0.23	0.08	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	14	0.23	0.08	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	14	0.23	0.08	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	14	0.23	0.08	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	14	0.23	0.08	0.23
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	13	1.37	0.56	1.27
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	13	1.37	0.56	1.27
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	13	1.37	0.56	1.27
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	13	1.37	0.56	1.27
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	13	1.37	0.56	1.27
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	13	1.37	0.56	1.27
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	13	0.97	0.5	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	13	0.97	0.5	0.76
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	13	0.87	0.57	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	13	0.87	0.57	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	13	0.87	0.57	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	13	0.87	0.57	0.69
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	13	0.68	0.37	0.57
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	13	0.54	0.33	0.59
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	13	0.54	0.33	0.59
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	13	0.54	0.33	0.59
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	13	0.54	0.33	0.59
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	12	1.22	0.49	1.21
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	12	1.22	0.49	1.21
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	12	1.22	0.49	1.21
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	12	0.65	0.26	0.66
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	12	0.65	0.26	0.66
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	12	0.65	0.26	0.66
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	12	0.65	0.3	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	12	0.5	0.18	0.54
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	12	0.5	0.18	0.54
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	12	0.46	0.21	0.42
(1,143)	1:28:A:GLY:H	1:61:A:GLY:HA3	12	0.46	0.21	0.42
(1,143)	1:28:A:GLY:H	1:61:A:GLY:HA2	12	0.46	0.21	0.42
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	12	0.35	0.21	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	12	0.35	0.21	0.3
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	12	0.3	0.27	0.15
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	12	0.3	0.27	0.15
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	12	0.29	0.06	0.3
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	12	0.29	0.06	0.3
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	12	0.29	0.06	0.3
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	12	0.24	0.09	0.26
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	12	0.24	0.09	0.26
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	12	0.24	0.09	0.26
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	12	0.24	0.09	0.26
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	12	0.24	0.09	0.26
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	12	0.24	0.09	0.26
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	12	0.17	0.04	0.18
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	12	0.17	0.04	0.18
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	11	1.77	0.73	1.81
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	11	1.77	0.73	1.81
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	11	0.97	0.4	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	11	0.97	0.4	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	11	0.97	0.4	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	11	0.97	0.4	1.17
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	11	0.95	0.6	0.93
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	11	0.66	0.38	0.68
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.51	0.17	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	11	0.51	0.17	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.51	0.17	0.47
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	11	0.5	0.36	0.34
(1,687)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	11	0.31	0.14	0.24
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	11	0.31	0.14	0.24
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	11	0.3	0.1	0.28
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	11	0.23	0.03	0.24
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	11	0.23	0.03	0.24
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	10	1.18	0.43	1.16
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	10	1.18	0.43	1.16
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	10	1.18	0.43	1.16
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	10	0.91	0.52	0.78
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	10	0.82	0.2	0.78
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	10	0.82	0.2	0.78
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	10	0.82	0.2	0.78
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	10	0.82	0.2	0.78
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	10	0.73	0.55	0.66
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	10	0.73	0.55	0.66
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	10	0.73	0.55	0.66
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	10	0.7	0.5	0.58
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	10	0.7	0.5	0.58
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	10	0.63	0.32	0.69
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	10	0.63	0.32	0.69
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	10	0.5	0.03	0.5
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	10	0.5	0.03	0.5
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	10	0.5	0.03	0.5
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	10	0.45	0.3	0.37
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	10	0.45	0.3	0.37
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	10	0.45	0.3	0.37
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	10	0.37	0.14	0.38
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	10	0.37	0.14	0.38
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	10	0.37	0.14	0.38
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	10	0.37	0.18	0.34
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	10	0.37	0.18	0.34
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	10	0.35	0.11	0.32
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	10	0.35	0.11	0.32
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	10	0.34	0.18	0.32
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	10	0.34	0.18	0.32
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	10	0.34	0.18	0.32
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	10	0.34	0.18	0.32
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	10	0.34	0.11	0.29
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	10	0.34	0.11	0.29
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	10	0.34	0.11	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	10	0.34	0.11	0.29
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	10	0.33	0.15	0.32
(1,730)	1:6:A:LYS:HD3	1:33:A:CYS:HA	10	0.32	0.13	0.34
(1,730)	1:6:A:LYS:HD2	1:33:A:CYS:HA	10	0.32	0.13	0.34
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD3	10	0.32	0.13	0.34
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD2	10	0.32	0.13	0.34
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	10	0.3	0.19	0.26
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	10	0.23	0.07	0.24
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG21	10	0.22	0.08	0.22
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG22	10	0.22	0.08	0.22
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG23	10	0.22	0.08	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG21	10	0.22	0.08	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG22	10	0.22	0.08	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG23	10	0.22	0.08	0.22
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	0.16	0.04	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	0.16	0.04	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	10	0.16	0.04	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	10	0.16	0.04	0.16
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	10	0.14	0.02	0.14
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	10	0.12	0.02	0.12
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	10	0.12	0.02	0.12
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	10	0.12	0.02	0.12
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	9	1.03	0.53	1.02
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	9	0.69	0.08	0.7
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	9	0.69	0.08	0.7
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	9	0.63	0.39	0.57
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	9	0.63	0.39	0.57
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	9	0.63	0.39	0.57
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	9	0.58	0.27	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	9	0.58	0.27	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	9	0.58	0.27	0.58
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	9	0.5	0.13	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	9	0.5	0.13	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	9	0.5	0.13	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	9	0.5	0.13	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	9	0.5	0.13	0.54
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	9	0.49	0.18	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	9	0.49	0.18	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	9	0.49	0.18	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	9	0.49	0.18	0.49
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	9	0.4	0.06	0.4
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	9	0.4	0.06	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	9	0.37	0.24	0.26
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	9	0.37	0.24	0.26
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	9	0.37	0.24	0.26
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	9	0.37	0.24	0.26
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	9	0.32	0.12	0.34
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	9	0.32	0.12	0.34
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	9	0.31	0.08	0.34
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE3	9	0.31	0.08	0.34
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	1.15	0.64	1.12
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	8	1.15	0.64	1.12
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	8	0.66	0.47	0.61
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	8	0.66	0.47	0.61
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	8	0.66	0.47	0.61
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	8	0.66	0.47	0.61
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	8	0.56	0.11	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	8	0.56	0.11	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	8	0.56	0.11	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	8	0.56	0.11	0.53
(1,358)	1:32:A:THR:H	1:37:A:LYS:HD2	8	0.5	0.17	0.52
(1,358)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.5	0.17	0.52
(1,358)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.5	0.17	0.52
(1,358)	1:32:A:THR:H	1:37:A:LYS:HD3	8	0.5	0.17	0.52
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	8	0.49	0.2	0.43
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	8	0.49	0.2	0.43
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	8	0.46	0.23	0.38
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	8	0.46	0.23	0.38
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	8	0.46	0.23	0.38
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	8	0.46	0.23	0.38
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	8	0.46	0.26	0.42
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	8	0.46	0.26	0.42
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	8	0.46	0.26	0.42
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	8	0.43	0.23	0.34
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	8	0.43	0.23	0.34
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	8	0.43	0.23	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	8	0.27	0.16	0.22
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	8	0.16	0.03	0.16
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	8	0.16	0.03	0.16
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	8	0.11	0.0	0.11
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	7	1.01	0.04	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	7	1.01	0.04	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	7	1.01	0.04	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	7	1.01	0.04	1.0
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	7	0.93	0.68	1.48
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	7	0.62	0.18	0.6
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	7	0.62	0.18	0.6
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	7	0.62	0.18	0.6
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	7	0.62	0.18	0.6
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	7	0.55	0.3	0.51
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	7	0.52	0.23	0.54
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	7	0.52	0.23	0.54
(1,837)	1:42:A:THR:HG23	1:54:A:GLY:HA2	7	0.5	0.41	0.39
(1,837)	1:42:A:THR:HG21	1:54:A:GLY:HA2	7	0.5	0.41	0.39
(1,837)	1:42:A:THR:HG22	1:54:A:GLY:HA2	7	0.5	0.41	0.39
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	7	0.48	0.3	0.51
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	7	0.48	0.3	0.51
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	7	0.48	0.3	0.51
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	7	0.48	0.3	0.51
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	7	0.48	0.3	0.51
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	7	0.48	0.3	0.51
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	7	0.47	0.18	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	7	0.47	0.18	0.53
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	7	0.43	0.13	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	7	0.43	0.38	0.24
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	7	0.42	0.24	0.38
(1,287)	1:58:A:CYS:H	1:59:A:LYS:HG3	7	0.37	0.19	0.43
(1,287)	1:58:A:CYS:H	1:59:A:LYS:HG2	7	0.37	0.19	0.43
(1,287)	1:37:A:LYS:HG2	1:58:A:CYS:H	7	0.37	0.19	0.43
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	7	0.27	0.08	0.32
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	7	0.27	0.08	0.32
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	7	0.27	0.08	0.32
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	7	0.26	0.12	0.29
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	7	0.26	0.12	0.29
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	7	0.26	0.12	0.29
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	7	0.25	0.0	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	7	0.25	0.0	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	7	0.25	0.0	0.25
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	7	0.24	0.11	0.19
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	7	0.24	0.11	0.19
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	7	0.23	0.08	0.19
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	7	0.23	0.08	0.19
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	7	0.2	0.09	0.15
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	7	0.18	0.06	0.15
(1,952)	1:14:A:CYS:HA	1:36:A:CYS:HB2	7	0.18	0.06	0.15
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	7	0.15	0.05	0.12
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	7	0.15	0.05	0.12
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	7	0.12	0.01	0.12
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	7	0.12	0.01	0.12
(1,865)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	6	0.86	0.28	0.86
(1,865)	1:6:A:LYS:HG2	1:15:A:ARG:HA	6	0.86	0.28	0.86
(1,865)	1:6:A:LYS:HG3	1:15:A:ARG:HA	6	0.86	0.28	0.86
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	6	0.85	0.52	1.06
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	6	0.85	0.52	1.06
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	6	0.85	0.52	1.06
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	6	0.84	0.29	1.0
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	6	0.84	0.29	1.0
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	6	0.84	0.29	1.0
(1,425)	1:9:A:LYS:HB2	1:31:A:CYS:HA	6	0.7	0.43	0.62
(1,425)	1:31:A:CYS:HA	1:37:A:LYS:HD2	6	0.7	0.43	0.62
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	6	0.68	0.17	0.76
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	6	0.68	0.17	0.76
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	6	0.68	0.17	0.76
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	6	0.68	0.17	0.76
(1,923)	1:9:A:LYS:HB2	1:29:A:GLU:H	6	0.64	0.28	0.68
(1,923)	1:9:A:LYS:HD2	1:29:A:GLU:H	6	0.64	0.28	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	6	0.58	0.23	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	6	0.58	0.23	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	6	0.58	0.23	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	6	0.58	0.23	0.62
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	6	0.54	0.17	0.54
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	6	0.54	0.17	0.54
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	6	0.54	0.17	0.54
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	6	0.3	0.25	0.15
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	6	0.26	0.1	0.25
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	6	0.26	0.1	0.25
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	6	0.26	0.1	0.25
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	6	0.25	0.09	0.25
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	6	0.25	0.09	0.25
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	6	0.25	0.14	0.22
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	6	0.25	0.14	0.22
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	6	0.23	0.02	0.22
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	6	0.23	0.02	0.22
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	6	0.19	0.09	0.16
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	6	0.19	0.09	0.16
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	6	0.19	0.09	0.16
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	6	0.19	0.09	0.16
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	6	0.17	0.05	0.17
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	6	0.17	0.05	0.17
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	5	1.31	0.55	1.54
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG2	5	1.31	0.55	1.54
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	5	1.31	0.55	1.54
(4,619)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	5	1.11	0.37	1.01
(4,451)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	1.08	0.85	1.2
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	5	1.0	0.38	1.07
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	5	1.0	0.38	1.07
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	5	1.0	0.38	1.07
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	5	1.0	0.38	1.07
(1,744)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	5	0.89	0.12	0.88
(1,744)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	5	0.89	0.12	0.88
(1,744)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	5	0.89	0.12	0.88
(1,744)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	5	0.89	0.12	0.88
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	5	0.53	0.17	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	5	0.53	0.17	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	5	0.53	0.17	0.65
(1,418)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	5	0.53	0.31	0.4
(1,418)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	5	0.53	0.31	0.4
(1,418)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	5	0.53	0.31	0.4
(1,988)	1:6:A:LYS:HE2	1:15:A:ARG:HA	5	0.51	0.23	0.57
(1,988)	1:6:A:LYS:HE3	1:15:A:ARG:HA	5	0.51	0.23	0.57
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	5	0.51	0.23	0.57
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	5	0.51	0.23	0.57
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	5	0.51	0.23	0.57
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	5	0.51	0.23	0.57
(4,341)	1:50:A:LYS:HB3	1:52:A:CYS:H	5	0.5	0.15	0.53
(4,341)	1:50:A:LYS:HB2	1:52:A:CYS:H	5	0.5	0.15	0.53
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	5	0.49	0.3	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	5	0.49	0.3	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	5	0.49	0.3	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	5	0.49	0.3	0.41
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.44	0.2	0.45
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG2	5	0.44	0.2	0.45
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.44	0.2	0.45
(4,866)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	5	0.39	0.17	0.46
(4,79)	1:45:A:GLY:HA3	1:46:A:CYS:H	5	0.38	0.01	0.38
(4,79)	1:45:A:GLY:HA2	1:46:A:CYS:H	5	0.38	0.01	0.38
(1,883)	1:9:A:LYS:HA	1:9:A:LYS:HE3	5	0.28	0.07	0.29
(1,883)	1:9:A:LYS:HA	1:9:A:LYS:HE2	5	0.28	0.07	0.29
(1,883)	1:32:A:THR:HA	1:37:A:LYS:HE2	5	0.28	0.07	0.29
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	5	0.26	0.0	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB2	5	0.26	0.0	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	5	0.26	0.0	0.26
(1,497)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	5	0.19	0.04	0.19
(1,497)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	5	0.19	0.04	0.19
(1,185)	1:42:A:THR:HG21	1:45:A:GLY:H	5	0.16	0.02	0.15
(1,185)	1:42:A:THR:HG22	1:45:A:GLY:H	5	0.16	0.02	0.15
(1,185)	1:42:A:THR:HG23	1:45:A:GLY:H	5	0.16	0.02	0.15
(4,202)	1:42:A:THR:HG21	1:45:A:GLY:H	5	0.16	0.02	0.15
(4,202)	1:42:A:THR:HG22	1:45:A:GLY:H	5	0.16	0.02	0.15
(4,202)	1:42:A:THR:HG23	1:45:A:GLY:H	5	0.16	0.02	0.15
(1,35)	1:42:A:THR:H	1:54:A:GLY:H	5	0.14	0.01	0.14
(4,37)	1:42:A:THR:H	1:54:A:GLY:H	5	0.14	0.01	0.14
(1,766)	1:39:A:CYS:HB3	1:55:A:PRO:HD2	5	0.13	0.01	0.13
(1,117)	1:11:A:THR:H	1:28:A:GLY:H	5	0.12	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,128)	1:11:A:THR:H	1:28:A:GLY:H	5	0.12	0.02	0.13
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	4	1.35	0.51	1.59
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	4	1.35	0.51	1.59
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	4	1.35	0.51	1.59
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	4	1.08	0.19	1.1
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG2	4	1.08	0.19	1.1
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	4	1.08	0.19	1.1
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	4	0.4	0.07	0.42
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	4	0.4	0.07	0.42
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	4	0.4	0.07	0.42
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB2	4	0.37	0.19	0.37
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB3	4	0.37	0.19	0.37
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	4	0.32	0.09	0.29
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	4	0.32	0.09	0.29
(4,806)	1:62:A:SER:HA	1:64:A:CYS:HB2	4	0.29	0.06	0.3
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	4	0.27	0.09	0.29
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	4	0.27	0.09	0.29
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	4	0.27	0.09	0.29
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	4	0.27	0.09	0.29
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	4	0.21	0.06	0.2
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG2	4	0.21	0.06	0.2
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	4	0.21	0.06	0.2
(1,179)	1:19:A:CYS:H	1:21:A:CYS:H	4	0.2	0.05	0.18
(4,709)	1:14:A:CYS:H	1:15:A:ARG:HG2	4	0.18	0.06	0.18
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG2	4	0.17	0.03	0.18
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG3	4	0.17	0.03	0.18
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG3	4	0.17	0.03	0.18
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG2	4	0.17	0.03	0.18
(1,161)	1:31:A:CYS:H	1:32:A:THR:HB	4	0.16	0.06	0.13
(4,173)	1:31:A:CYS:H	1:32:A:THR:HB	4	0.16	0.06	0.13
(4,279)	1:39:A:CYS:HA	1:40:A:ASN:HD22	4	0.14	0.02	0.14
(1,595)	1:21:A:CYS:H	1:36:A:CYS:HB2	4	0.13	0.01	0.14
(4,686)	1:21:A:CYS:H	1:36:A:CYS:HB2	4	0.13	0.01	0.14
(1,140)	1:41:A:CYS:H	1:66:A:CYS:HA	4	0.12	0.01	0.12
(4,150)	1:41:A:CYS:H	1:66:A:CYS:HA	4	0.12	0.01	0.12
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG2	3	0.69	0.4	0.96
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG3	3	0.69	0.4	0.96
(1,229)	1:9:A:LYS:HE2	1:29:A:GLU:H	3	0.57	0.09	0.64
(1,229)	1:9:A:LYS:HE3	1:29:A:GLU:H	3	0.57	0.09	0.64
(1,930)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	3	0.52	0.24	0.62
(1,930)	1:8:A:GLU:HA	1:9:A:LYS:HG2	3	0.52	0.24	0.62
(1,930)	1:6:A:LYS:HG3	1:15:A:ARG:HA	3	0.52	0.24	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	3	0.46	0.08	0.42
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	3	0.46	0.08	0.42
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	3	0.46	0.08	0.42
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	3	0.46	0.08	0.42
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA3	3	0.43	0.2	0.41
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA2	3	0.43	0.2	0.41
(4,116)	1:22:A:GLY:H	1:36:A:CYS:HB3	3	0.38	0.25	0.29
(4,899)	1:42:A:THR:HB	1:53:A:THR:HB	3	0.36	0.16	0.25
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	3	0.34	0.17	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	3	0.34	0.17	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	3	0.34	0.17	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	3	0.34	0.17	0.31
(1,843)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	3	0.32	0.1	0.3
(4,980)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	3	0.32	0.1	0.3
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	3	0.28	0.16	0.23
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	3	0.28	0.16	0.23
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	3	0.28	0.16	0.23
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	3	0.28	0.16	0.23
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	3	0.27	0.09	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	3	0.27	0.09	0.31
(4,1114)	1:22:A:GLY:HA3	1:25:A:CYS:HB2	3	0.27	0.09	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	3	0.27	0.09	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB3	3	0.27	0.09	0.31
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	3	0.23	0.08	0.24
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	3	0.23	0.08	0.24
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	3	0.23	0.08	0.24
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	3	0.23	0.08	0.24
(1,971)	1:16:A:SER:HB2	1:17:A:GLU:H	3	0.17	0.04	0.18
(1,971)	1:16:A:SER:HB3	1:17:A:GLU:H	3	0.17	0.04	0.18
(4,1182)	1:16:A:SER:HB2	1:17:A:GLU:H	3	0.17	0.04	0.18
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	3	0.17	0.04	0.18
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	3	0.17	0.04	0.18
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	3	0.16	0.05	0.17
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	3	0.16	0.05	0.17
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	3	0.15	0.05	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	3	0.15	0.05	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	3	0.15	0.05	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	3	0.15	0.05	0.12
(1,715)	1:19:A:CYS:HB2	1:35:A:ALA:HA	3	0.15	0.02	0.14
(1,910)	1:21:A:CYS:HB3	1:25:A:CYS:H	3	0.14	0.01	0.13
(4,1096)	1:21:A:CYS:HB3	1:25:A:CYS:H	3	0.14	0.01	0.13
(1,110)	1:11:A:THR:H	1:12:A:SER:HA	3	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,121)	1:11:A:THR:H	1:12:A:SER:HA	3	0.13	0.02	0.12
(1,134)	1:41:A:CYS:H	1:54:A:GLY:HA2	3	0.12	0.01	0.12
(4,144)	1:41:A:CYS:H	1:54:A:GLY:HA2	3	0.12	0.01	0.12
(1,282)	1:55:A:PRO:HA	1:58:A:CYS:H	3	0.12	0.01	0.11
(4,311)	1:55:A:PRO:HA	1:58:A:CYS:H	3	0.12	0.01	0.11
(4,590)	1:64:A:CYS:H	1:67:A:LYS:HE2	2	1.22	0.09	1.22
(4,590)	1:64:A:CYS:H	1:67:A:LYS:HE3	2	1.22	0.09	1.22
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	2	0.81	0.27	0.81
(4,1176)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	2	0.81	0.27	0.81
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	2	0.81	0.27	0.81
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	2	0.81	0.27	0.81
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG3	2	0.81	0.27	0.81
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	2	0.76	0.26	0.76
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	2	0.76	0.26	0.76
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE3	2	0.76	0.26	0.76
(4,1029)	1:25:A:CYS:HB3	1:26:A:GLN:HG2	2	0.72	0.04	0.72
(4,1029)	1:25:A:CYS:HB3	1:26:A:GLN:HG3	2	0.72	0.04	0.72
(1,668)	1:25:A:CYS:HA	1:26:A:GLN:HG3	2	0.65	0.03	0.65
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB2	2	0.64	0.31	0.64
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB2	2	0.64	0.31	0.64
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB3	2	0.64	0.31	0.64
(4,103)	1:31:A:CYS:H	1:33:A:CYS:H	2	0.62	0.38	0.62
(4,881)	1:38:A:THR:H	1:38:A:THR:HG21	2	0.56	0.07	0.56
(4,881)	1:38:A:THR:H	1:38:A:THR:HG22	2	0.56	0.07	0.56
(4,881)	1:38:A:THR:H	1:38:A:THR:HG23	2	0.56	0.07	0.56
(4,595)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	2	0.55	0.04	0.55
(4,595)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	0.55	0.04	0.55
(4,595)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	0.55	0.04	0.55
(4,595)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	2	0.55	0.04	0.55
(1,748)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	2	0.55	0.32	0.55
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	2	0.55	0.32	0.55
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA2	2	0.55	0.32	0.55
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	2	0.55	0.32	0.55
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA2	2	0.55	0.32	0.55
(4,217)	1:7:A:GLY:HA2	1:10:A:CYS:H	2	0.52	0.37	0.52
(1,821)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	2	0.51	0.05	0.51
(1,821)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	2	0.51	0.05	0.51
(1,874)	1:23:A:SER:HB2	1:24:A:LYS:HB2	2	0.5	0.29	0.5
(1,163)	1:31:A:CYS:H	1:37:A:LYS:HD2	2	0.5	0.16	0.5
(1,974)	1:49:A:GLY:HA3	1:50:A:LYS:HD3	2	0.47	0.24	0.47
(1,974)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	2	0.47	0.24	0.47
(1,968)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	2	0.44	0.21	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,968)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	2	0.44	0.21	0.44
(4,584)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	2	0.38	0.05	0.38
(1,969)	1:12:A:SER:HA	1:15:A:ARG:HD2	2	0.37	0.0	0.37
(1,969)	1:12:A:SER:HA	1:15:A:ARG:HD3	2	0.37	0.0	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD2	2	0.37	0.0	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD3	2	0.37	0.0	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD2	2	0.37	0.0	0.37
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB3	2	0.36	0.07	0.36
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB2	2	0.36	0.07	0.36
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB3	2	0.36	0.07	0.36
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB2	2	0.36	0.07	0.36
(1,407)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	2	0.32	0.04	0.32
(4,954)	1:16:A:SER:HB2	1:20:A:GLN:HE21	2	0.31	0.13	0.31
(4,954)	1:16:A:SER:HB3	1:20:A:GLN:HE21	2	0.31	0.13	0.31
(4,954)	1:16:A:SER:HB2	1:20:A:GLN:HE22	2	0.31	0.13	0.31
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG21	2	0.3	0.02	0.3
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG22	2	0.3	0.02	0.3
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG23	2	0.3	0.02	0.3
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG21	2	0.3	0.02	0.3
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG22	2	0.3	0.02	0.3
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG23	2	0.3	0.02	0.3
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB3	2	0.26	0.14	0.26
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB2	2	0.26	0.14	0.26
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB3	2	0.26	0.14	0.26
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB2	2	0.26	0.14	0.26
(4,1024)	1:23:A:SER:HB2	1:24:A:LYS:HB2	2	0.26	0.08	0.26
(4,1024)	1:23:A:SER:HB3	1:24:A:LYS:HB2	2	0.26	0.08	0.26
(1,965)	1:37:A:LYS:HG3	1:55:A:PRO:HA	2	0.25	0.09	0.25
(4,399)	1:56:A:ASP:HB3	1:57:A:SER:HA	2	0.22	0.0	0.22
(1,106)	1:22:A:GLY:H	1:36:A:CYS:HB3	2	0.22	0.07	0.22
(4,6)	1:15:A:ARG:HG3	1:16:A:SER:H	2	0.19	0.03	0.19
(4,1115)	1:15:A:ARG:HG3	1:16:A:SER:H	2	0.19	0.03	0.19
(4,80)	1:46:A:CYS:H	1:51:A:GLU:HA	2	0.18	0.03	0.18
(1,232)	1:9:A:LYS:HG2	1:29:A:GLU:H	2	0.16	0.04	0.16
(1,232)	1:9:A:LYS:HG3	1:29:A:GLU:H	2	0.16	0.04	0.16
(4,315)	1:56:A:ASP:HB2	1:58:A:CYS:H	2	0.16	0.01	0.16
(4,315)	1:56:A:ASP:HB2	1:58:A:CYS:H	2	0.16	0.01	0.16
(4,315)	1:56:A:ASP:HB3	1:58:A:CYS:H	2	0.16	0.01	0.16
(4,315)	1:56:A:ASP:HB3	1:58:A:CYS:H	2	0.16	0.01	0.16
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA3	2	0.16	0.06	0.16
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA2	2	0.16	0.06	0.16
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA3	2	0.16	0.06	0.16

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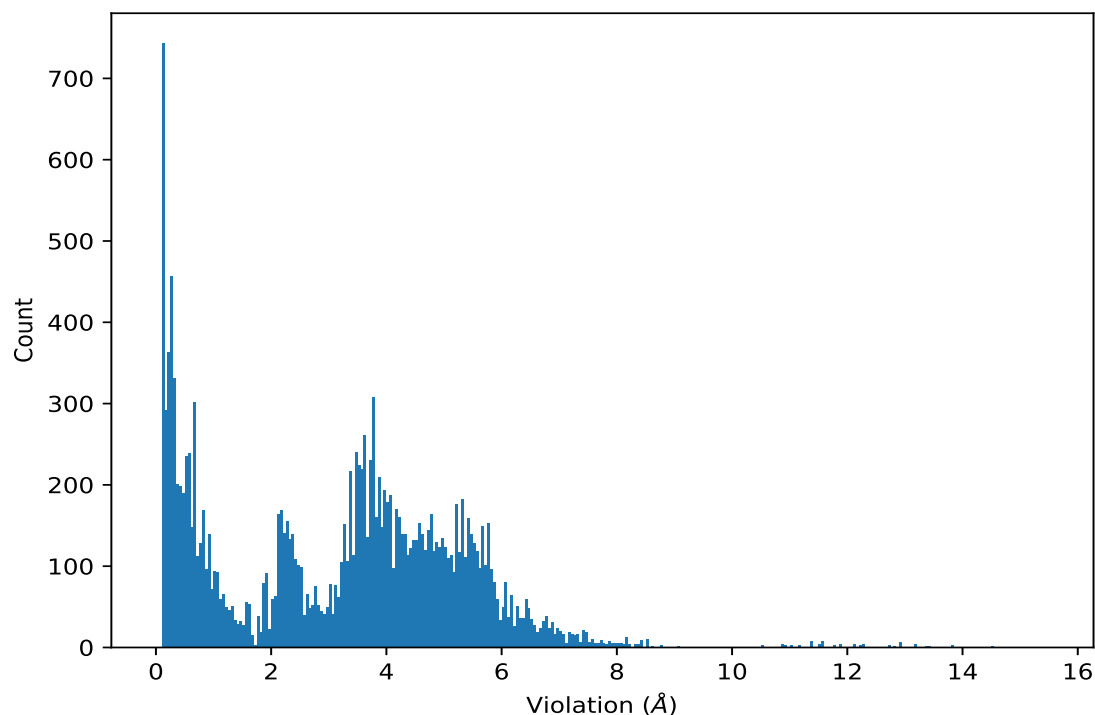
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA2	2	0.16	0.06	0.16
(1,460)	1:11:A:THR:HA	1:26:A:GLN:HB2	2	0.16	0.02	0.16
(4,524)	1:11:A:THR:HA	1:26:A:GLN:HB2	2	0.16	0.02	0.16
(1,331)	1:42:A:THR:H	1:53:A:THR:HA	2	0.16	0.02	0.16
(4,367)	1:42:A:THR:H	1:53:A:THR:HA	2	0.16	0.02	0.16
(1,813)	1:18:A:PRO:HB2	1:19:A:CYS:HB2	2	0.14	0.01	0.14
(1,928)	1:31:A:CYS:H	1:37:A:LYS:HD3	2	0.14	0.02	0.14
(1,928)	1:15:A:ARG:HG3	1:16:A:SER:H	2	0.14	0.02	0.14
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB2	2	0.14	0.01	0.14
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB2	2	0.14	0.01	0.14
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB3	2	0.14	0.01	0.14
(1,24)	1:21:A:CYS:HA	1:25:A:CYS:H	2	0.14	0.02	0.14
(4,26)	1:21:A:CYS:HA	1:25:A:CYS:H	2	0.14	0.02	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD2	2	0.14	0.01	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD3	2	0.14	0.01	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD2	2	0.14	0.01	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD3	2	0.14	0.01	0.14
(1,333)	1:41:A:CYS:HB2	1:42:A:THR:H	2	0.12	0.01	0.12
(1,684)	1:14:A:CYS:HA	1:20:A:GLN:HB2	2	0.12	0.01	0.12
(4,787)	1:14:A:CYS:HA	1:20:A:GLN:HB2	2	0.12	0.01	0.12
(1,390)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	2	0.12	0.01	0.12
(1,390)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	2	0.12	0.01	0.12
(1,963)	1:38:A:THR:HG21	1:67:A:LYS:HA	2	0.12	0.02	0.12
(1,963)	1:38:A:THR:HG22	1:67:A:LYS:HA	2	0.12	0.02	0.12
(1,963)	1:38:A:THR:HG23	1:67:A:LYS:HA	2	0.12	0.02	0.12
(4,1172)	1:38:A:THR:HG21	1:67:A:LYS:HA	2	0.12	0.02	0.12
(4,1172)	1:38:A:THR:HG22	1:67:A:LYS:HA	2	0.12	0.02	0.12
(4,1172)	1:38:A:THR:HG23	1:67:A:LYS:HA	2	0.12	0.02	0.12
(1,50)	1:61:A:GLY:H	1:64:A:CYS:HB3	2	0.11	0.01	0.11
(4,56)	1:61:A:GLY:H	1:64:A:CYS:HB3	2	0.11	0.01	0.11
(1,464)	1:16:A:SER:HA	1:20:A:GLN:HG3	2	0.11	0.0	0.11
(4,528)	1:16:A:SER:HA	1:20:A:GLN:HG3	2	0.11	0.0	0.11
(4,578)	1:16:A:SER:HB3	1:20:A:GLN:HB2	2	0.11	0.0	0.11
(4,578)	1:16:A:SER:HB2	1:20:A:GLN:HB2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	13	15.5
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	10	14.75
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	1	14.51
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	5	14.51
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	8	14.42
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	3	14.06
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	13	14.03
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	13	13.84
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	13	13.84
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	13	13.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	15	13.63
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	19	13.56
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	18	13.5
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	17	13.45
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	14	13.42
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	9	13.38
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	5	13.37
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	4	13.31
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	1	13.24
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	10	13.17
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	10	13.17
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	10	13.17
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	10	13.16
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	20	13.1
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	6	12.95
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	5	12.93
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	5	12.93
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	5	12.93
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	1	12.92
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	1	12.92
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	1	12.92
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	3	12.87
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	2	12.85
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	12	12.81
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	11	12.76
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	3	12.73
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	3	12.73
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	3	12.73
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	8	12.45
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	16	12.29
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	8	12.25
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	8	12.25
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	8	12.25
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	17	12.21
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	17	12.21
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	17	12.21
(4,477)	1:31:A:CYS:HA	1:67:A:LYS:HB3	7	12.13
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	15	12.11
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	15	12.11
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	15	12.11
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	17	12.05
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	14	12.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	15	11.95
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	18	11.88
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	18	11.88
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	18	11.88
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	18	11.86
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	9	11.76
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	9	11.76
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	9	11.76
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	20	11.59
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	20	11.59
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	20	11.59
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	9	11.59
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	14	11.58
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	14	11.58
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	14	11.58
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	20	11.56
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	19	11.54
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	4	11.51
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	4	11.51
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	4	11.51
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	4	11.39
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	6	11.39
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	19	11.37
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	19	11.37
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	19	11.37
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	11	11.36
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	11	11.36
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	11	11.36
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	2	11.22
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	6	11.16
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	6	11.16
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	6	11.16
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	11	11.08
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	16	11.04
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	16	11.04
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	16	11.04
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	2	10.9
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	2	10.9
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	2	10.9
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	7	10.88
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	7	10.88
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	7	10.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	12	10.88
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	7	10.73
(4,177)	1:31:A:CYS:H	1:67:A:LYS:HB3	16	10.69
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	12	10.5
(4,871)	1:30:A:GLY:HA3	1:67:A:LYS:HB3	12	10.5
(4,871)	1:30:A:GLY:HA2	1:67:A:LYS:HB3	12	10.5
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	3	9.17
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	2	9.07
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	2	9.07
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	7	8.95
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	12	8.78
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	17	8.77
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	18	8.75
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	14	8.74
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	5	8.7
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	8	8.64
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	1	8.63
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	2	8.58
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	8	8.53
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	13	8.53
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	13	8.53
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	13	8.53
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	4	8.52
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	8	8.51
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	7	8.51
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	7	8.51
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	7	8.51
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	9	8.51
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	17	8.48
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	6	8.44
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	9	8.43
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	9	8.43
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	9	8.43
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	16	8.42
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	5	8.42
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	5	8.42
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	5	8.42
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	7	8.4
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	4	8.39
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	11	8.38
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	7	8.38
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	9	8.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	17	8.34
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	16	8.33
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	14	8.31
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	7	8.3
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	9	8.24
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	10	8.24
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	6	8.22
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	8	8.22
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	16	8.19
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	17	8.19
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	12	8.18
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	14	8.18
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	4	8.18
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	16	8.17
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	4	8.17
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	1	8.17
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	3	8.15
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	4	8.15
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	3	8.15
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	3	8.15
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	3	8.15
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	12	8.13
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	12	8.13
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	12	8.13
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	10	8.13
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	2	8.09
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	15	8.07
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	3	8.06
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	7	8.06
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	17	8.06
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	3	8.06
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	8	8.03
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	4	8.01
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	4	8.01
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	4	8.01
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	18	8.01
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	3	7.99
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	18	7.98
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	18	7.98
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	19	7.97
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	14	7.95
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	9	7.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	10	7.94
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	17	7.93
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	17	7.93
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	20	7.9
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	8	7.88
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	6	7.88
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	6	7.88
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	6	7.88
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	5	7.88
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	5	7.88
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	19	7.88
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	19	7.88
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	3	7.85
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	3	7.85
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	1	7.85
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	14	7.82
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	1	7.77
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	1	7.77
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	5	7.76
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	2	7.75
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	18	7.75
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	18	7.75
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	6	7.74
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	9	7.73
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	15	7.72
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	15	7.72
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	15	7.72
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	9	7.72
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	20	7.71
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	15	7.71
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	12	7.71
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	4	7.69
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	4	7.69
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	9	7.67
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	9	7.67
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	3	7.65
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	15	7.63
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	8	7.61
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	10	7.61
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	10	7.61
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	10	7.61
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	17	7.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	15	7.6
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	12	7.59
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	14	7.59
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	10	7.58
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	2	7.56
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	2	7.56
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	13	7.56
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	14	7.56
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	14	7.56
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	2	7.56
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	2	7.56
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	17	7.55
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	17	7.55
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	11	7.53
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	4	7.52
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	4	7.52
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	8	7.52
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	1	7.52
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	16	7.49
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	16	7.49
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	16	7.49
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	12	7.49
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	12	7.49
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	1	7.49
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	1	7.49
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	1	7.49
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	8	7.49
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	7	7.49
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	1	7.49
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	13	7.46
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	2	7.45
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	2	7.45
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	2	7.45
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	20	7.45
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	20	7.45
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	20	7.45
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	9	7.45
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	7	7.44
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	7	7.44
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	12	7.44
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	12	7.44
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	10	7.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	10	7.44
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	7	7.44
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	8	7.44
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	7	7.43
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	7	7.43
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	9	7.42
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	13	7.42
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	6	7.42
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	5	7.42
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	7	7.42
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	5	7.41
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	15	7.41
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	15	7.41
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	13	7.41
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	9	7.41
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	14	7.4
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	16	7.38
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	2	7.37
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	16	7.37
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	14	7.36
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	13	7.36
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	4	7.36
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	11	7.36
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	18	7.34
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	6	7.34
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	6	7.34
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	18	7.34
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	6	7.34
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	4	7.34
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	2	7.33
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	16	7.33
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	4	7.32
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	3	7.32
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	14	7.32
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	14	7.31
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	14	7.31
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	14	7.31
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	16	7.31
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	2	7.31
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	14	7.31
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	6	7.29
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	20	7.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	3	7.28
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	14	7.28
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	2	7.28
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	19	7.27
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	15	7.27
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	5	7.27
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	1	7.27
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	18	7.26
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	18	7.26
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	11	7.26
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	10	7.26
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	4	7.25
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	7	7.25
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	5	7.24
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	14	7.24
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	17	7.24
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	19	7.24
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	1	7.23
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	3	7.23
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	3	7.23
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	3	7.23
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	20	7.23
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	20	7.22
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	5	7.22
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	18	7.21
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	8	7.21
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	8	7.2
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	8	7.2
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	6	7.2
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	7	7.19
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	7	7.19
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	20	7.18
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	20	7.18
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	20	7.18
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	18	7.16
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	18	7.16
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	18	7.16
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	4	7.16
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	16	7.16
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	6	7.15
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	14	7.15
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	14	7.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	14	7.15
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	8	7.15
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	2	7.15
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	16	7.15
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	1	7.15
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	11	7.15
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	11	7.14
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	3	7.13
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	15	7.13
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	7.12
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	12	7.11
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	6	7.1
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	4	7.1
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	3	7.1
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	14	7.09
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	17	7.09
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	15	7.08
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	1	7.08
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	1	7.08
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	1	7.08
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	5	7.08
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	5	7.08
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	5	7.08
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	13	7.07
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	10	7.06
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	18	7.06
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	9	7.06
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	3	7.06
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	13	7.05
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	5	7.04
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	9	7.03
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	12	7.03
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	12	7.03
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	12	7.03
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	8	7.03
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	9	7.03
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	9	7.02
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	5	7.02
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	1	7.02
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	16	7.01
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	10	7.01
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	16	7.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	16	7.01
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	10	7.0
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	11	7.0
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	11	7.0
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	11	7.0
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	19	7.0
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	2	6.99
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	20	6.98
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	4	6.98
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	6	6.98
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	17	6.98
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	7	6.98
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	14	6.97
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	14	6.97
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	8	6.97
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	8	6.97
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	8	6.97
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	13	6.97
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	1	6.97
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	18	6.97
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	14	6.97
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	5	6.96
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	11	6.96
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	17	6.96
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	20	6.95
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	12	6.95
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	13	6.95
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	14	6.95
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	16	6.95
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	16	6.95
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	2	6.94
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	17	6.94
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	8	6.94
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	8	6.94
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	4	6.94
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	2	6.93
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	9	6.92
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	1	6.92
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	20	6.92
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	9	6.92
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	8	6.92
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	6	6.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	6	6.91
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	2	6.91
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	15	6.91
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	5	6.9
(4,629)	1:31:A:CYS:HB3	1:38:A:THR:H	12	6.9
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	7	6.89
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	7	6.89
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	7	6.89
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	10	6.89
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	10	6.89
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	10	6.89
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	13	6.89
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	13	6.89
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	13	6.89
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	13	6.89
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	13	6.89
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	13	6.89
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	13	6.89
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	13	6.89
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	13	6.89
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	3	6.89
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	3	6.89
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	18	6.89
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	19	6.88
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	15	6.88
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	15	6.88
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	15	6.88
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	1	6.88
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	1	6.88
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	1	6.88
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	10	6.88
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	10	6.88
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	19	6.88
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	7	6.87
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	1	6.87
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	1	6.87
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	14	6.85
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	14	6.85
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	14	6.85
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	10	6.85
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	7	6.85
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	18	6.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	18	6.85
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	18	6.85
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	18	6.85
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	3	6.85
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	5	6.84
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	1	6.84
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	17	6.84
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	17	6.84
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	17	6.84
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	6	6.84
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	18	6.83
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	17	6.83
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	2	6.82
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	7	6.82
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	7	6.81
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	15	6.81
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	18	6.81
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	18	6.81
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	15	6.8
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	5	6.8
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	9	6.8
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	9	6.8
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	9	6.8
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	9	6.8
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	11	6.8
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	11	6.8
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	4	6.8
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	15	6.79
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	6	6.79
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	14	6.79
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	19	6.79
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	7	6.79
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	11	6.79
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	10	6.78
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	2	6.78
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	10	6.78
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	8	6.78
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	8	6.78
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	8	6.78
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	8	6.78
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	6	6.78
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	14	6.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	12	6.77
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	19	6.77
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	19	6.76
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	19	6.76
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	19	6.76
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	19	6.76
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	8	6.76
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	8	6.76
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	8	6.76
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	18	6.75
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	18	6.75
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	18	6.75
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	18	6.75
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	14	6.75
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	8	6.75
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	11	6.74
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	4	6.74
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	4	6.74
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	20	6.74
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	7	6.73
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	3	6.73
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	11	6.73
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	20	6.73
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	11	6.73
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	1	6.73
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	1	6.73
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	1	6.73
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	10	6.73
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	1	6.73
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	10	6.72
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	10	6.72
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	10	6.72
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	6	6.72
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	6	6.72
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	6	6.72
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	4	6.72
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	7	6.72
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	15	6.71
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	6	6.71
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	2	6.71
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	2	6.71
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	2	6.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	17	6.71
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	13	6.71
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	20	6.7
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	7	6.7
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	9	6.7
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	19	6.7
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	5	6.69
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	5	6.69
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	16	6.69
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	19	6.68
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	19	6.68
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	19	6.68
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	20	6.68
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	20	6.68
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	8	6.67
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	8	6.67
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	5	6.67
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	8	6.67
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	8	6.67
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	16	6.67
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	16	6.67
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	5	6.67
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	20	6.67
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	3	6.66
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	3	6.66
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	4	6.66
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	15	6.66
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	4	6.65
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	5	6.65
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	16	6.65
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	18	6.64
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	6.64
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	8	6.64
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	3	6.63
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	2	6.63
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	2	6.63
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	2	6.63
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	12	6.62
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	12	6.62
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	12	6.62
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	12	6.62
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	13	6.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	13	6.62
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	16	6.62
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	2	6.62
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	6	6.62
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	6	6.62
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	17	6.61
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	9	6.61
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	19	6.6
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	20	6.6
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	14	6.6
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	14	6.6
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	19	6.6
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	16	6.6
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	16	6.6
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	16	6.6
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	16	6.6
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	11	6.59
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	18	6.59
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	18	6.59
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	18	6.59
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	6	6.59
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	6	6.59
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	20	6.59
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	19	6.58
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	15	6.58
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	1	6.57
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	1	6.57
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	1	6.57
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	14	6.57
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	14	6.57
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	14	6.57
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	13	6.56
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	3	6.56
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	1	6.56
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	10	6.56
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	4	6.55
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	1	6.55
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	3	6.55
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	19	6.55
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	10	6.55
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	1	6.54
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	1	6.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	1	6.54
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	18	6.54
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	13	6.53
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	16	6.53
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	1	6.53
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	1	6.53
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	8	6.53
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	8	6.53
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	8	6.53
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	15	6.53
(4,471)	1:48:A:CYS:HB3	1:64:A:CYS:HA	14	6.53
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	8	6.53
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	14	6.52
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	14	6.52
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	5	6.52
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	16	6.52
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	3	6.51
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	3	6.51
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	3	6.51
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	13	6.51
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	13	6.51
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	6	6.51
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	6	6.51
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	6	6.51
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	17	6.51
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	3	6.51
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	7	6.5
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	20	6.5
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	6	6.49
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	6	6.49
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	6	6.49
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	6	6.49
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	3	6.49
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	9	6.49
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	9	6.49
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	7	6.49
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	12	6.49
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	15	6.49
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	18	6.49
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	7	6.49
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	6.48
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	4	6.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	6	6.48
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	6	6.48
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	6	6.48
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	10	6.48
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	18	6.48
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	18	6.48
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	18	6.48
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	12	6.47
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	12	6.47
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	19	6.47
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	19	6.47
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	15	6.47
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	20	6.47
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	20	6.47
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	20	6.47
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	9	6.47
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	20	6.46
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	20	6.46
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	20	6.46
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	2	6.46
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	12	6.46
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	5	6.45
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	10	6.45
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	10	6.45
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	10	6.45
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	14	6.45
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	18	6.45
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	18	6.45
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	20	6.45
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	20	6.45
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	20	6.45
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	6	6.45
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	3	6.45
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	17	6.45
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	3	6.44
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	14	6.44
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	12	6.44
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	20	6.44
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	13	6.44
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	18	6.44
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	3	6.44
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	6	6.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	5	6.43
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	12	6.43
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	12	6.43
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	4	6.43
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	15	6.42
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	15	6.42
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	15	6.42
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	17	6.42
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	17	6.42
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	17	6.42
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	19	6.42
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	19	6.42
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	19	6.42
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	9	6.42
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	9	6.42
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	8	6.42
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	16	6.42
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	3	6.42
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	12	6.41
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	4	6.41
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	3	6.41
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	3	6.41
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	2	6.41
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	4	6.41
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	9	6.41
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	9	6.41
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	9	6.41
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	9	6.41
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	9	6.41
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	9	6.41
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	9	6.41
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	9	6.41
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	9	6.41
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	13	6.41
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	3	6.41
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	3	6.41
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	11	6.4
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	11	6.4
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	11	6.4
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	11	6.4
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	8	6.4
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	19	6.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	16	6.4
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	16	6.4
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	16	6.4
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	19	6.4
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	3	6.4
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	3	6.4
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	3	6.4
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	17	6.4
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	16	6.4
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	16	6.4
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	2	6.39
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	2	6.39
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	2	6.39
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	2	6.39
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	9	6.39
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	6.39
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	2	6.39
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	6.39
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	12	6.39
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	16	6.39
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	16	6.39
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	16	6.39
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	16	6.39
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	9	6.38
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	9	6.38
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	9	6.38
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	13	6.38
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	7	6.38
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	20	6.38
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	20	6.38
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	7	6.38
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	5	6.37
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	8	6.37
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	8	6.37
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	8	6.37
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	8	6.37
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	8	6.37
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	8	6.37
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	8	6.37
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	8	6.37
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	8	6.37
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	8	6.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	8	6.37
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	8	6.37
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	17	6.37
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	11	6.36
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	19	6.35
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	12	6.35
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	12	6.35
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	14	6.34
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	19	6.34
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	17	6.34
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	9	6.34
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	9	6.34
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	9	6.34
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	9	6.34
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	14	6.33
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	17	6.33
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	18	6.33
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	18	6.33
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	3	6.33
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	18	6.33
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	18	6.33
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	20	6.33
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	15	6.33
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	8	6.33
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	8	6.33
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	20	6.32
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	16	6.32
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	13	6.32
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	13	6.32
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	19	6.32
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	11	6.32
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	11	6.32
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	11	6.32
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	5	6.32
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	9	6.32
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	14	6.32
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	16	6.32
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	10	6.31
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	8	6.31
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	15	6.31
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	2	6.3
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	2	6.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	2	6.3
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	16	6.3
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	16	6.3
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	16	6.3
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	7	6.3
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	13	6.3
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	13	6.3
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	18	6.29
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	18	6.29
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	17	6.29
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	17	6.29
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	17	6.29
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	10	6.29
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	10	6.29
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	19	6.28
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	8	6.28
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	8	6.28
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	8	6.28
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	8	6.28
(4,981)	1:40:A:ASN:HB2	1:48:A:CYS:HB2	6	6.28
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	2	6.28
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	1	6.27
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	2	6.27
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	2	6.27
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	8	6.27
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG21	4	6.27
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG22	4	6.27
(4,1049)	1:37:A:LYS:HE3	1:38:A:THR:HG23	4	6.27
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	6	6.27
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	7	6.27
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	13	6.27
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	15	6.27
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	13	6.26
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	13	6.26
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	11	6.26
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	11	6.26
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	16	6.26
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	10	6.26
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	3	6.26
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	3	6.26
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	3	6.26
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	2	6.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	11	6.25
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	19	6.25
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	7	6.25
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	10	6.25
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	10	6.25
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	10	6.25
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	13	6.25
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	17	6.24
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	2	6.23
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	2	6.23
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	2	6.23
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	11	6.23
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	18	6.23
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	7	6.22
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	7	6.22
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	7	6.22
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	8	6.22
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	8	6.22
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	9	6.22
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	14	6.22
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	13	6.21
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	11	6.21
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	8	6.21
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	6.21
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	1	6.2
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	20	6.2
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	12	6.2
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	12	6.2
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	12	6.2
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	14	6.2
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	14	6.2
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	14	6.2
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	12	6.2
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	16	6.19
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	10	6.19
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	11	6.19
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	11	6.19
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	11	6.19
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	4	6.19
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	20	6.19
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	20	6.19
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	2	6.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	2	6.18
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	2	6.18
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	15	6.18
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	1	6.18
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	1	6.18
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	4	6.18
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	6	6.18
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	19	6.18
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	19	6.18
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	19	6.18
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	19	6.18
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	19	6.18
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	19	6.18
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	19	6.18
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	19	6.18
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	19	6.18
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	15	6.18
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	18	6.18
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	12	6.18
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	4	6.17
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	11	6.17
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	10	6.17
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	10	6.17
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	10	6.17
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	13	6.17
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	20	6.17
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	4	6.16
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	4	6.16
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	4	6.16
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	12	6.16
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	12	6.16
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	12	6.16
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	12	6.16
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	5	6.16
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	5	6.16
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	1	6.16
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	13	6.16
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	13	6.16
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	13	6.16
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	13	6.16
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	13	6.16
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	13	6.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	13	6.16
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	13	6.16
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	13	6.16
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	13	6.16
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	13	6.16
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	13	6.16
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	6	6.16
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	6	6.16
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	6	6.16
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	6	6.16
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	8	6.15
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	10	6.15
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	8	6.15
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	12	6.14
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	14	6.14
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	14	6.14
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	12	6.14
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	12	6.14
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	12	6.14
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	6	6.14
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	10	6.14
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	17	6.13
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	20	6.13
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	20	6.13
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	16	6.13
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	9	6.13
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	10	6.13
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	6.12
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	8	6.12
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	15	6.12
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	16	6.12
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	16	6.12
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	16	6.12
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	16	6.12
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	16	6.12
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	16	6.12
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	16	6.12
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	16	6.12
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	16	6.12
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	6.12
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	7	6.12
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	2	6.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	16	6.11
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	16	6.11
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	16	6.11
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	6	6.11
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	2	6.11
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	18	6.11
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	6	6.11
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	3	6.11
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	13	6.11
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	20	6.1
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	20	6.1
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	14	6.1
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	14	6.1
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	14	6.1
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	14	6.1
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	14	6.1
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	14	6.1
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	14	6.1
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	14	6.1
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	14	6.1
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	14	6.1
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	14	6.1
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	14	6.1
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	20	6.1
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	20	6.1
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	20	6.1
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	7	6.1
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	2	6.1
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	2	6.1
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	19	6.1
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	19	6.1
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	1	6.1
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	9	6.1
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	11	6.1
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	17	6.09
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	1	6.09
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	1	6.09
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	1	6.09
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	1	6.09
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	1	6.09
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	1	6.09
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	1	6.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	1	6.09
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	1	6.09
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	1	6.09
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	1	6.09
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	1	6.09
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	4	6.09
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	4	6.09
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	4	6.09
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	20	6.09
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	15	6.08
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	15	6.08
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	15	6.08
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	18	6.08
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	9	6.08
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	1	6.08
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	3	6.08
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	3	6.08
(4,1061)	1:35:A:ALA:H	1:37:A:LYS:HD3	15	6.07
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	8	6.07
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	8	6.07
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	8	6.07
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	8	6.07
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	8	6.07
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	8	6.07
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	8	6.07
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	8	6.07
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	8	6.07
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	1	6.07
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	1	6.07
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	1	6.07
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	6	6.07
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	18	6.07
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	5	6.07
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	19	6.06
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	19	6.06
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	14	6.06
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	14	6.06
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	14	6.06
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	14	6.06
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	14	6.06
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	14	6.06
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	14	6.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	14	6.06
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	14	6.06
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	2	6.06
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	2	6.06
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	20	6.06
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	20	6.06
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	10	6.05
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	17	6.05
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	17	6.05
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	17	6.05
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	14	6.05
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	1	6.05
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	12	6.04
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	7	6.04
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	7	6.04
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	7	6.04
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	2	6.04
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	15	6.03
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	3	6.03
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	7	6.03
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	7	6.03
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	2	6.03
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	9	6.03
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	15	6.03
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	7	6.03
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	12	6.02
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	19	6.02
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	1	6.02
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	3	6.02
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	9	6.02
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	9	6.02
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	9	6.02
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	11	6.01
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	11	6.01
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	11	6.01
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	15	6.01
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	19	6.01
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	14	6.01
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	11	6.01
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	9	6.01
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	14	6.01
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	8	6.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	18	6.01
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	18	6.01
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	18	6.01
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	7	6.01
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	8	6.0
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	11	6.0
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	11	6.0
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	4	6.0
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	4	6.0
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	4	6.0
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	11	6.0
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	11	6.0
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	13	6.0
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	16	6.0
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	17	5.99
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	17	5.99
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	17	5.99
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	18	5.99
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	18	5.99
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	18	5.99
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	14	5.99
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	1	5.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	1	5.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	1	5.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	1	5.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	1	5.99
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	20	5.99
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	12	5.98
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	12	5.98
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	12	5.98
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	19	5.98
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	16	5.98
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	16	5.98
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	16	5.98
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	5	5.97
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	5	5.97
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	5	5.97
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	5	5.97
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	5	5.97
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	10	5.97
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	19	5.97
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	9	5.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	15	5.95
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	15	5.95
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	16	5.95
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	3	5.95
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	3	5.95
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	18	5.95
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	18	5.94
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	18	5.94
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	18	5.94
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	4	5.94
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	3	5.94
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	16	5.93
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	16	5.93
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	16	5.93
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	16	5.93
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	13	5.93
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	11	5.93
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	19	5.93
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	19	5.93
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	19	5.93
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	19	5.93
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	19	5.93
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	19	5.93
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	19	5.93
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	19	5.93
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	19	5.93
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	19	5.93
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	19	5.93
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	19	5.93
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	1	5.93
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	7	5.93
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	7	5.93
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	18	5.93
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	16	5.92
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	16	5.92
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	9	5.92
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	18	5.92
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	9	5.92
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	1	5.92
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	1	5.92
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	1	5.92
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	19	5.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	7	5.92
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	7	5.92
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	7	5.92
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	7	5.92
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	14	5.92
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	18	5.91
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	16	5.91
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.91
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.91
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	20	5.91
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	14	5.91
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	11	5.9
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	13	5.9
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	5	5.9
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	5	5.9
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	9	5.9
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	15	5.9
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	4	5.9
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	7	5.9
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	12	5.9
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	3	5.9
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	10	5.9
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	14	5.9
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	17	5.89
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	5	5.89
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	3	5.89
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	7	5.89
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	7	5.89
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	7	5.89
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	8	5.89
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	8	5.89
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	8	5.89
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	5	5.89
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	7	5.88
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	7	5.88
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	3	5.88
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	3	5.88
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	3	5.88
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	16	5.88
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	16	5.88
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	16	5.88
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	16	5.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	2	5.88
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	8	5.88
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	5	5.88
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	19	5.88
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	11	5.87
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	12	5.87
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	9	5.87
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	7	5.87
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	7	5.87
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	6	5.87
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	4	5.87
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	4	5.87
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	4	5.87
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	13	5.87
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	13	5.87
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	13	5.87
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	20	5.87
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	20	5.87
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	20	5.87
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	1	5.87
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	10	5.87
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	19	5.87
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	15	5.87
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	16	5.87
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	12	5.87
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	12	5.87
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	12	5.87
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	14	5.86
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	14	5.86
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	14	5.86
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	17	5.86
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	2	5.86
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	2	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	3	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	3	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	3	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	3	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	3	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	3	5.86
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	3	5.86
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	3	5.86
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	3	5.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	20	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	20	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	20	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	20	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	20	5.86
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	20	5.86
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	20	5.86
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	20	5.86
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	20	5.86
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	19	5.86
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	1	5.86
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	1	5.86
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	5	5.86
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	5	5.86
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	16	5.86
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	16	5.86
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	5.86
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	5.86
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	17	5.86
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	9	5.86
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	19	5.85
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	20	5.85
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	19	5.85
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	19	5.85
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	13	5.85
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	5.85
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	18	5.85
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	18	5.85
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	18	5.85
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	18	5.85
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	9	5.85
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	13	5.85
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	5.85
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	8	5.85
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	8	5.85
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	10	5.85
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	10	5.85
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	10	5.85
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	10	5.85
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	6	5.85
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	14	5.85
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	15	5.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	15	5.84
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	6	5.84
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	6	5.84
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	6	5.84
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	18	5.84
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	15	5.84
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	10	5.84
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	10	5.84
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	20	5.83
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	20	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	2	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	2	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	2	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	9	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	9	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	9	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	15	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	15	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	15	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	19	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	19	5.83
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	19	5.83
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	12	5.83
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	19	5.83
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	10	5.83
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	10	5.83
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	16	5.82
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	16	5.82
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	16	5.82
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	16	5.82
(4,1041)	1:37:A:LYS:HD3	1:38:A:THR:HA	12	5.82
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	6	5.82
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	6	5.82
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	11	5.82
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	11	5.82
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	11	5.82
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	11	5.82
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	10	5.82
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	10	5.82
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	10	5.82
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	10	5.82
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	10	5.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	10	5.82
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	10	5.82
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	10	5.82
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	10	5.82
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	10	5.82
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	10	5.82
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	10	5.82
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	8	5.82
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	8	5.82
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	8	5.82
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	6	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	10	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	10	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	10	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	14	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	14	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	14	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	17	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	17	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	17	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	18	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	18	5.82
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	18	5.82
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	11	5.82
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	5	5.81
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	9	5.81
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	9	5.81
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	9	5.81
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	14	5.81
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	19	5.81
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	19	5.81
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	19	5.81
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	5	5.8
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	5	5.8
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	10	5.8
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	10	5.8
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	10	5.8
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	10	5.8
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	15	5.8
(4,938)	1:41:A:CYS:HB2	1:55:A:PRO:HD3	2	5.8
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	5	5.8
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	5	5.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	5	5.8
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	13	5.8
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	13	5.8
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	13	5.8
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	8	5.8
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	8	5.8
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	8	5.8
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	4	5.8
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	4	5.8
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	14	5.8
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	14	5.8
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	2	5.8
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	2	5.8
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	2	5.8
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	5	5.79
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	5	5.79
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	5	5.79
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	10	5.79
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	7	5.79
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	7	5.79
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	7	5.79
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	7	5.79
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	7	5.79
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	7	5.79
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	7	5.79
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	7	5.79
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	7	5.79
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	11	5.79
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	11	5.79
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	15	5.79
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	15	5.79
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	8	5.79
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	15	5.79
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	15	5.79
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	15	5.79
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	10	5.79
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	17	5.79
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	3	5.79
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	3	5.79
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	4	5.79
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	17	5.79
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	9	5.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	12	5.79
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	12	5.79
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	8	5.79
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	5	5.78
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	5	5.78
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	5	5.78
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	8	5.78
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	17	5.78
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	17	5.78
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	17	5.78
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	17	5.78
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	17	5.78
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	4	5.78
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	14	5.78
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	5.78
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	5	5.78
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	11	5.78
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	4	5.78
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	4	5.78
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	12	5.78
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	12	5.78
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	15	5.78
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	11	5.78
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	11	5.78
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	11	5.78
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	11	5.78
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	8	5.77
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	8	5.77
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	8	5.77
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	1	5.77
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	19	5.77
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	2	5.77
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	2	5.77
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	2	5.77
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	14	5.77
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	7	5.77
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	15	5.77
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	16	5.77
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	15	5.77
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	9	5.77
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	9	5.77
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	9	5.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	13	5.76
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	13	5.76
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	13	5.76
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	6	5.76
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	6	5.76
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	6	5.76
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	7	5.76
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	7	5.76
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	7	5.76
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.76
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	20	5.76
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	20	5.76
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	20	5.76
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	3	5.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	16	5.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	16	5.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	16	5.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	16	5.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	16	5.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	16	5.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	16	5.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	16	5.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	16	5.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	16	5.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	16	5.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	16	5.76
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	17	5.76
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	17	5.76
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	18	5.76
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	18	5.76
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	18	5.76
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	16	5.76
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	16	5.76
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	16	5.76
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	6	5.76
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	17	5.76
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	15	5.76
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	15	5.76
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	15	5.76
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	1	5.75
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	1	5.75
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	1	5.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	20	5.75
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	11	5.75
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	11	5.75
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	11	5.75
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	11	5.75
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	11	5.75
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	11	5.75
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	11	5.75
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	11	5.75
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	11	5.75
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	6	5.75
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	19	5.75
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	5	5.75
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	11	5.75
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	10	5.75
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	10	5.75
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	10	5.75
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	19	5.74
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	19	5.74
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	19	5.74
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	19	5.74
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	14	5.74
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	3	5.74
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	6	5.74
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	9	5.74
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	4	5.74
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	4	5.74
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	19	5.74
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	2	5.73
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	2	5.73
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	2	5.73
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	2	5.73
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	5.73
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	5.73
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	2	5.73
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	10	5.73
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	5	5.73
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	5.73
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	5.73
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	17	5.73
(4,504)	1:39:A:CYS:H	1:58:A:CYS:HB2	11	5.73
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	5	5.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	1	5.73
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	11	5.73
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	3	5.73
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	9	5.73
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	8	5.73
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	8	5.73
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	8	5.73
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	17	5.73
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	18	5.72
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	18	5.72
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	18	5.72
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	18	5.72
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	4	5.72
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	4	5.72
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	4	5.72
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	4	5.72
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	4	5.72
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	4	5.72
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	4	5.72
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	4	5.72
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	4	5.72
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	4	5.72
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	4	5.72
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	4	5.72
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	10	5.72
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	10	5.72
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	12	5.72
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	4	5.72
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	4	5.72
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	4	5.72
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	15	5.72
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	2	5.72
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	15	5.72
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	9	5.72
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	12	5.71
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	12	5.71
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	12	5.71
(4,1161)	1:14:A:CYS:HA	1:36:A:CYS:HB2	20	5.71
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	7	5.71
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	9	5.71
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	17	5.71
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	17	5.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	17	5.71
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	17	5.71
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	17	5.71
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	17	5.71
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	17	5.71
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	17	5.71
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	17	5.71
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	20	5.71
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	13	5.71
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	19	5.71
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	14	5.71
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	19	5.71
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	19	5.71
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	5	5.71
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	15	5.71
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	18	5.71
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	1	5.71
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	9	5.7
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	9	5.7
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	16	5.7
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	16	5.7
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	16	5.7
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	10	5.7
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	10	5.7
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	10	5.7
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	10	5.7
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	10	5.7
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	10	5.7
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	10	5.7
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	10	5.7
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	10	5.7
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	9	5.7
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	9	5.7
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	8	5.7
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	8	5.7
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	11	5.69
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	11	5.69
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	11	5.69
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	13	5.69
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	13	5.69
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	13	5.69
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	13	5.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	5	5.69
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	4	5.69
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	16	5.69
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	16	5.69
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	16	5.69
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	1	5.69
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	18	5.69
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	18	5.69
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	12	5.69
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	12	5.69
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	12	5.69
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	12	5.69
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	2	5.69
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	15	5.69
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	19	5.69
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	10	5.69
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	11	5.69
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	14	5.69
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	19	5.68
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	19	5.68
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	4	5.68
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	4	5.68
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	2	5.68
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	19	5.68
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	19	5.68
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	18	5.68
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	18	5.68
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	20	5.68
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	17	5.68
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	17	5.68
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	6	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	1	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	1	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	1	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	1	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	11	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	11	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	11	5.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	11	5.68
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	12	5.68
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	8	5.68
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	6	5.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	6	5.68
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	6	5.68
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	14	5.68
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	14	5.68
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	14	5.68
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	16	5.68
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	9	5.68
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	13	5.67
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	13	5.67
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	6	5.67
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	6	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	5	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	5	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	5	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	5	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	5	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	5	5.67
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	5	5.67
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	5	5.67
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	5	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	6	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	6	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	6	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	6	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	6	5.67
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	6	5.67
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	6	5.67
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	6	5.67
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	6	5.67
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	3	5.67
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	3	5.67
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	20	5.67
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	20	5.67
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	20	5.67
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	20	5.67
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	4	5.67
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	13	5.67
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	17	5.67
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	17	5.67
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	3	5.67
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	3	5.67
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	5	5.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	20	5.67
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	20	5.67
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	20	5.67
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	12	5.67
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	12	5.67
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	14	5.67
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	17	5.67
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	7	5.67
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	9	5.67
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	7	5.67
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	4	5.66
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	4	5.66
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	4	5.66
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	8	5.66
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	8	5.66
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	8	5.66
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	10	5.66
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	17	5.66
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	15	5.66
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	15	5.66
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	15	5.66
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	15	5.66
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	15	5.66
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	15	5.66
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	15	5.66
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	15	5.66
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	15	5.66
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	9	5.66
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	17	5.66
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	17	5.66
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	17	5.66
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	9	5.66
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	12	5.66
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	12	5.66
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	12	5.66
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	4	5.66
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	6	5.66
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	14	5.66
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	16	5.66
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	2	5.66
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	14	5.66
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	14	5.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	14	5.66
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	17	5.65
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	17	5.65
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	17	5.65
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	7	5.65
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	11	5.65
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	11	5.65
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	11	5.65
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	11	5.65
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	17	5.65
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	5	5.65
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	18	5.65
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	18	5.65
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	19	5.65
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	16	5.65
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	20	5.65
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	10	5.64
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	5	5.64
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	12	5.64
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	12	5.64
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	12	5.64
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	12	5.64
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	12	5.64
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	12	5.64
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	12	5.64
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	12	5.64
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	12	5.64
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	12	5.64
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	2	5.64
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	2	5.64
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	16	5.64
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	16	5.64
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	16	5.64
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	16	5.64
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	1	5.64
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	6	5.64
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	6	5.64
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	6	5.64
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	19	5.64
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	6	5.64
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	6	5.64
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	16	5.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	7	5.64
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	12	5.64
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	12	5.64
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	5.64
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	19	5.64
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	20	5.64
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	12	5.64
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	5	5.64
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	19	5.63
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	2	5.63
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	2	5.63
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	2	5.63
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	5	5.63
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	5	5.63
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	12	5.63
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	6	5.63
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	4	5.63
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	4	5.63
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	9	5.62
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	9	5.62
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	9	5.62
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	10	5.62
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	10	5.62
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	10	5.62
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	19	5.62
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	19	5.62
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	19	5.62
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	3	5.62
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	4	5.62
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	4	5.62
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	9	5.62
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	13	5.62
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	13	5.62
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	13	5.62
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	13	5.62
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	13	5.62
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	7	5.62
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	7	5.62
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	9	5.62
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	9	5.62
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	9	5.62
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	9	5.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	19	5.62
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	14	5.62
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	14	5.62
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	14	5.62
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	16	5.62
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	7	5.62
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	7	5.62
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	7	5.62
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	10	5.62
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	10	5.62
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	10	5.62
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	10	5.62
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	2	5.62
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	13	5.62
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	19	5.62
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	7	5.61
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	10	5.61
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	10	5.61
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	10	5.61
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	19	5.61
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	19	5.61
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	19	5.61
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	1	5.61
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	13	5.61
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	2	5.61
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	18	5.61
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	5.61
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	1	5.61
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	1	5.61
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	6	5.61
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	10	5.6
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	3	5.6
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	3	5.6
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	2	5.6
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	2	5.6
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	2	5.6
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	2	5.6
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	2	5.6
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	2	5.6
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	2	5.6
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	2	5.6
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	2	5.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	15	5.6
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	7	5.6
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	7	5.6
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	12	5.6
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	12	5.6
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	5	5.6
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	5	5.6
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	5	5.6
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	11	5.6
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	11	5.6
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	4	5.6
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	4	5.6
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	15	5.6
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	15	5.6
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	10	5.6
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	11	5.6
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	11	5.6
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	11	5.6
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	7	5.6
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	9	5.6
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	14	5.6
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	16	5.6
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	6	5.6
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	14	5.6
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	20	5.59
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	14	5.59
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	14	5.59
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	14	5.59
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	6	5.59
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	7	5.59
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	7	5.59
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	8	5.59
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	8	5.59
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	8	5.59
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	8	5.59
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	10	5.59
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	17	5.59
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	15	5.59
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	8	5.58
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	8	5.58
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	8	5.58
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	1	5.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	1	5.58
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	1	5.58
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	1	5.58
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	1	5.58
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	1	5.58
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	1	5.58
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	1	5.58
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	1	5.58
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	9	5.58
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	9	5.58
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	10	5.58
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	10	5.58
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	3	5.58
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	4	5.58
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	17	5.58
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	3	5.58
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	10	5.57
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	3	5.57
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	18	5.57
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	18	5.57
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	18	5.57
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	10	5.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	11	5.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	11	5.57
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	14	5.57
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	7	5.57
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	7	5.57
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	7	5.57
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	7	5.57
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	18	5.57
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	2	5.57
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	3	5.57
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	3	5.57
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	20	5.57
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	15	5.57
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	2	5.57
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	4	5.57
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	13	5.56
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	13	5.56
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	13	5.56
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	15	5.56
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	2	5.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	6	5.56
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	2	5.56
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	2	5.56
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	2	5.56
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	2	5.56
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	2	5.56
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	2	5.56
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	2	5.56
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	2	5.56
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	2	5.56
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	2	5.56
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	2	5.56
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	2	5.56
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	4	5.56
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	10	5.56
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	16	5.56
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	1	5.56
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	1	5.56
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	13	5.56
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	3	5.56
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	20	5.56
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	3	5.56
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	3	5.56
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	2	5.55
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	19	5.55
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	19	5.55
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	1	5.55
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	3	5.55
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	20	5.55
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	5	5.55
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	5	5.55
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	5	5.55
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	5	5.55
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	6	5.55
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	12	5.55
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	13	5.55
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	15	5.54
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	17	5.54
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	12	5.54
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	12	5.54
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	19	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	4	5.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	4	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	4	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	7	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	7	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	7	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	9	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	9	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	9	5.54
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	5	5.54
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	2	5.54
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	2	5.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	13	5.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	13	5.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	13	5.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	13	5.54
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	3	5.54
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	3	5.54
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	3	5.54
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	3	5.54
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	17	5.54
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	16	5.54
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	13	5.53
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	13	5.53
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	13	5.53
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	4	5.53
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	4	5.53
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	4	5.53
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	4	5.53
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	4	5.53
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	4	5.53
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	4	5.53
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	4	5.53
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	4	5.53
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	12	5.53
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	10	5.53
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	19	5.53
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	8	5.53
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	2	5.53
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	2	5.53
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	2	5.53
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	2	5.53
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	17	5.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	19	5.53
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	13	5.53
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	13	5.53
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	13	5.53
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	17	5.52
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	8	5.52
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	8	5.52
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	8	5.52
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	8	5.52
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	8	5.52
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	14	5.52
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	14	5.52
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	16	5.52
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	16	5.52
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	15	5.52
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	9	5.52
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	17	5.52
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	17	5.52
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	17	5.52
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	17	5.52
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	9	5.52
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	2	5.52
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	20	5.52
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	16	5.52
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	1	5.51
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	1	5.51
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	1	5.51
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	1	5.51
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	18	5.51
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	18	5.51
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	18	5.51
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG21	18	5.51
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG22	18	5.51
(4,1047)	1:37:A:LYS:HE2	1:38:A:THR:HG23	18	5.51
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG21	18	5.51
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG22	18	5.51
(4,1047)	1:37:A:LYS:HE3	1:38:A:THR:HG23	18	5.51
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	13	5.51
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	13	5.51
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	18	5.51
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	20	5.51
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	9	5.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	4	5.51
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	7	5.51
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	17	5.51
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	2	5.51
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	2	5.51
(4,564)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	16	5.51
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	20	5.51
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	20	5.51
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	8	5.51
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	12	5.51
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	12	5.51
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	1	5.5
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	1	5.5
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	1	5.5
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	12	5.5
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	12	5.5
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	1	5.5
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	14	5.5
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	1	5.5
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	10	5.5
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	5	5.5
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	5	5.5
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	19	5.5
(4,400)	1:54:A:GLY:HA2	1:56:A:ASP:HB2	3	5.5
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	6	5.5
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	19	5.5
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	14	5.49
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	16	5.49
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	5	5.49
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	5	5.49
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	5	5.49
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	13	5.49
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	15	5.49
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	11	5.49
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	17	5.49
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	17	5.49
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	17	5.49
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	19	5.49
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	20	5.49
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	2	5.49
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	13	5.49
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	13	5.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	8	5.48
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	19	5.48
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	10	5.48
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	10	5.48
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	10	5.48
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	13	5.48
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	13	5.48
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	13	5.48
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	19	5.48
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	19	5.48
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	19	5.48
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	19	5.48
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	12	5.48
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	4	5.48
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	16	5.48
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	9	5.48
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	9	5.48
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	4	5.48
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	15	5.48
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	15	5.48
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	15	5.48
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	8	5.48
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	8	5.48
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	8	5.48
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	8	5.48
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	7	5.48
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	18	5.48
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	11	5.48
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	11	5.48
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	11	5.48
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	11	5.48
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	15	5.48
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	3	5.47
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	3	5.47
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	3	5.47
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	5	5.47
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	17	5.47
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	18	5.47
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	15	5.47
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	15	5.47
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	3	5.47
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	3	5.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	3	5.47
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	16	5.47
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	17	5.47
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	16	5.47
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	16	5.47
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	4	5.47
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	4	5.47
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	7	5.47
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	12	5.47
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	12	5.47
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	1	5.46
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	1	5.46
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	1	5.46
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	1	5.46
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	12	5.46
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	12	5.46
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	12	5.46
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	12	5.46
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	17	5.46
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	19	5.46
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	19	5.46
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	20	5.46
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	20	5.46
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	20	5.46
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	13	5.46
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	13	5.46
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	13	5.46
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	2	5.46
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	18	5.46
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	9	5.46
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	9	5.46
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	8	5.46
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	8	5.46
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	8	5.46
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	17	5.46
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	11	5.46
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	15	5.46
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	18	5.46
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	18	5.46
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	12	5.46
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	6	5.46
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	7	5.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	7	5.46
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	7	5.46
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	7	5.46
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	9	5.45
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	9	5.45
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	9	5.45
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	14	5.45
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	14	5.45
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	14	5.45
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	14	5.45
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	2	5.45
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	14	5.45
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	3	5.45
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	3	5.45
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	3	5.45
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	4	5.45
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	11	5.45
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	16	5.45
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	20	5.45
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	18	5.45
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	14	5.45
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	6	5.45
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	6	5.45
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	6	5.45
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	6	5.45
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	6	5.45
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	6	5.45
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	6	5.45
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	6	5.45
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	6	5.45
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	6	5.45
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	6	5.45
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	6	5.45
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	10	5.45
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	6	5.45
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	3	5.45
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	7	5.45
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	10	5.45
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	5	5.45
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	11	5.44
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	11	5.44
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	11	5.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	11	5.44
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	6	5.44
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	6	5.44
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	6	5.44
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	6	5.44
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	19	5.44
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	15	5.44
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	15	5.44
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	15	5.44
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	9	5.44
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	9	5.44
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	9	5.44
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	5.44
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	5	5.44
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	8	5.44
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	11	5.44
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	10	5.44
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	1	5.44
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	10	5.44
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	11	5.44
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	5	5.44
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	13	5.44
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	8	5.44
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	20	5.43
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	1	5.43
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	1	5.43
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	8	5.43
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	18	5.43
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	18	5.43
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	18	5.43
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	18	5.43
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	18	5.43
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	18	5.43
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	18	5.43
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	18	5.43
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	18	5.43
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	18	5.43
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	18	5.43
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	18	5.43
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	18	5.43
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	18	5.43
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	19	5.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	19	5.43
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	19	5.43
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	19	5.43
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	4	5.43
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	15	5.43
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	15	5.43
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	14	5.43
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	10	5.43
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	12	5.43
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	17	5.43
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	18	5.43
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	2	5.42
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	18	5.42
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	18	5.42
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	12	5.42
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	12	5.42
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	12	5.42
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	8	5.42
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	8	5.42
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	15	5.42
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	15	5.42
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	15	5.42
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	17	5.42
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	15	5.42
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	15	5.42
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	5	5.42
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	5	5.42
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	5	5.42
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	5	5.42
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	5	5.42
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	5	5.42
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	17	5.42
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	17	5.42
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	17	5.42
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	17	5.42
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	17	5.42
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	17	5.42
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	8	5.42
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	4	5.42
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	8	5.42
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	9	5.42
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	17	5.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	4	5.42
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	8	5.41
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	8	5.41
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	8	5.41
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	8	5.41
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	1	5.41
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	6	5.41
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	6	5.41
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	6	5.41
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	5	5.41
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	5	5.41
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	5.41
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	20	5.41
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	5.41
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	17	5.41
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	17	5.41
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	17	5.41
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	15	5.41
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	15	5.41
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	15	5.41
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	15	5.41
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	15	5.41
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	15	5.41
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	15	5.41
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	15	5.41
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	15	5.41
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	15	5.41
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	15	5.41
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	15	5.41
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	15	5.41
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	15	5.41
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	16	5.41
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	16	5.41
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	16	5.41
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	16	5.41
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	16	5.41
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	16	5.41
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	6	5.41
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	18	5.41
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	4	5.41
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	11	5.4
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	11	5.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	9	5.4
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	14	5.4
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	5	5.4
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	14	5.4
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	20	5.4
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	20	5.4
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	20	5.4
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	15	5.4
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	20	5.4
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	20	5.4
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	4	5.4
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	8	5.4
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	8	5.4
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	8	5.4
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	8	5.4
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	8	5.4
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	8	5.4
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	9	5.4
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	9	5.4
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	9	5.4
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	9	5.4
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	9	5.4
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	9	5.4
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	2	5.4
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	2	5.4
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	15	5.4
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	2	5.4
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	13	5.4
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	10	5.4
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	12	5.4
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	2	5.39
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	2	5.39
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	2	5.39
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	2	5.39
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	18	5.39
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	14	5.39
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	14	5.39
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	14	5.39
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	14	5.39
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	14	5.39
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	14	5.39
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	18	5.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	18	5.39
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	18	5.39
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	12	5.39
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	12	5.39
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	12	5.39
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	12	5.39
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	15	5.39
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	6	5.39
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	6	5.39
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	6	5.39
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	6	5.39
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	6	5.39
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	6	5.39
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	16	5.39
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	16	5.39
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	18	5.39
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	9	5.39
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	9	5.39
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	14	5.39
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	1	5.39
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	7	5.39
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	17	5.38
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	17	5.38
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	3	5.38
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	15	5.38
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	15	5.38
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	15	5.38
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	15	5.38
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	15	5.38
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	15	5.38
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	5	5.38
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	18	5.38
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	4	5.38
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	11	5.38
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	8	5.38
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	7	5.38
(4,1203)	1:38:A:THR:HG21	1:55:A:PRO:HB2	8	5.37
(4,1203)	1:38:A:THR:HG22	1:55:A:PRO:HB2	8	5.37
(4,1203)	1:38:A:THR:HG23	1:55:A:PRO:HB2	8	5.37
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	9	5.37
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	11	5.37
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	18	5.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	8	5.37
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	2	5.37
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	2	5.37
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	2	5.37
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	2	5.37
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	2	5.37
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	2	5.37
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	18	5.37
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	18	5.37
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	18	5.37
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	18	5.37
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	18	5.37
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	18	5.37
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	11	5.37
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	14	5.37
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	11	5.36
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	11	5.36
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	11	5.36
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	10	5.36
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	10	5.36
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	10	5.36
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	10	5.36
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	10	5.36
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	10	5.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	11	5.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	11	5.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	11	5.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	11	5.36
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	8	5.36
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	6	5.36
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	6	5.36
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	6	5.36
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	11	5.36
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	11	5.36
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	11	5.36
(4,991)	1:52:A:CYS:HB2	1:54:A:GLY:HA3	9	5.36
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	15	5.36
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	15	5.36
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	15	5.36
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	10	5.36
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	10	5.36
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	3	5.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	3	5.36
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	3	5.36
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	3	5.36
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	3	5.36
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	3	5.36
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	4	5.36
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	4	5.36
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	4	5.36
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	4	5.36
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	4	5.36
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	4	5.36
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	20	5.36
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	20	5.36
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	4	5.36
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	2	5.36
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	6	5.35
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	8	5.35
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	8	5.35
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	8	5.35
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	8	5.35
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	16	5.35
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	16	5.35
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	16	5.35
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	1	5.35
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	9	5.35
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	9	5.35
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	9	5.35
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	9	5.35
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	9	5.35
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	9	5.35
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	9	5.35
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	9	5.35
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	9	5.35
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	9	5.35
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	9	5.35
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	9	5.35
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	15	5.35
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	15	5.35
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	17	5.35
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	17	5.35
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	10	5.35
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	10	5.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	10	5.35
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	10	5.35
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	10	5.35
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	10	5.35
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	17	5.35
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	15	5.35
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	15	5.35
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	15	5.35
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	15	5.35
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	15	5.35
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	7	5.35
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	15	5.35
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	7	5.35
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	4	5.34
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	4	5.34
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	4	5.34
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	4	5.34
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	7	5.34
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	7	5.34
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	7	5.34
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	6	5.34
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	16	5.34
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	7	5.34
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	7	5.34
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	7	5.34
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	7	5.34
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	3	5.34
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	3	5.34
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	5	5.34
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	16	5.34
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	3	5.34
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	10	5.34
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	12	5.34
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	12	5.34
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	12	5.34
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	12	5.34
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	12	5.34
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	12	5.34
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	12	5.34
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	12	5.34
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	12	5.34
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	12	5.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	12	5.34
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	12	5.34
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	4	5.34
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	3	5.34
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	6	5.34
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	15	5.33
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	15	5.33
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	15	5.33
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	16	5.33
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	16	5.33
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	16	5.33
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	5	5.33
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	5	5.33
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	5	5.33
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	4	5.33
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	9	5.33
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	9	5.33
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	9	5.33
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	8	5.33
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	16	5.33
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	16	5.33
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	8	5.33
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	7	5.33
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	12	5.33
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	13	5.33
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	18	5.33
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	18	5.33
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	18	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	1	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	1	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	1	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	1	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	1	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	1	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	7	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	7	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	7	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	7	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	7	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	7	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	14	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	14	5.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	14	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	14	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	14	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	14	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	19	5.33
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	19	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	19	5.33
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	19	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	19	5.33
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	19	5.33
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	1	5.33
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	2	5.33
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	6	5.33
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	20	5.33
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	11	5.33
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	2	5.33
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	6	5.33
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	15	5.33
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	6	5.33
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	16	5.32
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	2	5.32
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	2	5.32
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	2	5.32
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	2	5.32
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	10	5.32
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	18	5.32
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	18	5.32
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	18	5.32
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	18	5.32
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	18	5.32
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	18	5.32
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	5	5.32
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	5	5.32
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	6	5.32
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	6	5.32
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	2	5.32
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	5	5.32
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	20	5.32
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	5	5.32
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	14	5.31
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	14	5.31
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	14	5.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	19	5.31
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	19	5.31
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	19	5.31
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	20	5.31
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	3	5.31
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	5	5.31
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	5	5.31
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	5	5.31
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	5	5.31
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	10	5.31
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	10	5.31
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	8	5.31
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	10	5.31
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	20	5.31
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	13	5.31
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	13	5.31
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	12	5.31
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	12	5.31
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	12	5.31
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	12	5.31
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	12	5.31
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	12	5.31
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	8	5.31
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	8	5.31
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	13	5.31
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	13	5.31
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	6	5.31
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	6	5.31
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	10	5.31
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	17	5.3
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	17	5.3
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	17	5.3
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	17	5.3
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	15	5.3
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	15	5.3
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	9	5.3
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	9	5.3
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	9	5.3
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	9	5.3
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	9	5.3
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	5	5.3
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	5	5.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	5	5.3
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	12	5.3
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	13	5.3
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	13	5.3
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	13	5.3
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	13	5.3
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	13	5.3
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	13	5.3
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	5	5.3
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	5	5.3
(4,318)	1:55:A:PRO:HB3	1:58:A:CYS:H	1	5.3
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	5	5.3
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	5	5.29
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	5	5.29
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	5	5.29
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	5	5.29
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	9	5.29
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	9	5.29
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	9	5.29
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	10	5.29
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	2	5.29
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	7	5.29
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	19	5.29
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	14	5.29
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	14	5.29
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	16	5.29
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	16	5.29
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	19	5.29
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	19	5.29
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	1	5.29
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	13	5.29
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	16	5.29
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	17	5.29
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	19	5.29
(4,198)	1:58:A:CYS:H	1:60:A:CYS:H	2	5.29
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	16	5.29
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	17	5.29
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	19	5.29
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	18	5.29
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	8	5.29
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	9	5.29
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	4	5.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	11	5.28
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	11	5.28
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	19	5.28
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	17	5.28
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	20	5.28
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	13	5.28
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	13	5.28
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	3	5.28
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	19	5.27
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	19	5.27
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	19	5.27
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	5.27
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	1	5.27
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	1	5.27
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	11	5.27
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	5	5.27
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	5	5.27
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	5	5.27
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	5	5.27
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	17	5.27
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	17	5.27
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	18	5.27
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	18	5.27
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	18	5.27
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	16	5.27
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	5	5.27
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	1	5.27
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	12	5.26
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	12	5.26
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	12	5.26
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	5	5.26
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	18	5.26
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	5	5.26
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	4	5.26
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	8	5.26
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	8	5.26
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	8	5.26
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	9	5.26
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	19	5.26
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB2	11	5.26
(4,506)	1:39:A:CYS:H	1:58:A:CYS:HB3	11	5.26
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	19	5.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	1	5.26
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	12	5.26
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	1	5.26
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	17	5.25
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	17	5.25
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	17	5.25
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	10	5.25
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	20	5.25
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	20	5.25
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	20	5.25
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	20	5.25
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	4	5.25
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	3	5.25
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	3	5.25
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	3	5.25
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	10	5.25
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	10	5.25
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	10	5.25
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	9	5.25
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	9	5.25
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	13	5.25
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	3	5.24
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	3	5.24
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	3	5.24
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	3	5.24
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	14	5.24
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	15	5.24
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	14	5.24
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	11	5.24
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	11	5.24
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	16	5.24
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	15	5.24
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	15	5.24
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	15	5.24
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	15	5.24
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	15	5.24
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	11	5.24
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	11	5.24
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	3	5.24
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	9	5.24
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	8	5.24
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	3	5.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	3	5.24
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	3	5.24
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	11	5.24
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	11	5.24
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	11	5.24
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	11	5.24
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	11	5.24
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	11	5.24
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	8	5.24
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	16	5.24
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	1	5.24
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	11	5.24
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	10	5.24
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	15	5.24
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	11	5.23
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	1	5.23
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	1	5.23
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	1	5.23
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	1	5.23
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	3	5.23
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	9	5.23
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	1	5.23
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	6	5.23
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	6	5.23
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	6	5.23
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	6	5.23
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	14	5.23
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	3	5.23
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	3	5.23
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	3	5.23
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	3	5.23
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	3	5.23
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	3	5.23
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	3	5.23
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	3	5.23
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	14	5.23
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	14	5.23
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	14	5.23
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB2	20	5.23
(4,533)	1:11:A:THR:HG21	1:12:A:SER:HB3	20	5.23
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB2	20	5.23
(4,533)	1:11:A:THR:HG22	1:12:A:SER:HB3	20	5.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB2	20	5.23
(4,533)	1:11:A:THR:HG23	1:12:A:SER:HB3	20	5.23
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	19	5.23
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	18	5.23
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	6	5.23
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	3	5.23
(4,196)	1:19:A:CYS:H	1:21:A:CYS:H	7	5.23
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	6	5.23
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	6	5.23
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	6	5.23
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	13	5.22
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	13	5.22
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	13	5.22
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	10	5.22
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	10	5.22
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	10	5.22
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	20	5.22
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	20	5.22
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	20	5.22
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	17	5.22
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	11	5.22
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	8	5.22
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	8	5.22
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	8	5.22
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	11	5.22
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	8	5.22
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	3	5.22
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	3	5.22
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	3	5.22
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	3	5.22
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	2	5.22
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	14	5.22
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	14	5.22
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	14	5.22
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	9	5.22
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	8	5.22
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	8	5.22
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	3	5.22
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	18	5.21
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	18	5.21
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	18	5.21
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	6	5.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	6	5.21
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	6	5.21
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	6	5.21
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	12	5.21
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	20	5.21
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	2	5.21
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	17	5.21
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	15	5.21
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	15	5.21
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	14	5.21
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	8	5.21
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	1	5.21
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	17	5.21
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	17	5.21
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	3	5.21
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	3	5.21
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	3	5.21
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	14	5.21
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	14	5.21
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	14	5.21
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	14	5.21
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	17	5.21
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	9	5.2
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	9	5.2
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	8	5.2
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	8	5.2
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	18	5.2
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	18	5.2
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	18	5.2
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	7	5.2
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	10	5.2
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	10	5.2
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	17	5.2
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	5	5.2
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	5	5.2
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	5	5.2
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	5	5.2
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	5	5.2
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	5	5.2
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	5	5.2
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	5	5.2
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	5	5.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	5	5.2
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	5	5.2
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	5	5.2
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	16	5.2
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	16	5.2
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	16	5.2
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	5	5.2
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	11	5.2
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	5	5.2
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	5	5.2
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	14	5.2
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	14	5.2
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	14	5.2
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	14	5.2
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	14	5.2
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	20	5.2
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	20	5.2
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	20	5.2
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	19	5.2
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	19	5.2
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	19	5.2
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	1	5.2
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	1	5.2
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	10	5.2
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	8	5.2
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	16	5.2
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	16	5.2
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	16	5.2
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	8	5.2
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	2	5.19
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	2	5.19
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	5	5.19
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	15	5.19
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	13	5.19
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	2	5.19
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	7	5.19
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	4	5.19
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	14	5.19
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	20	5.19
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	18	5.19
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	19	5.19
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	6	5.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	7	5.18
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	7	5.18
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	7	5.18
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	20	5.18
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	20	5.18
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	20	5.18
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	20	5.18
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	6	5.18
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	6	5.18
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	6	5.18
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	6	5.18
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	16	5.18
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	15	5.18
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	3	5.18
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	13	5.18
(4,653)	1:21:A:CYS:HB3	1:24:A:LYS:HG3	12	5.18
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	18	5.18
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	13	5.18
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	18	5.18
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	10	5.18
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	1	5.18
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	1	5.18
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	1	5.18
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	14	5.18
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	15	5.18
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	18	5.18
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	5	5.18
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	19	5.18
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	18	5.18
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	7	5.17
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	12	5.17
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	2	5.17
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	2	5.17
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	12	5.17
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	12	5.17
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	8	5.17
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	6	5.17
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	12	5.17
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	19	5.17
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	13	5.17
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	10	5.17
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	10	5.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,42)	1:14:A:CYS:HB2	1:26:A:GLN:H	18	5.17
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	6	5.16
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	6	5.16
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	6	5.16
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	19	5.16
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	19	5.16
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	19	5.16
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	19	5.16
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	12	5.16
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	6	5.16
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	6	5.16
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	6	5.16
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	4	5.16
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	8	5.16
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	15	5.16
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	15	5.16
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	11	5.16
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	5	5.15
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	5	5.15
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	5	5.15
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	19	5.15
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	3	5.15
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	3	5.15
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	3	5.15
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	3	5.15
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	9	5.15
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	9	5.15
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	9	5.15
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	9	5.15
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	20	5.15
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	4	5.15
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	4	5.15
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	8	5.15
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	8	5.15
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	19	5.15
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	7	5.15
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	7	5.15
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	13	5.15
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	13	5.14
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	13	5.14
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	13	5.14
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	13	5.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	2	5.14
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	2	5.14
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	2	5.14
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	11	5.14
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	15	5.14
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	1	5.14
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	16	5.14
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	16	5.14
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	1	5.14
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	10	5.14
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	4	5.14
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	7	5.14
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	19	5.14
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	19	5.14
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	19	5.14
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	5.14
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	5.14
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	10	5.14
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	6	5.14
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	20	5.14
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	13	5.14
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	13	5.14
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	13	5.14
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	13	5.14
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	4	5.13
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	4	5.13
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	4	5.13
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	18	5.13
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	6	5.13
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	18	5.13
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	1	5.13
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	10	5.13
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	10	5.13
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	10	5.13
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	1	5.13
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	6	5.13
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	14	5.13
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	3	5.13
(4,900)	1:46:A:CYS:HA	1:53:A:THR:HB	20	5.13
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	4	5.13
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	10	5.13
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	6	5.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	8	5.13
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	15	5.13
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	2	5.13
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	2	5.13
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	8	5.13
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	18	5.13
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	3	5.12
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	3	5.12
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	3	5.12
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	12	5.12
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	12	5.12
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	12	5.12
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	11	5.12
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	9	5.12
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	11	5.12
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	11	5.12
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	11	5.12
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	11	5.12
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	7	5.12
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	19	5.12
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	2	5.12
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	2	5.12
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	1	5.12
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	1	5.12
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	1	5.12
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	7	5.12
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	17	5.12
(4,500)	1:23:A:SER:HA	1:24:A:LYS:HB3	12	5.12
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	15	5.12
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	15	5.12
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	15	5.12
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	9	5.12
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	15	5.12
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	15	5.12
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	15	5.12
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	15	5.12
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	11	5.12
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	11	5.12
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	11	5.12
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	9	5.12
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	1	5.12
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	2	5.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	2	5.11
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	2	5.11
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	6	5.11
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	6	5.11
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	6	5.11
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	16	5.11
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	12	5.11
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	17	5.11
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	19	5.11
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	7	5.11
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	7	5.11
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	7	5.11
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	4	5.11
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	5	5.11
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	9	5.11
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	13	5.11
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	20	5.11
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	5	5.11
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	12	5.11
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	10	5.11
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	20	5.11
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	1	5.11
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	1	5.11
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	1	5.11
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	1	5.11
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	9	5.11
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	9	5.1
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	9	5.1
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	9	5.1
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	9	5.1
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	9	5.1
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	9	5.1
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	18	5.1
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	18	5.1
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	5	5.1
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	18	5.1
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	12	5.1
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	4	5.1
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	13	5.1
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	16	5.1
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	4	5.1
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	4	5.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	4	5.1
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	4	5.1
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	7	5.1
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	7	5.1
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	7	5.1
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	15	5.1
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	20	5.1
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	5	5.1
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	5	5.1
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	5	5.1
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	20	5.1
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	3	5.09
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	3	5.09
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	3	5.09
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	13	5.09
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	2	5.09
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	12	5.09
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	13	5.09
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	13	5.09
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	13	5.09
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	16	5.09
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	18	5.09
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	19	5.09
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	17	5.09
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	17	5.09
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	5	5.09
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	13	5.09
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	2	5.09
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	4	5.09
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	20	5.08
(4,1187)	1:49:A:GLY:HA2	1:50:A:LYS:HD2	20	5.08
(4,1187)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	20	5.08
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	1	5.08
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	9	5.08
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	11	5.08
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	11	5.08
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	19	5.08
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	4	5.08
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	18	5.08
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	14	5.08
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	17	5.08
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	2	5.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	2	5.08
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	2	5.08
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	20	5.08
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	20	5.08
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	20	5.08
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	14	5.08
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	3	5.08
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	11	5.08
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	2	5.08
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	20	5.08
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	20	5.08
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	20	5.08
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	2	5.07
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	17	5.07
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	17	5.07
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	20	5.07
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	11	5.07
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	3	5.07
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	1	5.07
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	11	5.07
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	7	5.07
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	7	5.07
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	7	5.07
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	11	5.07
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	11	5.07
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	11	5.07
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	15	5.07
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	11	5.07
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	17	5.07
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	12	5.07
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	4	5.07
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	19	5.06
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	19	5.06
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	19	5.06
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	19	5.06
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	3	5.06
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	7	5.06
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	8	5.06
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	17	5.06
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	5	5.06
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	5	5.06
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	5	5.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	5	5.06
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	5	5.06
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	2	5.06
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	6	5.06
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	17	5.06
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	8	5.06
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	2	5.06
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	1	5.06
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	16	5.06
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	11	5.06
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	13	5.05
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	4	5.05
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	18	5.05
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	14	5.05
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	4	5.05
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	13	5.05
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	5	5.05
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	10	5.05
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	13	5.05
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	1	5.05
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	7	5.05
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	7	5.05
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	7	5.05
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	12	5.05
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	13	5.04
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	13	5.04
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	13	5.04
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	9	5.04
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	3	5.04
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	7	5.04
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	10	5.04
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	7	5.04
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	12	5.04
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	14	5.04
(4,517)	1:54:A:GLY:HA2	1:55:A:PRO:HB3	9	5.04
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	8	5.04
(4,317)	1:39:A:CYS:HB3	1:58:A:CYS:H	5	5.04
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	6	5.04
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	12	5.04
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	12	5.04
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	12	5.04
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	12	5.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	14	5.04
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	14	5.04
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	4	5.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	1	5.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	1	5.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	1	5.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	1	5.03
(4,1038)	1:37:A:LYS:HD2	1:38:A:THR:HA	13	5.03
(4,1038)	1:37:A:LYS:HD3	1:38:A:THR:HA	13	5.03
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	17	5.03
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	10	5.03
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	14	5.03
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	14	5.03
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	14	5.03
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	11	5.03
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	11	5.03
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	13	5.03
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	13	5.03
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	13	5.03
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	19	5.03
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	16	5.03
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	16	5.02
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	16	5.02
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	16	5.02
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	20	5.02
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	15	5.02
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	7	5.02
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	20	5.02
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	20	5.02
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	19	5.02
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	19	5.02
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	19	5.02
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	6	5.02
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	5.02
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	20	5.02
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	5.02
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	20	5.02
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	8	5.02
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	4	5.02
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	14	5.02
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	11	5.01
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	10	5.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	1	5.01
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	4	5.01
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	17	5.01
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	16	5.01
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	5	5.01
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	2	5.01
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	16	5.01
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	7	5.01
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	7	5.01
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	1	5.01
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	1	5.01
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	1	5.01
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	1	5.01
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	9	5.01
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	7	5.01
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	3	5.01
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	3	5.01
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	3	5.01
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	16	5.0
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	16	5.0
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	16	5.0
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	7	5.0
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	7	5.0
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	7	5.0
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	7	5.0
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	6	5.0
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	1	5.0
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	1	5.0
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	1	5.0
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	6	5.0
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	18	5.0
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	19	5.0
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	3	5.0
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	3	5.0
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	3	5.0
(4,966)	1:64:A:CYS:H	1:67:A:LYS:HA	1	5.0
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	20	5.0
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	20	5.0
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	20	5.0
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	20	5.0
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	20	5.0
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	13	5.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	13	5.0
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	13	5.0
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	13	5.0
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	2	5.0
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	19	5.0
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	2	5.0
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	2	5.0
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	6	5.0
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	10	4.99
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	15	4.99
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	15	4.99
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	15	4.99
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	15	4.99
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	2	4.99
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	20	4.99
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	13	4.99
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	4	4.99
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	4	4.99
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	4	4.99
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	4	4.99
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	4	4.99
(4,1081)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	9	4.98
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	6	4.98
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	6	4.98
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	16	4.98
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	19	4.98
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	19	4.98
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	12	4.98
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	9	4.98
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	8	4.98
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	8	4.98
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	17	4.98
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	17	4.98
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	17	4.98
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	17	4.98
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	17	4.98
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	17	4.98
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	17	4.98
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	17	4.98
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	17	4.98
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	17	4.98
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	17	4.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	17	4.98
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	6	4.98
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	6	4.98
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	6	4.98
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	6	4.98
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	6	4.98
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	6	4.98
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	6	4.98
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	6	4.98
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	2	4.98
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	1	4.98
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	17	4.98
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	17	4.98
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	17	4.98
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	17	4.98
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	12	4.98
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	4	4.98
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	14	4.97
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	14	4.97
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	14	4.97
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	2	4.97
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	5	4.97
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	5	4.97
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	16	4.97
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	16	4.97
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	16	4.97
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	11	4.97
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	11	4.97
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	11	4.97
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	18	4.97
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	1	4.97
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	1	4.97
(4,505)	1:6:A:LYS:H	1:10:A:CYS:HB2	12	4.97
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	11	4.97
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	2	4.97
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	4.97
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	4.97
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	15	4.97
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	13	4.97
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	18	4.97
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	13	4.97
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	12	4.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	14	4.96
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	14	4.96
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	14	4.96
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	14	4.96
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	4	4.96
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	4	4.96
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	4	4.96
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	15	4.96
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	15	4.96
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	15	4.96
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	7	4.96
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	8	4.96
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	8	4.96
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	1	4.96
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	1	4.96
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	7	4.96
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	7	4.96
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	20	4.96
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	20	4.96
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	20	4.96
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	20	4.96
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	20	4.96
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	20	4.96
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	20	4.96
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	20	4.96
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	20	4.96
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	20	4.96
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	20	4.96
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	20	4.96
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	13	4.96
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	8	4.96
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	8	4.96
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	8	4.96
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	13	4.96
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	16	4.96
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	20	4.96
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	18	4.95
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	18	4.95
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	18	4.95
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	18	4.95
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	4.95
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	10	4.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	10	4.95
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	10	4.95
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	1	4.95
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	10	4.95
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	10	4.95
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	10	4.95
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	10	4.95
(4,893)	1:50:A:LYS:HA	1:51:A:GLU:HA	6	4.95
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	3	4.95
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	3	4.95
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	3	4.95
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	3	4.95
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	20	4.95
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	20	4.95
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	6	4.95
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	11	4.95
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	3	4.95
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	1	4.94
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	1	4.94
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	1	4.94
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	17	4.94
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	17	4.94
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	17	4.94
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	13	4.94
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	13	4.94
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	17	4.94
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	17	4.94
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	18	4.94
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	18	4.94
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	17	4.94
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	17	4.94
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	3	4.94
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	17	4.94
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	17	4.94
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	16	4.94
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	11	4.94
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	11	4.94
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	11	4.94
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	4	4.94
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	4	4.94
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	4	4.94
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	17	4.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	6	4.94
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	6	4.94
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	6	4.94
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	18	4.93
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	16	4.93
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	16	4.93
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	19	4.93
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	19	4.93
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	19	4.93
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	19	4.93
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	9	4.93
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	9	4.93
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	14	4.93
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	14	4.93
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	14	4.93
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	14	4.93
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	15	4.93
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	7	4.93
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	7	4.93
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	1	4.93
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	10	4.93
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	10	4.93
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	14	4.93
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	5	4.93
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	1	4.92
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	1	4.92
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	1	4.92
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	13	4.92
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	13	4.92
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	13	4.92
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	13	4.92
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	13	4.92
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	13	4.92
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	14	4.92
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	14	4.92
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	14	4.92
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	6	4.92
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	15	4.92
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	7	4.92
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	7	4.92
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	9	4.92
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	9	4.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	9	4.92
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	7	4.92
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	9	4.92
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	9	4.92
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	9	4.92
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	9	4.92
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	15	4.92
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	15	4.92
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	17	4.92
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	6	4.92
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	14	4.91
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	14	4.91
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	15	4.91
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	12	4.91
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	7	4.91
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	7	4.91
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	7	4.91
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	14	4.91
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	1	4.91
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	1	4.91
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	17	4.91
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	11	4.91
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	11	4.91
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	11	4.91
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	10	4.91
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	9	4.9
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	9	4.9
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	9	4.9
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	4	4.9
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	13	4.9
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	13	4.9
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	13	4.9
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	13	4.9
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	5	4.9
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	5	4.9
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	2	4.9
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	10	4.9
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	19	4.9
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	12	4.9
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	12	4.9
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	12	4.9
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	12	4.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	12	4.9
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	12	4.9
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	15	4.9
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	9	4.9
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	4.9
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	2	4.9
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	4.9
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	2	4.9
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	2	4.9
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	2	4.9
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	3	4.9
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	5	4.9
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	5	4.9
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	5	4.9
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	10	4.9
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	9	4.89
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	1	4.89
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	5	4.89
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	16	4.89
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	3	4.89
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	10	4.89
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	10	4.89
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	10	4.89
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	5	4.89
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	4	4.89
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	4	4.89
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	4	4.89
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	11	4.89
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	17	4.89
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	17	4.89
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	17	4.89
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	20	4.89
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	7	4.89
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	8	4.88
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	8	4.88
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	8	4.88
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	9	4.88
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	9	4.88
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	9	4.88
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	9	4.88
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	19	4.88
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	20	4.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	20	4.88
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	20	4.88
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	18	4.88
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	18	4.88
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	18	4.88
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	18	4.88
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	6	4.88
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	3	4.88
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	3	4.88
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	3	4.88
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	3	4.88
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	3	4.88
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	3	4.88
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	3	4.88
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	3	4.88
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	3	4.88
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	3	4.88
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	3	4.88
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	3	4.88
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD3	19	4.88
(4,847)	1:33:A:CYS:HA	1:37:A:LYS:HD2	19	4.88
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	9	4.88
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	9	4.88
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	20	4.88
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	20	4.88
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	9	4.88
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	9	4.88
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	20	4.88
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	20	4.88
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	18	4.88
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	17	4.88
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	14	4.88
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	14	4.88
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	14	4.88
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	15	4.87
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	15	4.87
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	15	4.87
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	16	4.87
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	16	4.87
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	16	4.87
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	16	4.87
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	20	4.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	1	4.87
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	1	4.87
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	1	4.87
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	17	4.87
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	6	4.87
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	19	4.87
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	7	4.87
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	7	4.87
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	4	4.87
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	6	4.87
(4,1030)	1:18:A:PRO:HB3	1:19:A:CYS:HB2	17	4.87
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	14	4.87
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	5	4.87
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	11	4.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	1	4.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	1	4.87
(4,321)	1:37:A:LYS:HG2	1:58:A:CYS:H	11	4.87
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	6	4.87
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	10	4.87
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	20	4.87
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	1	4.86
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	1	4.86
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	1	4.86
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	1	4.86
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	4	4.86
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	4	4.86
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	4	4.86
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	7	4.86
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	3	4.86
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	10	4.86
(4,983)	1:48:A:CYS:HB2	1:50:A:LYS:HB2	20	4.86
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	11	4.86
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	14	4.86
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	7	4.86
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	7	4.86
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	7	4.86
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	7	4.86
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	7	4.86
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	7	4.86
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	7	4.86
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	7	4.86
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	7	4.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	7	4.86
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	7	4.86
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	7	4.86
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	12	4.86
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	12	4.86
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	12	4.86
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	18	4.86
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	12	4.86
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	12	4.86
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	12	4.86
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	12	4.86
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	15	4.86
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	17	4.86
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	18	4.86
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	12	4.86
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	10	4.86
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	10	4.86
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	10	4.86
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	12	4.86
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	10	4.85
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	10	4.85
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	10	4.85
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	4	4.85
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	4	4.85
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	17	4.85
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	17	4.85
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	16	4.85
(4,949)	1:48:A:CYS:HB3	1:50:A:LYS:HB2	20	4.85
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	10	4.85
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	13	4.85
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	12	4.85
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	9	4.85
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	15	4.85
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	14	4.85
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	20	4.85
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	20	4.85
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	20	4.85
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	20	4.85
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	4	4.85
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	10	4.85
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	7	4.85
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	4	4.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	4	4.85
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	4	4.85
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	6	4.84
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	6	4.84
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	6	4.84
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	11	4.84
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	2	4.84
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	14	4.84
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	10	4.84
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	10	4.84
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	2	4.84
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	9	4.84
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	15	4.84
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	15	4.84
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	15	4.84
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	6	4.84
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	6	4.84
(4,393)	1:32:A:THR:H	1:37:A:LYS:HD3	6	4.84
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	5	4.84
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	5	4.84
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	2	4.84
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	8	4.84
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	19	4.84
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	19	4.84
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	19	4.84
(4,110)	1:19:A:CYS:HB3	1:35:A:ALA:H	7	4.84
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	20	4.83
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	20	4.83
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	20	4.83
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	14	4.83
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	14	4.83
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	14	4.83
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	14	4.83
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	1	4.83
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	5	4.83
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	5	4.83
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	5	4.83
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	7	4.83
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	7	4.83
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	1	4.83
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	12	4.83
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	19	4.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	6	4.83
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	17	4.83
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	5	4.83
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	4	4.82
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	4	4.82
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	4	4.82
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	12	4.82
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	12	4.82
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	12	4.82
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	18	4.82
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	18	4.82
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	18	4.82
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	19	4.82
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	19	4.82
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	19	4.82
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	4	4.82
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	15	4.82
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	15	4.82
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	15	4.82
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	15	4.82
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	15	4.82
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	15	4.82
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	2	4.82
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	2	4.82
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	19	4.82
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	2	4.82
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	2	4.82
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	2	4.82
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	2	4.82
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	3	4.82
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	1	4.82
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	1	4.82
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	8	4.82
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	1	4.82
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	9	4.82
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	9	4.82
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	9	4.82
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	17	4.81
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	9	4.81
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	9	4.81
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	15	4.81
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	18	4.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	4	4.81
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	4	4.81
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	4	4.81
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	5	4.81
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	13	4.81
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	5	4.81
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	7	4.81
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	20	4.81
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	16	4.81
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	5	4.81
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	9	4.81
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	18	4.81
(4,1134)	1:32:A:THR:H	1:37:A:LYS:HG2	13	4.8
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	6	4.8
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	12	4.8
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	3	4.8
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	6	4.8
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	14	4.8
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	14	4.8
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	15	4.8
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	15	4.8
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	7	4.8
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	12	4.8
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	3	4.8
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	3	4.8
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	12	4.8
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	12	4.8
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	12	4.8
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	12	4.8
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	20	4.8
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	11	4.8
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	1	4.8
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	14	4.8
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	17	4.8
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	20	4.79
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	4.79
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	16	4.79
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	16	4.79
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	2	4.79
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	7	4.79
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	8	4.79
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	12	4.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	12	4.79
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	12	4.79
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	15	4.79
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	15	4.79
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	15	4.79
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	1	4.79
(4,276)	1:39:A:CYS:HB3	1:56:A:ASP:H	11	4.79
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	6	4.79
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	20	4.79
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	10	4.78
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	18	4.78
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	8	4.78
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	2	4.78
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	2	4.78
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	9	4.78
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	5	4.78
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	15	4.78
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	9	4.78
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	16	4.78
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	2	4.78
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	10	4.78
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	14	4.78
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	15	4.78
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	15	4.78
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	15	4.78
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	9	4.78
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	15	4.78
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	13	4.78
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	2	4.78
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	7	4.78
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	7	4.78
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	7	4.78
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	5	4.78
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	3	4.77
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	3	4.77
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	3	4.77
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	15	4.77
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	15	4.77
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	15	4.77
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	12	4.77
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	16	4.77
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	16	4.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	16	4.77
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	9	4.77
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	12	4.77
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	12	4.77
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	12	4.77
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	12	4.77
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	13	4.77
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	11	4.77
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	11	4.77
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	20	4.77
(4,791)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	3	4.77
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	4	4.77
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	6	4.77
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	6	4.77
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	7	4.77
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	2	4.77
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	2	4.77
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	2	4.77
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	7	4.77
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	8	4.77
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	15	4.76
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	15	4.76
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	15	4.76
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	15	4.76
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	17	4.76
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	3	4.76
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	8	4.76
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	12	4.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	11	4.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	11	4.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	11	4.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	11	4.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	11	4.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	11	4.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB2	11	4.76
(4,855)	1:11:A:THR:HG21	1:62:A:SER:HB3	11	4.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB2	11	4.76
(4,855)	1:11:A:THR:HG22	1:62:A:SER:HB3	11	4.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB2	11	4.76
(4,855)	1:11:A:THR:HG23	1:62:A:SER:HB3	11	4.76
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	6	4.76
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	19	4.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	20	4.76
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	2	4.76
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	10	4.76
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	10	4.76
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	10	4.76
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	10	4.76
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	3	4.76
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	3	4.76
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	3	4.76
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	2	4.75
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	2	4.75
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	2	4.75
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	17	4.75
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	17	4.75
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	17	4.75
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	7	4.75
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	2	4.75
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	2	4.75
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	2	4.75
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	2	4.75
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	10	4.75
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	10	4.75
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	19	4.75
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	3	4.75
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	4	4.75
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	4	4.75
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	4	4.75
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	4	4.75
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	4	4.75
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	16	4.75
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	16	4.75
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	16	4.75
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	1	4.75
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	1	4.75
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	1	4.75
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	5	4.75
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	6	4.75
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	6	4.75
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	3	4.75
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	3	4.75
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	3	4.75
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	14	4.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	8	4.75
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	8	4.75
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	8	4.75
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	18	4.75
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	18	4.75
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	18	4.75
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	20	4.75
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	20	4.75
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	11	4.74
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	11	4.74
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	11	4.74
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	9	4.74
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	11	4.74
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	8	4.74
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	19	4.74
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	19	4.74
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	19	4.74
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	19	4.74
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	13	4.74
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	13	4.74
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	13	4.74
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	16	4.74
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	16	4.74
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	16	4.74
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	9	4.74
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	7	4.74
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	7	4.74
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	7	4.74
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	8	4.74
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	12	4.74
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	12	4.74
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	12	4.74
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	5	4.73
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	5	4.73
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	5	4.73
(4,1204)	1:38:A:THR:HG21	1:39:A:CYS:HB2	7	4.73
(4,1204)	1:38:A:THR:HG22	1:39:A:CYS:HB2	7	4.73
(4,1204)	1:38:A:THR:HG23	1:39:A:CYS:HB2	7	4.73
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	10	4.73
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	10	4.73
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	10	4.73
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	8	4.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	7	4.73
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	7	4.73
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	7	4.73
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	7	4.73
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	10	4.73
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	1	4.73
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	1	4.73
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	4	4.73
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	4	4.73
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	6	4.73
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	6	4.73
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	11	4.73
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	11	4.73
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	4	4.73
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	4	4.73
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	6	4.73
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	6	4.73
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	11	4.73
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	11	4.73
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB1	11	4.73
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB2	11	4.73
(4,768)	1:33:A:CYS:HB2	1:34:A:ALA:HB3	11	4.73
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	13	4.73
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	13	4.73
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	13	4.73
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	3	4.73
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	11	4.73
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	7	4.73
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	4	4.72
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	5	4.72
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	15	4.72
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	15	4.72
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	8	4.72
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	4	4.72
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	16	4.72
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	4	4.72
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	18	4.72
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	3	4.72
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	3	4.72
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	2	4.72
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	3	4.72
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	17	4.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	16	4.71
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	5	4.71
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	18	4.71
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	18	4.71
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	5	4.71
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	6	4.71
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	6	4.71
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	14	4.71
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	14	4.71
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	20	4.71
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	20	4.71
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	11	4.71
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	11	4.71
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	12	4.71
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	13	4.71
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	13	4.71
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	7	4.71
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	16	4.71
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	16	4.71
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	16	4.71
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	16	4.71
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	16	4.71
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	12	4.71
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	16	4.71
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	8	4.71
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	8	4.71
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	8	4.71
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	12	4.71
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	14	4.7
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	4	4.7
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	4	4.7
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	4	4.7
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	4	4.7
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB1	11	4.7
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB2	11	4.7
(4,1055)	1:33:A:CYS:H	1:34:A:ALA:HB3	11	4.7
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	4.7
(4,1015)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	16	4.7
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	19	4.7
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	19	4.7
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	7	4.7
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	2	4.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	2	4.7
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	2	4.7
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	10	4.7
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	10	4.7
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	18	4.7
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	18	4.7
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	10	4.7
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	10	4.7
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	18	4.7
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	18	4.7
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	17	4.7
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	2	4.7
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	17	4.7
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	17	4.7
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	17	4.7
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	17	4.7
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	18	4.7
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	2	4.7
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	5	4.7
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	4.7
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	5	4.7
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	5	4.7
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	5	4.7
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	8	4.7
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	9	4.7
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	13	4.7
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	15	4.69
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	15	4.69
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	12	4.69
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	12	4.69
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	19	4.69
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	19	4.69
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	19	4.69
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG21	19	4.69
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG22	19	4.69
(4,822)	1:39:A:CYS:HB3	1:42:A:THR:HG23	19	4.69
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	13	4.69
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	19	4.69
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	19	4.69
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	6	4.69
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	15	4.69
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	15	4.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	15	4.69
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	8	4.69
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	8	4.69
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	16	4.69
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	14	4.68
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	7	4.68
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	7	4.68
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	12	4.68
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	12	4.68
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	8	4.68
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	8	4.68
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	16	4.68
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	16	4.68
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	16	4.68
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	16	4.68
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	7	4.68
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	7	4.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	14	4.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	14	4.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	14	4.68
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	14	4.68
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	14	4.68
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	16	4.68
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	1	4.68
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	1	4.68
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	1	4.68
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	15	4.67
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	8	4.67
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	8	4.67
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	17	4.67
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	3	4.67
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	9	4.67
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	15	4.67
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	15	4.67
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	15	4.67
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	1	4.67
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	11	4.67
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	8	4.67
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	9	4.67
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	6	4.67
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	7	4.67
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	7	4.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	7	4.67
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	9	4.67
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	20	4.67
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	20	4.67
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	20	4.67
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	17	4.66
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	17	4.66
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	17	4.66
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	17	4.66
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	17	4.66
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	17	4.66
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	17	4.66
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	3	4.66
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	7	4.66
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	11	4.66
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	13	4.66
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	1	4.66
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	1	4.66
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	1	4.66
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	1	4.66
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	7	4.66
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	6	4.66
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	18	4.66
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	16	4.66
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	17	4.66
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	17	4.66
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	17	4.66
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	3	4.66
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	6	4.66
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	6	4.66
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	6	4.66
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	18	4.66
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	8	4.65
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	14	4.65
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	7	4.65
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	7	4.65
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	7	4.65
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	7	4.65
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	7	4.65
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	7	4.65
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	7	4.65
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	7	4.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	18	4.65
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	18	4.65
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	18	4.65
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	7	4.65
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	7	4.65
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	8	4.65
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	8	4.65
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	15	4.65
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	15	4.65
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	7	4.65
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	7	4.65
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	8	4.65
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	8	4.65
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	15	4.65
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	15	4.65
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	18	4.65
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	11	4.65
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	8	4.65
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	15	4.65
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	9	4.65
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	7	4.64
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	7	4.64
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	18	4.64
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	18	4.64
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	18	4.64
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	18	4.64
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	18	4.64
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	5	4.64
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	5	4.64
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	5	4.64
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	17	4.64
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	17	4.64
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	17	4.64
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	17	4.64
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	7	4.64
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	5	4.64
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	5	4.64
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	5	4.64
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	5	4.64
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	5	4.64
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	5	4.64
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	5	4.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	5	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	2	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	2	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	2	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	2	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	3	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	3	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	3	4.64
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	3	4.64
(4,323)	1:37:A:LYS:HG2	1:58:A:CYS:H	11	4.64
(4,323)	1:37:A:LYS:HG3	1:58:A:CYS:H	11	4.64
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	19	4.64
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	19	4.64
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	19	4.64
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	2	4.64
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	2	4.64
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	2	4.64
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	15	4.63
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	15	4.63
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	2	4.63
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	10	4.63
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	20	4.63
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	20	4.63
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	14	4.63
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	6	4.63
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	6	4.63
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	12	4.63
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	12	4.63
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	16	4.63
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	16	4.63
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	4	4.63
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	10	4.63
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	10	4.63
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	10	4.63
(4,842)	1:20:A:GLN:HA	1:22:A:GLY:HA3	5	4.63
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	15	4.63
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	15	4.63
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	14	4.63
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	14	4.63
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	14	4.63
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	14	4.63
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	13	4.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	8	4.63
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	9	4.63
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	20	4.63
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	15	4.63
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	1	4.63
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	15	4.62
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	1	4.62
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	1	4.62
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	1	4.62
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	6	4.62
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	4	4.62
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	17	4.62
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	17	4.62
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	17	4.62
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	17	4.62
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	8	4.62
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	8	4.62
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	17	4.62
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	17	4.62
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	13	4.62
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	13	4.62
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	13	4.62
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	11	4.62
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	3	4.62
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	3	4.62
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	3	4.62
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	3	4.62
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	12	4.62
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	12	4.62
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	12	4.62
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	9	4.62
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	4	4.62
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	17	4.62
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	19	4.62
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	17	4.62
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	17	4.62
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	17	4.62
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	17	4.62
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	17	4.62
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	16	4.62
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	16	4.62
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	16	4.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	15	4.61
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	12	4.61
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	16	4.61
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	9	4.61
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	9	4.61
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	9	4.61
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	9	4.61
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	17	4.61
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	13	4.61
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	13	4.61
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	13	4.61
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	12	4.61
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	12	4.61
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	2	4.61
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	14	4.61
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	14	4.61
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	14	4.61
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	17	4.61
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	17	4.61
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	17	4.61
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	14	4.61
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	8	4.61
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	20	4.61
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	4	4.61
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	4	4.61
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	4	4.61
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	4	4.61
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	20	4.61
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	20	4.61
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	20	4.61
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	10	4.61
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	11	4.61
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	17	4.61
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	11	4.6
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	18	4.6
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	6	4.6
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	5	4.6
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	4.6
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	16	4.6
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	16	4.6
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	5	4.6
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	5	4.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	3	4.6
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	3	4.6
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	11	4.6
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	11	4.6
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	20	4.6
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	4.6
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	10	4.6
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	2	4.6
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	6	4.6
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	6	4.6
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	6	4.6
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	6	4.6
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	20	4.6
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	7	4.6
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	7	4.6
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	7	4.6
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	11	4.59
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	15	4.59
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	6	4.59
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	17	4.59
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	17	4.59
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	17	4.59
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	17	4.59
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	7	4.59
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	17	4.59
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	14	4.59
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	6	4.59
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	12	4.59
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	4	4.59
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	4	4.59
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	4	4.59
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	4	4.59
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	4	4.59
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	3	4.59
(4,810)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	13	4.59
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	10	4.59
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	1	4.59
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	1	4.59
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	1	4.59
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	1	4.59
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	1	4.59
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	1	4.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	1	4.59
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	1	4.59
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	19	4.59
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	19	4.59
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	19	4.59
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	19	4.59
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	5	4.59
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	5	4.59
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	5	4.59
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	2	4.59
(4,300)	1:66:A:CYS:H	1:67:A:LYS:HE3	2	4.59
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	14	4.59
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	1	4.59
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	13	4.59
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	3	4.59
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	3	4.59
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	3	4.59
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	9	4.59
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	15	4.59
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	15	4.59
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	17	4.58
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	8	4.58
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	12	4.58
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	20	4.58
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	17	4.58
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	19	4.58
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	9	4.58
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	16	4.58
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	11	4.58
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	17	4.58
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	17	4.58
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	10	4.58
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	6	4.58
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	17	4.58
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	17	4.58
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	17	4.58
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	3	4.58
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	3	4.58
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	3	4.57
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	7	4.57
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	7	4.57
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	7	4.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	1	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	1	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	1	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	9	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	9	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	14	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	14	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	19	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	19	4.57
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	9	4.57
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	9	4.57
(4,919)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	8	4.57
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	9	4.57
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	9	4.57
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	19	4.57
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	6	4.57
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	6	4.57
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	6	4.57
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	3	4.57
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	1	4.57
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	8	4.57
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	12	4.57
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	16	4.57
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	20	4.56
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	20	4.56
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	15	4.56
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	15	4.56
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	9	4.56
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	9	4.56
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	9	4.56
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	3	4.56
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	2	4.56
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	2	4.56
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	2	4.56
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	2	4.56
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	19	4.56
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	8	4.56
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	8	4.56
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	8	4.56
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	17	4.56
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	20	4.56
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	12	4.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	12	4.56
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	12	4.56
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	18	4.56
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	18	4.56
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	18	4.56
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	15	4.55
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	19	4.55
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	4.55
(4,1013)	1:7:A:GLY:HA2	1:9:A:LYS:HG3	16	4.55
(4,1013)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	16	4.55
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	18	4.55
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	18	4.55
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	20	4.55
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	20	4.55
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	6	4.55
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	19	4.55
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	17	4.55
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	7	4.55
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	4	4.54
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	4	4.54
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	5	4.54
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	5	4.54
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	3	4.54
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	3	4.54
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	20	4.54
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	18	4.54
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	18	4.54
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	18	4.54
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	3	4.54
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	3	4.54
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	19	4.54
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	19	4.54
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	17	4.54
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	17	4.54
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	19	4.54
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	6	4.54
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	6	4.54
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	3	4.54
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	16	4.54
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	16	4.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	18	4.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	18	4.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	18	4.54
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	18	4.54
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	4.54
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	3	4.54
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	4.54
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	13	4.54
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	9	4.54
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	9	4.54
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	9	4.54
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	4	4.54
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	7	4.53
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	12	4.53
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	13	4.53
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	13	4.53
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	18	4.53
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	18	4.53
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	2	4.53
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	6	4.53
(4,593)	1:45:A:GLY:HA3	1:46:A:CYS:HB3	6	4.53
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	9	4.53
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	9	4.53
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	4	4.53
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	2	4.53
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	3	4.53
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	3	4.53
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	2	4.53
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	12	4.53
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	12	4.53
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	13	4.52
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	13	4.52
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	13	4.52
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	5	4.52
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	5	4.52
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	11	4.52
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	17	4.52
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	17	4.52
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	17	4.52
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	17	4.52
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	5	4.52
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	3	4.52
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	3	4.52
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	3	4.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	3	4.52
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	3	4.52
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	3	4.52
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	2	4.52
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	2	4.52
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	11	4.52
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	5	4.52
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	5	4.52
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	9	4.52
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	9	4.52
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	3	4.52
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	7	4.52
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	3	4.52
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	7	4.52
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	1	4.52
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	8	4.52
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	18	4.51
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	4	4.51
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	11	4.51
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	8	4.51
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	8	4.51
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	10	4.51
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	10	4.51
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	6	4.51
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	6	4.51
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	6	4.51
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	20	4.51
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	20	4.51
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	20	4.51
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	9	4.51
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	9	4.51
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	9	4.51
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	19	4.51
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	19	4.51
(4,319)	1:39:A:CYS:HB2	1:58:A:CYS:H	5	4.51
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	20	4.51
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	15	4.51
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	13	4.51
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	13	4.51
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	13	4.51
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	7	4.5
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	7	4.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	7	4.5
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	7	4.5
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	7	4.5
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	10	4.5
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	13	4.5
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	1	4.5
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	16	4.5
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	16	4.5
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	1	4.5
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	1	4.5
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	2	4.5
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	2	4.5
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	8	4.5
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	8	4.5
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	8	4.5
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	5	4.5
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	4	4.5
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	4	4.5
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	12	4.5
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	19	4.5
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	16	4.5
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	3	4.5
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	13	4.5
(4,218)	1:10:A:CYS:H	1:27:A:CYS:HA	15	4.5
(4,1202)	1:38:A:THR:HG21	1:39:A:CYS:HB3	8	4.49
(4,1202)	1:38:A:THR:HG22	1:39:A:CYS:HB3	8	4.49
(4,1202)	1:38:A:THR:HG23	1:39:A:CYS:HB3	8	4.49
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	1	4.49
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	1	4.49
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	1	4.49
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	17	4.49
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	17	4.49
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	10	4.49
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	12	4.49
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	12	4.49
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	12	4.49
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	5	4.49
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	5	4.49
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	9	4.49
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	9	4.49
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	9	4.49
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	9	4.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	9	4.49
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	9	4.49
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	9	4.49
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	9	4.49
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	9	4.49
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	12	4.49
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	17	4.49
(4,599)	1:30:A:GLY:HA3	1:32:A:THR:HB	17	4.49
(4,599)	1:30:A:GLY:HA2	1:32:A:THR:HB	17	4.49
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	4	4.49
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	4	4.49
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	19	4.49
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	13	4.49
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	13	4.49
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	13	4.49
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	13	4.49
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	8	4.49
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG2	13	4.49
(4,322)	1:58:A:CYS:H	1:59:A:LYS:HG3	13	4.49
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	12	4.49
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	1	4.49
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA3	1	4.49
(4,154)	1:28:A:GLY:H	1:61:A:GLY:HA2	1	4.49
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	4	4.49
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	4	4.49
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	4	4.49
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	6	4.49
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	6	4.49
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	5	4.48
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	9	4.48
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	9	4.48
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	9	4.48
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	9	4.48
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	8	4.48
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	3	4.48
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	7	4.48
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	1	4.48
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	1	4.48
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	1	4.48
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	6	4.48
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	6	4.48
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	18	4.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	12	4.48
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	4	4.48
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	11	4.48
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	3	4.47
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	3	4.47
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	3	4.47
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	9	4.47
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	14	4.47
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	18	4.47
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	16	4.47
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	5	4.47
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	5	4.47
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	5	4.47
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	13	4.47
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	10	4.47
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	9	4.46
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	9	4.46
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	10	4.46
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	10	4.46
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	16	4.46
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	16	4.46
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	6	4.46
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	6	4.46
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	3	4.46
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	3	4.46
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	5	4.46
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	5	4.46
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	5	4.46
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	12	4.46
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	2	4.46
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	2	4.46
(4,956)	1:7:A:GLY:HA3	1:31:A:CYS:HB2	1	4.46
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	9	4.46
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	9	4.46
(4,809)	1:63:A:SER:HB2	1:64:A:CYS:HB2	16	4.46
(4,809)	1:63:A:SER:HB3	1:64:A:CYS:HB2	16	4.46
(4,807)	1:63:A:SER:HB2	1:64:A:CYS:HB2	16	4.46
(4,807)	1:63:A:SER:HB3	1:64:A:CYS:HB2	16	4.46
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	8	4.46
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	8	4.46
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	8	4.46
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	8	4.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	11	4.46
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	11	4.46
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	17	4.46
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	19	4.46
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	2	4.45
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	2	4.45
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	17	4.45
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	17	4.45
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	5	4.45
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	15	4.45
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	13	4.45
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	13	4.45
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	19	4.45
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	19	4.45
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	19	4.45
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	19	4.45
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	1	4.45
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	11	4.45
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	11	4.45
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	17	4.45
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	17	4.45
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	17	4.45
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	1	4.45
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	19	4.45
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	19	4.45
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	3	4.45
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	4	4.45
(4,401)	1:56:A:ASP:HB2	1:57:A:SER:HA	13	4.45
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	7	4.45
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	7	4.45
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	19	4.44
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	19	4.44
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	19	4.44
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	12	4.44
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	15	4.44
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	4	4.44
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	4	4.44
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	12	4.44
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	15	4.44
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	1	4.44
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	3	4.44
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	1	4.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	14	4.44
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	10	4.44
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	3	4.44
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	2	4.44
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	4	4.44
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	13	4.43
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	16	4.43
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	16	4.43
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB2	1	4.43
(4,939)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	1	4.43
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB1	1	4.43
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB2	1	4.43
(4,849)	1:33:A:CYS:HA	1:35:A:ALA:HB3	1	4.43
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	12	4.43
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	6	4.43
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	6	4.43
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	6	4.43
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	1	4.43
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	1	4.43
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	12	4.43
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	5	4.43
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	9	4.43
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	11	4.43
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	16	4.43
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	4	4.43
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	4	4.43
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	4	4.43
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	4	4.43
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	18	4.43
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	2	4.42
(4,1118)	1:54:A:GLY:HA2	1:55:A:PRO:HG2	19	4.42
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	8	4.42
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	8	4.42
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	8	4.42
(4,1048)	1:32:A:THR:HG21	1:37:A:LYS:HE3	11	4.42
(4,1048)	1:32:A:THR:HG22	1:37:A:LYS:HE3	11	4.42
(4,1048)	1:32:A:THR:HG23	1:37:A:LYS:HE3	11	4.42
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	17	4.42
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	4	4.42
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	4	4.42
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	4	4.42
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	4	4.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	15	4.42
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	15	4.42
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	2	4.42
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	2	4.42
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	19	4.42
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	10	4.42
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	18	4.42
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	19	4.42
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	3	4.42
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	20	4.42
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	8	4.42
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	16	4.42
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	16	4.42
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	16	4.42
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	6	4.41
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	4.41
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	20	4.41
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	4.41
(4,1078)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	13	4.41
(4,904)	1:38:A:THR:HB	1:55:A:PRO:HB3	5	4.41
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	5	4.41
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	9	4.41
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	9	4.41
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	1	4.41
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	4	4.41
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	6	4.41
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	5	4.41
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	13	4.41
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	13	4.41
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	13	4.41
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	14	4.41
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	12	4.41
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	5	4.41
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	16	4.4
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	10	4.4
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	10	4.4
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	15	4.4
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	15	4.4
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	10	4.4
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	10	4.4
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	19	4.4
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	19	4.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	11	4.4
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	11	4.4
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	11	4.4
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	5	4.4
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	12	4.4
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	17	4.4
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	15	4.4
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	15	4.4
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	15	4.4
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	15	4.4
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	5	4.4
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	5	4.4
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	5	4.4
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	19	4.4
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	5	4.4
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD2	5	4.4
(4,398)	1:58:A:CYS:HA	1:59:A:LYS:HD3	5	4.4
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	19	4.4
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	13	4.4
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	1	4.4
(4,127)	1:11:A:THR:H	1:27:A:CYS:H	5	4.4
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	11	4.4
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	8	4.4
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	8	4.4
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	11	4.4
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	11	4.4
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	2	4.39
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	3	4.39
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	3	4.39
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	14	4.39
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	14	4.39
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	14	4.39
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	4	4.39
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	11	4.39
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	11	4.39
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	17	4.39
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	14	4.39
(4,563)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	16	4.39
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	9	4.39
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	2	4.39
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	10	4.39
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	16	4.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	18	4.39
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	10	4.39
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	13	4.39
(4,1080)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	13	4.38
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	4	4.38
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	4	4.38
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	4	4.38
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	4	4.38
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	4	4.38
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	4	4.38
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	10	4.38
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	5	4.38
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	5	4.38
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	12	4.38
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	12	4.38
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	13	4.38
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	13	4.38
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	8	4.38
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	12	4.38
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	12	4.38
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	18	4.38
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	4.38
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	17	4.38
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	17	4.38
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	17	4.38
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	8	4.38
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	20	4.38
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	1	4.38
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	18	4.38
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	18	4.38
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	5	4.38
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	9	4.38
(4,313)	1:52:A:CYS:HB3	1:58:A:CYS:H	8	4.38
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	9	4.38
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	10	4.38
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	14	4.38
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	15	4.38
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	14	4.38
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	17	4.38
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	13	4.37
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	14	4.37
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	14	4.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	14	4.37
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	14	4.37
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	13	4.37
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	13	4.37
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	13	4.37
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	14	4.37
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	1	4.37
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	1	4.37
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	17	4.37
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	17	4.37
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	17	4.37
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	1	4.37
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	20	4.37
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	20	4.37
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	1	4.37
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	1	4.37
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	1	4.37
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	17	4.37
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	18	4.37
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	16	4.37
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	17	4.37
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	17	4.37
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	19	4.36
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	15	4.36
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	15	4.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	3	4.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	3	4.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	3	4.36
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	3	4.36
(4,1079)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	9	4.36
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	14	4.36
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	14	4.36
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	20	4.36
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	20	4.36
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	20	4.36
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	1	4.36
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	13	4.36
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	15	4.36
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	19	4.36
(4,626)	1:28:A:GLY:HA3	1:31:A:CYS:HB3	19	4.36
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	11	4.36
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	3	4.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	20	4.36
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	7	4.36
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	12	4.36
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	16	4.36
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	17	4.36
(4,455)	1:60:A:CYS:HB3	1:67:A:LYS:HD3	16	4.36
(4,395)	1:32:A:THR:H	1:37:A:LYS:HD2	19	4.36
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	3	4.36
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	9	4.36
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	16	4.36
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	19	4.36
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	3	4.36
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	8	4.36
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	12	4.36
(4,1139)	1:67:A:LYS:HA	1:67:A:LYS:HE2	16	4.35
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	16	4.35
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	18	4.35
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	18	4.35
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	18	4.35
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	18	4.35
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	18	4.35
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	18	4.35
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	13	4.35
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	16	4.35
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	16	4.35
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	3	4.35
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	8	4.35
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	11	4.35
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	13	4.35
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	14	4.35
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	16	4.35
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	10	4.35
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	14	4.35
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	12	4.35
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	5	4.35
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	6	4.35
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	15	4.35
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	4	4.35
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	4	4.35
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	6	4.34
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	2	4.34
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	10	4.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	10	4.34
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	10	4.34
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	10	4.34
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	10	4.34
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	10	4.34
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	6	4.34
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	6	4.34
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	15	4.34
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	15	4.34
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	15	4.34
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	4	4.34
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	18	4.34
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	4.34
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	18	4.34
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	4.34
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	18	4.34
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	18	4.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	7	4.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	7	4.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	7	4.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	7	4.34
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	14	4.34
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	11	4.34
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	11	4.34
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	8	4.34
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	8	4.34
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	8	4.34
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	15	4.34
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	14	4.34
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	13	4.34
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	9	4.34
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	17	4.34
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	1	4.34
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	1	4.34
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	7	4.34
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	3	4.33
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	11	4.33
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	4.33
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	17	4.33
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	15	4.33
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	15	4.33
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	15	4.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	20	4.33
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	20	4.33
(4,738)	1:12:A:SER:HA	1:16:A:SER:H	18	4.33
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	20	4.33
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	2	4.33
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	20	4.33
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	4	4.33
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	7	4.33
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	12	4.33
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	7	4.33
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	1	4.33
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	13	4.33
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	8	4.32
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	12	4.32
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	12	4.32
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	14	4.32
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	14	4.32
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	14	4.32
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	17	4.32
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	17	4.32
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	12	4.32
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	12	4.32
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	12	4.32
(4,922)	1:21:A:CYS:HA	1:36:A:CYS:HB3	7	4.32
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	8	4.32
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	8	4.32
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	8	4.32
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	5	4.32
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	6	4.32
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	12	4.32
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	11	4.32
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	14	4.32
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	19	4.32
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	6	4.32
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	18	4.32
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	1	4.31
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	1	4.31
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	1	4.31
(4,1144)	1:60:A:CYS:HB2	1:67:A:LYS:HD2	16	4.31
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	1	4.31
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	17	4.31
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	7	4.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	10	4.31
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	19	4.31
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	19	4.31
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	8	4.31
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	18	4.31
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	20	4.31
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	2	4.31
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	12	4.31
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	3	4.31
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	11	4.31
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	9	4.3
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	7	4.3
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	7	4.3
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	14	4.3
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	11	4.3
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	5	4.3
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	4	4.3
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	4	4.3
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	4	4.3
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	4	4.3
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	8	4.3
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	4.3
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	8	4.3
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	19	4.3
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	19	4.3
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	19	4.3
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	19	4.3
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	20	4.3
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	6	4.29
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	17	4.29
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	14	4.29
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	14	4.29
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	20	4.29
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	11	4.29
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	10	4.29
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	10	4.29
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	10	4.29
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	10	4.29
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	4	4.29
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	4	4.29
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	4	4.29
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	10	4.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	3	4.29
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	11	4.29
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	19	4.29
(4,239)	1:34:A:ALA:HB1	1:37:A:LYS:H	1	4.29
(4,239)	1:34:A:ALA:HB2	1:37:A:LYS:H	1	4.29
(4,239)	1:34:A:ALA:HB3	1:37:A:LYS:H	1	4.29
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	19	4.29
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	19	4.29
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	6	4.29
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	4	4.29
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	20	4.29
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	4	4.28
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	19	4.28
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	19	4.28
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	9	4.28
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	9	4.28
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	9	4.28
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	4	4.28
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	4	4.28
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	16	4.28
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	16	4.28
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	16	4.28
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	16	4.28
(4,740)	1:40:A:ASN:HA	1:66:A:CYS:HB2	16	4.28
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	1	4.28
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	1	4.28
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	1	4.28
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	1	4.28
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	1	4.28
(4,518)	1:54:A:GLY:HA3	1:55:A:PRO:HG2	8	4.28
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	3	4.28
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	3	4.28
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	3	4.28
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	15	4.28
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	3	4.28
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	2	4.28
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	2	4.28
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	20	4.28
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	2	4.28
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	9	4.28
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	9	4.28
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	4	4.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	17	4.27
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	15	4.27
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	6	4.27
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	6	4.27
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	6	4.27
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	5	4.27
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	5	4.27
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	5	4.27
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	20	4.27
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	20	4.27
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	8	4.27
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	8	4.27
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	12	4.27
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	12	4.27
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	12	4.27
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	12	4.27
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	13	4.27
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	13	4.27
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	20	4.27
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	20	4.27
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	15	4.27
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	9	4.27
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	2	4.27
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	5	4.27
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	5	4.27
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	6	4.27
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	6	4.26
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	6	4.26
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	5	4.26
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	5	4.26
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	19	4.26
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	2	4.26
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	2	4.26
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	8	4.26
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	8	4.26
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	14	4.26
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	17	4.26
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	7	4.26
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	7	4.26
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	7	4.26
(4,404)	1:41:A:CYS:HA	1:42:A:THR:HA	1	4.26
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	6	4.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	4	4.26
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	14	4.26
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	17	4.26
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	18	4.26
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	18	4.26
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	18	4.26
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	13	4.25
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	13	4.25
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	13	4.25
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	13	4.25
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	13	4.25
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	13	4.25
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	2	4.25
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	16	4.25
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	16	4.25
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	16	4.25
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	19	4.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	4.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	4.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	4.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	4.25
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	17	4.25
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	17	4.25
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	5	4.25
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	5	4.25
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	15	4.25
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	4	4.25
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	18	4.25
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	16	4.25
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	11	4.25
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	6	4.25
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	20	4.25
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	20	4.25
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	20	4.25
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	20	4.25
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	2	4.25
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	6	4.25
(4,32)	1:54:A:GLY:H	1:58:A:CYS:HA	5	4.25
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	20	4.25
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	20	4.25
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	3	4.25
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	3	4.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	3	4.24
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	3	4.24
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	12	4.24
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	12	4.24
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	12	4.24
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	12	4.24
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	15	4.24
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	15	4.24
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	15	4.24
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	15	4.24
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	7	4.24
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	7	4.24
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	7	4.24
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	4	4.24
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	4	4.24
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	12	4.24
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	12	4.24
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	12	4.24
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	13	4.24
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	13	4.24
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	13	4.24
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	14	4.24
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	14	4.24
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	14	4.24
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	16	4.24
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	16	4.24
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	16	4.24
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	11	4.24
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	5	4.24
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	5	4.24
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	17	4.24
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	17	4.24
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	7	4.24
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	4	4.24
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	12	4.24
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	12	4.24
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	13	4.24
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	13	4.24
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	11	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	11	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	12	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	12	4.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	14	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	14	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	18	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	18	4.23
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	11	4.23
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	11	4.23
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	1	4.23
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	6	4.23
(4,710)	1:15:A:ARG:HG2	1:16:A:SER:H	10	4.23
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	15	4.23
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	15	4.23
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	15	4.23
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	18	4.23
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	18	4.23
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	18	4.23
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	18	4.23
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	5	4.23
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	5	4.23
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	12	4.23
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	12	4.23
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	13	4.23
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	14	4.23
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	18	4.23
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	3	4.23
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	3	4.23
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	3	4.23
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	8	4.22
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	8	4.22
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	19	4.22
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	19	4.22
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	12	4.22
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	11	4.22
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	12	4.22
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	12	4.22
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	12	4.22
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	7	4.22
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	7	4.22
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	1	4.22
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	8	4.22
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	8	4.22
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	14	4.22
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	14	4.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	7	4.22
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	7	4.22
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	7	4.22
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	7	4.22
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	8	4.22
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	10	4.22
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	11	4.22
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	11	4.22
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	1	4.22
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	19	4.22
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	6	4.22
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	6	4.22
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	6	4.22
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	15	4.22
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	15	4.22
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	15	4.22
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	2	4.22
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	1	4.21
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	1	4.21
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	14	4.21
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	14	4.21
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	6	4.21
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	6	4.21
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	6	4.21
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	6	4.21
(4,974)	1:42:A:THR:HG21	1:55:A:PRO:HD3	19	4.21
(4,974)	1:42:A:THR:HG22	1:55:A:PRO:HD3	19	4.21
(4,974)	1:42:A:THR:HG23	1:55:A:PRO:HD3	19	4.21
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	3	4.21
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	19	4.21
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	19	4.21
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	19	4.21
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	2	4.21
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	2	4.21
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	10	4.21
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	10	4.21
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	11	4.21
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	11	4.21
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	2	4.21
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	17	4.21
(4,231)	1:33:A:CYS:H	1:36:A:CYS:H	11	4.21
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	13	4.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,104)	1:33:A:CYS:H	1:36:A:CYS:H	11	4.21
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	8	4.21
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	8	4.21
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	8	4.21
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	13	4.21
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	13	4.21
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	13	4.21
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	19	4.21
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	13	4.2
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	6	4.2
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	16	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	4	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	4	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	5	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	5	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	9	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	9	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	12	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	12	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	16	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	16	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	17	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	17	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	20	4.2
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	20	4.2
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	3	4.2
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	6	4.2
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	2	4.2
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	5	4.2
(4,168)	1:14:A:CYS:H	1:20:A:GLN:H	5	4.2
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	5	4.2
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	5	4.2
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	5	4.2
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	11	4.2
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	15	4.19
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	15	4.19
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	3	4.19
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	6	4.19
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	14	4.19
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	5	4.19
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	5	4.19
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	20	4.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	20	4.19
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	20	4.19
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	20	4.19
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	6	4.19
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	20	4.19
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	20	4.19
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	20	4.19
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	1	4.19
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	13	4.19
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	13	4.19
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	19	4.19
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	19	4.19
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	2	4.19
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	2	4.19
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	2	4.19
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	5	4.19
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	5	4.19
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	5	4.19
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	14	4.19
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	14	4.19
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	14	4.19
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	15	4.19
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	15	4.19
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	15	4.19
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	8	4.19
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	8	4.19
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	4	4.19
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	2	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	11	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	11	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	11	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	16	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	16	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	16	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	19	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	19	4.19
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	19	4.19
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	2	4.19
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	2	4.19
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	5	4.19
(4,1154)	1:37:A:LYS:HG3	1:38:A:THR:HA	17	4.18
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	6	4.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	7	4.18
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	7	4.18
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	7	4.18
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	7	4.18
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	3	4.18
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	3	4.18
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	3	4.18
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	9	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	3	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	3	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	6	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	6	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	7	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	7	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	8	4.18
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	8	4.18
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	12	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	5	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	5	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	5	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	5	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	6	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	6	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	6	4.18
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	6	4.18
(4,294)	1:64:A:CYS:HA	1:66:A:CYS:H	17	4.18
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	4	4.18
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	1	4.18
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	1	4.18
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	1	4.18
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	17	4.18
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	17	4.18
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	17	4.18
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	6	4.17
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	18	4.17
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA2	8	4.17
(4,917)	1:60:A:CYS:HB3	1:61:A:GLY:HA3	8	4.17
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	2	4.17
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	2	4.17
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	2	4.17
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	18	4.17
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	18	4.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	18	4.17
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	18	4.17
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	15	4.17
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	15	4.17
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	15	4.17
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	15	4.17
(4,329)	1:49:A:GLY:H	1:50:A:LYS:HB2	16	4.17
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	18	4.17
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	17	4.17
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	14	4.16
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	14	4.16
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	14	4.16
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	14	4.16
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	6	4.16
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	6	4.16
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	20	4.16
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	20	4.16
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	10	4.16
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	4	4.16
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	15	4.16
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	11	4.16
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	11	4.16
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	11	4.16
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	5	4.16
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	5	4.16
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	5	4.16
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	5	4.16
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	3	4.16
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	4	4.16
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	15	4.16
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	9	4.16
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	9	4.16
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	9	4.16
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	16	4.15
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	16	4.15
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	15	4.15
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	15	4.15
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	15	4.15
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	15	4.15
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	3	4.15
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	3	4.15
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	3	4.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	3	4.15
(4,1039)	1:37:A:LYS:HB3	1:38:A:THR:HA	13	4.15
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	16	4.15
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	16	4.15
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	16	4.15
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	16	4.15
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	1	4.15
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	1	4.15
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	1	4.15
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	2	4.15
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	2	4.15
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	3	4.15
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	2	4.15
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	2	4.15
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	2	4.15
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	4	4.15
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	12	4.15
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	12	4.15
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	12	4.15
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	18	4.15
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	18	4.15
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	18	4.15
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	8	4.15
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	8	4.15
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	19	4.15
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	18	4.15
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	5	4.15
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	19	4.15
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	14	4.15
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	14	4.15
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	14	4.15
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	17	4.15
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	7	4.15
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	7	4.15
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	18	4.15
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	18	4.15
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	7	4.14
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	20	4.14
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	4	4.14
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	4	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	2	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	2	4.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	2	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	2	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	10	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	10	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	10	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	10	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	12	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	12	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	12	4.14
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	12	4.14
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	1	4.14
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	10	4.14
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	10	4.14
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	10	4.14
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	19	4.14
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	19	4.14
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	19	4.14
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	19	4.14
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	19	4.14
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	19	4.14
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	19	4.14
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	19	4.14
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA2	1	4.14
(4,600)	1:44:A:ASP:HA	1:45:A:GLY:HA3	1	4.14
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD2	3	4.14
(4,568)	1:41:A:CYS:HB3	1:47:A:LYS:HD3	3	4.14
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	2	4.14
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	14	4.14
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	20	4.13
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	20	4.13
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	11	4.13
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	3	4.13
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	3	4.13
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	14	4.13
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	14	4.13
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	14	4.13
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	14	4.13
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	14	4.13
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	14	4.13
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	15	4.13
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	5	4.13
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	13	4.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	20	4.13
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	4.13
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	16	4.13
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	16	4.13
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	16	4.13
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	16	4.13
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	13	4.13
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	4	4.13
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	4	4.13
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	4	4.13
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	5	4.12
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	5	4.12
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	5	4.12
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	14	4.12
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	14	4.12
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	3	4.12
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	3	4.12
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	7	4.12
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	7	4.12
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	7	4.12
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	10	4.12
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	4.12
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	4.12
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	4.12
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	4.12
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	2	4.12
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	2	4.12
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	13	4.12
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	9	4.12
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	9	4.12
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	9	4.12
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	10	4.12
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	1	4.12
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	9	4.12
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	15	4.12
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	3	4.11
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	3	4.11
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	11	4.11
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	11	4.11
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	7	4.11
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	7	4.11
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	5	4.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	5	4.11
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	5	4.11
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	4	4.11
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	12	4.11
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	10	4.11
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	19	4.11
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	19	4.11
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	10	4.11
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	6	4.1
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	6	4.1
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	6	4.1
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	10	4.1
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	4	4.1
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	4	4.1
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	4	4.1
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	4	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	5	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	5	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	5	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	5	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	18	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	18	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	18	4.1
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	18	4.1
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	8	4.1
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	8	4.1
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	14	4.1
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	14	4.1
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	14	4.1
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	14	4.1
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	14	4.1
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	14	4.1
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	20	4.1
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	6	4.1
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	4	4.1
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	2	4.1
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	2	4.1
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	2	4.1
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	18	4.1
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	4	4.09
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	4	4.09
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	4	4.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	16	4.09
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	16	4.09
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	16	4.09
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	15	4.09
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	15	4.09
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	3	4.09
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	17	4.09
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	17	4.09
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	17	4.09
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	12	4.09
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	2	4.09
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	2	4.09
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	7	4.09
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	11	4.09
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	15	4.09
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	16	4.09
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	18	4.09
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	20	4.09
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	20	4.09
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	20	4.09
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	6	4.09
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	19	4.09
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	14	4.09
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	14	4.09
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	3	4.08
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	3	4.08
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	3	4.08
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	17	4.08
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	17	4.08
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	17	4.08
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	17	4.08
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	17	4.08
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	17	4.08
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	6	4.08
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	6	4.08
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	13	4.08
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	13	4.08
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	13	4.08
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	13	4.08
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	4	4.08
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	4	4.08
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	4	4.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	4	4.08
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	4	4.08
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	4	4.08
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	3	4.08
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	3	4.08
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	3	4.08
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	3	4.08
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	4	4.08
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	10	4.08
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	10	4.08
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	10	4.08
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	1	4.08
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	2	4.07
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	2	4.07
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	2	4.07
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	2	4.07
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	19	4.07
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	9	4.07
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	9	4.07
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	9	4.07
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	18	4.07
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	18	4.07
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	18	4.07
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	16	4.07
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	16	4.07
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	15	4.07
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	15	4.07
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	15	4.07
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	6	4.07
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	6	4.07
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	6	4.07
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	7	4.07
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	9	4.07
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	20	4.07
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	20	4.07
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	20	4.07
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	20	4.07
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	8	4.07
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	8	4.07
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	8	4.07
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	6	4.07
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	6	4.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	2	4.07
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	7	4.07
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	9	4.07
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	8	4.07
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	14	4.07
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	3	4.07
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	9	4.07
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	18	4.06
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	18	4.06
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	18	4.06
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	19	4.06
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	20	4.06
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	1	4.06
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	1	4.06
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	20	4.06
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	9	4.06
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	9	4.06
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	9	4.06
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	18	4.06
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	18	4.06
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	11	4.06
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	11	4.06
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	11	4.06
(4,552)	1:40:A:ASN:HB2	1:67:A:LYS:HA	10	4.06
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	20	4.06
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	7	4.06
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	7	4.06
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	15	4.06
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	15	4.06
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	20	4.06
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	4	4.06
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	9	4.06
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	4.05
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	4.05
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	4.05
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	4.05
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	5	4.05
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	11	4.05
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	11	4.05
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	11	4.05
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	11	4.05
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	7	4.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	15	4.05
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	9	4.05
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	9	4.05
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	9	4.05
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	9	4.05
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	9	4.05
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	9	4.05
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	7	4.05
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	7	4.05
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	7	4.05
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	8	4.05
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	8	4.05
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	8	4.05
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	14	4.05
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	14	4.05
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	14	4.05
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	16	4.05
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	16	4.05
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	16	4.05
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	13	4.05
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	9	4.05
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	9	4.05
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	19	4.05
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	19	4.05
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	9	4.05
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	15	4.05
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	11	4.05
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	1	4.05
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	4	4.04
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	4	4.04
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	4	4.04
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	4	4.04
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	5	4.04
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	5	4.04
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	5	4.04
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	7	4.04
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	7	4.04
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	7	4.04
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	7	4.04
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	12	4.04
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	12	4.04
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	12	4.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,499)	1:63:A:SER:HA	1:67:A:LYS:HG3	13	4.04
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	11	4.04
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	11	4.04
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	12	4.04
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	18	4.04
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	18	4.04
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	18	4.04
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	18	4.04
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	6	4.04
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	13	4.04
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	13	4.04
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	18	4.04
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	7	4.04
(4,8)	1:15:A:ARG:HG2	1:16:A:SER:H	10	4.04
(4,8)	1:15:A:ARG:HG3	1:16:A:SER:H	10	4.04
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	5	4.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	5	4.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD2	5	4.03
(4,1090)	1:58:A:CYS:HA	1:59:A:LYS:HD3	5	4.03
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	8	4.03
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	8	4.03
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	8	4.03
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	8	4.03
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	8	4.03
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	8	4.03
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	5	4.03
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	5	4.03
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	5	4.03
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	13	4.03
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	13	4.03
(4,858)	1:11:A:THR:HG21	1:14:A:CYS:HB3	8	4.03
(4,858)	1:11:A:THR:HG22	1:14:A:CYS:HB3	8	4.03
(4,858)	1:11:A:THR:HG23	1:14:A:CYS:HB3	8	4.03
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	2	4.03
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	2	4.03
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	16	4.03
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	16	4.03
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	16	4.03
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	16	4.03
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	14	4.03
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	3	4.03
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	7	4.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	10	4.03
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	10	4.03
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	10	4.03
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	10	4.03
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	8	4.03
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	11	4.02
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	11	4.02
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	11	4.02
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	11	4.02
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	4	4.02
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	4	4.02
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	4	4.02
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	13	4.02
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	13	4.02
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	13	4.02
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	18	4.02
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	18	4.02
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	18	4.02
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	19	4.02
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	19	4.02
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	19	4.02
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	11	4.02
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	11	4.02
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	11	4.02
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	20	4.02
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	9	4.02
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	17	4.02
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	17	4.02
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	7	4.02
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	7	4.02
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	7	4.02
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	5	4.02
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	3	4.01
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	3	4.01
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	3	4.01
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	15	4.01
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	15	4.01
(4,1121)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	8	4.01
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA2	17	4.01
(4,1004)	1:4:A:LYS:HB2	1:5:A:GLY:HA3	17	4.01
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	19	4.01
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	19	4.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	1	4.01
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	1	4.01
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	1	4.01
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	10	4.01
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	10	4.01
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	10	4.01
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	8	4.01
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	17	4.01
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	7	4.01
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	7	4.01
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	7	4.01
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	1	4.01
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	1	4.01
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	1	4.01
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	1	4.01
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	1	4.01
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	1	4.01
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	19	4.01
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	18	4.01
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	18	4.01
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	20	4.01
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	20	4.01
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	20	4.01
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	5	4.01
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	9	4.01
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	9	4.01
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	9	4.01
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	9	4.01
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	12	4.01
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	12	4.01
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	12	4.01
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	12	4.01
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	17	4.01
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	19	4.01
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	8	4.0
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	8	4.0
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	8	4.0
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	8	4.0
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	2	4.0
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	2	4.0
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	2	4.0
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	18	4.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	18	4.0
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	8	4.0
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	8	4.0
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	8	4.0
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	8	4.0
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	15	4.0
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	15	4.0
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	15	4.0
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	15	4.0
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	19	4.0
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	19	4.0
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	19	4.0
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	19	4.0
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	19	4.0
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	19	4.0
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	19	4.0
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	19	4.0
(4,1034)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	12	4.0
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	6	4.0
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	10	4.0
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	16	4.0
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	9	4.0
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	9	4.0
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	9	4.0
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	1	4.0
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	12	4.0
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	12	4.0
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	17	4.0
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	17	4.0
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	12	4.0
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	12	4.0
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	12	4.0
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	12	4.0
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	14	4.0
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	14	4.0
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	14	4.0
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	14	4.0
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	1	4.0
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	10	4.0
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	8	3.99
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	8	3.99
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	8	3.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	8	3.99
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	16	3.99
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	16	3.99
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	14	3.99
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	14	3.99
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	14	3.99
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	14	3.99
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	2	3.99
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	3	3.99
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	3	3.99
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	2	3.99
(4,765)	1:54:A:GLY:HA3	1:56:A:ASP:HB2	3	3.99
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	6	3.99
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	6	3.99
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	6	3.99
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	2	3.99
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	2	3.99
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	2	3.99
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	2	3.99
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	2	3.99
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	2	3.99
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	2	3.99
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	2	3.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	19	3.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	19	3.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	19	3.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	19	3.99
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	10	3.99
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	10	3.99
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	10	3.99
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	6	3.99
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	6	3.99
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	6	3.99
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	6	3.99
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	9	3.99
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	12	3.99
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA2	12	3.99
(4,48)	1:44:A:ASP:H	1:45:A:GLY:HA3	12	3.99
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	3.98
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	10	3.98
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	10	3.98
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	10	3.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	11	3.98
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	11	3.98
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	11	3.98
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	15	3.98
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	15	3.98
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	15	3.98
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	9	3.98
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	10	3.98
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	10	3.98
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	10	3.98
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	15	3.98
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	15	3.98
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	15	3.98
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	2	3.98
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	2	3.98
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	2	3.98
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	10	3.98
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	10	3.98
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	10	3.98
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	10	3.98
(4,340)	1:51:A:GLU:HB2	1:52:A:CYS:H	17	3.98
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	1	3.98
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	1	3.98
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	1	3.98
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	1	3.98
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	18	3.98
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	18	3.98
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	18	3.98
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	18	3.98
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	18	3.98
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	19	3.98
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	10	3.98
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	16	3.98
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	12	3.97
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	12	3.97
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	20	3.97
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	2	3.97
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	3	3.97
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	4	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	3.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	3.97
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	11	3.97
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	11	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	3.97
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	3.97
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	3.97
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	3.97
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	5	3.97
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	5	3.97
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	5	3.97
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	18	3.97
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	18	3.97
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	18	3.97
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	1	3.97
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	1	3.97
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	1	3.97
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	1	3.97
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	6	3.97
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	6	3.97
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	6	3.97
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	4	3.97
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	4	3.97
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	4	3.97
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	4	3.97
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	17	3.97
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	17	3.97
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	17	3.97
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	17	3.97
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	5	3.97
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	5	3.97
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	3	3.96
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	13	3.96
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	9	3.96
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	9	3.96
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	9	3.96
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	9	3.96
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	15	3.96
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	15	3.96
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	15	3.96
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	15	3.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	15	3.96
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	15	3.96
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	15	3.96
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	15	3.96
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	15	3.96
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	6	3.96
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	8	3.96
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	15	3.96
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	15	3.96
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	15	3.96
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	4	3.96
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	4	3.96
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	11	3.96
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	11	3.96
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	11	3.96
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	11	3.96
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	6	3.96
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	8	3.96
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	9	3.96
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	9	3.96
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	3	3.96
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	2	3.96
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	3	3.96
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	3	3.95
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	3	3.95
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	3	3.95
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	3	3.95
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	18	3.95
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	11	3.95
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	11	3.95
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	5	3.95
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	5	3.95
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	15	3.95
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	15	3.95
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	20	3.95
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	20	3.95
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	20	3.95
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	20	3.95
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	3	3.95
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	3	3.95
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	3	3.95
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	14	3.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	14	3.95
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	14	3.95
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	14	3.95
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	14	3.95
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	14	3.95
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	14	3.95
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	14	3.95
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	11	3.95
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	13	3.95
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	19	3.95
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	16	3.95
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	16	3.95
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	16	3.95
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	5	3.95
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	5	3.95
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	20	3.95
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	20	3.95
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	20	3.95
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	20	3.95
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	10	3.95
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	10	3.95
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	14	3.95
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	5	3.95
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	7	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	7	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	7	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	7	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	9	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	9	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	9	3.94
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	9	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	5	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	5	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	5	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	10	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	10	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	10	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	19	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	19	3.94
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	19	3.94
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	8	3.94
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	8	3.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	8	3.94
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	8	3.94
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	5	3.94
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	19	3.94
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	19	3.94
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	9	3.94
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	9	3.94
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	9	3.94
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	9	3.94
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	9	3.94
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	9	3.94
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	9	3.94
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	20	3.94
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	19	3.94
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	19	3.94
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	19	3.94
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	19	3.94
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	19	3.94
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	10	3.94
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	4	3.94
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	4	3.94
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	7	3.94
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	7	3.94
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	7	3.93
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	20	3.93
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	20	3.93
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	20	3.93
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	11	3.93
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	11	3.93
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	14	3.93
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	14	3.93
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	13	3.93
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	13	3.93
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	3.93
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	3.93
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	3.93
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	3.93
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	19	3.93
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	19	3.93
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	15	3.93
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	12	3.93
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	12	3.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	12	3.93
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	12	3.93
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	3	3.93
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	3	3.93
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	3	3.93
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	3	3.93
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	14	3.93
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	1	3.92
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	1	3.92
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	1	3.92
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	18	3.92
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	18	3.92
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	18	3.92
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	13	3.92
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	13	3.92
(4,1126)	1:7:A:GLY:HA2	1:9:A:LYS:HG2	8	3.92
(4,1126)	1:7:A:GLY:HA3	1:9:A:LYS:HG2	8	3.92
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	13	3.92
(4,1076)	1:37:A:LYS:HB3	1:55:A:PRO:HG2	13	3.92
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	11	3.92
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	11	3.92
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	11	3.92
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	19	3.92
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	19	3.92
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	14	3.92
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	14	3.92
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	14	3.92
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	3.92
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	3.92
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	3.92
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	3.92
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	8	3.92
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	8	3.92
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	2	3.92
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	4	3.92
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	20	3.92
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	20	3.92
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	13	3.92
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	13	3.92
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	13	3.92
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	8	3.92
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	8	3.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	8	3.92
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	8	3.92
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	18	3.92
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	16	3.92
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	16	3.92
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	18	3.92
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	18	3.92
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	18	3.92
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	18	3.92
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	16	3.91
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	6	3.91
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	6	3.91
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	6	3.91
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	13	3.91
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	13	3.91
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	13	3.91
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	8	3.91
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	15	3.91
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	15	3.91
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	6	3.91
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	6	3.91
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	4	3.91
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	4	3.91
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	4	3.91
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	4	3.91
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	4	3.91
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	4	3.91
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	4	3.91
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	11	3.91
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	11	3.91
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	11	3.91
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	7	3.91
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	14	3.91
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	15	3.91
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	15	3.91
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	15	3.91
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	19	3.91
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	19	3.91
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	19	3.91
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	16	3.91
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	14	3.91
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	19	3.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	19	3.91
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	19	3.91
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	19	3.91
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	5	3.9
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	5	3.9
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	5	3.9
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	5	3.9
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	11	3.9
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	5	3.9
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	5	3.9
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	5	3.9
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	5	3.9
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	5	3.9
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	5	3.9
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	5	3.9
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	5	3.9
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	5	3.9
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	5	3.9
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	10	3.9
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	10	3.9
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	10	3.9
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	10	3.9
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	10	3.9
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	10	3.9
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	6	3.9
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	6	3.9
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD3	6	3.9
(4,476)	1:31:A:CYS:HA	1:37:A:LYS:HD2	6	3.9
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	2	3.9
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	14	3.9
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	14	3.9
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	14	3.9
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	12	3.9
(4,39)	1:26:A:GLN:H	1:27:A:CYS:HB2	13	3.9
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	15	3.89
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	15	3.89
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	15	3.89
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	13	3.89
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	13	3.89
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	13	3.89
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	13	3.89
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	13	3.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	13	3.89
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	13	3.89
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	13	3.89
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	4	3.89
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	4	3.89
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	4	3.89
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	4	3.89
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	9	3.89
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	6	3.89
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	6	3.89
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	6	3.89
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	15	3.89
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	15	3.89
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	18	3.89
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	18	3.89
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	15	3.89
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	15	3.89
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	2	3.89
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	2	3.89
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	2	3.89
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	2	3.89
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	13	3.89
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	13	3.89
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	13	3.89
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	13	3.89
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	14	3.89
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	15	3.89
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	6	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	6	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	14	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	14	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	14	3.88
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	14	3.88
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	4	3.88
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	4	3.88
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	4	3.88
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD2	15	3.88
(4,1025)	1:23:A:SER:HB2	1:24:A:LYS:HD3	15	3.88
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD2	15	3.88
(4,1025)	1:23:A:SER:HB3	1:24:A:LYS:HD3	15	3.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	17	3.88
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	17	3.88
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	17	3.88
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	17	3.88
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	17	3.88
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	17	3.88
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	17	3.88
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	18	3.88
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	9	3.88
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	9	3.88
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	9	3.88
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	9	3.88
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	9	3.88
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	9	3.88
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	9	3.88
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	9	3.88
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	16	3.88
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	16	3.88
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	16	3.88
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	20	3.88
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	20	3.88
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	20	3.88
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	12	3.88
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	4	3.88
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	12	3.88
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	11	3.88
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	12	3.87
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	12	3.87
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	12	3.87
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	5	3.87
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	8	3.87
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	10	3.87
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	10	3.87
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	11	3.87
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	11	3.87
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	11	3.87
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	11	3.87
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	11	3.87
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	11	3.87
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	13	3.87
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	13	3.87
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	13	3.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	13	3.87
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	13	3.87
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	13	3.87
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	13	3.87
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	4	3.87
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	8	3.87
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	19	3.87
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	19	3.87
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	19	3.87
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	19	3.87
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	3.87
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	3.87
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	3.87
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	3.87
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	16	3.87
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	16	3.87
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	15	3.87
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	15	3.87
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	15	3.87
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	15	3.87
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	15	3.87
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	15	3.87
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	15	3.87
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	15	3.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	15	3.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	15	3.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	15	3.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	15	3.87
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	13	3.87
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	13	3.87
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	13	3.87
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	9	3.87
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	9	3.87
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	4	3.87
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	4	3.87
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	17	3.87
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	17	3.87
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	17	3.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	8	3.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	8	3.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	14	3.87
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	14	3.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	15	3.87
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	1	3.86
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	1	3.86
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	1	3.86
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	1	3.86
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	20	3.86
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	20	3.86
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	20	3.86
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	4	3.86
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	4	3.86
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	7	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	7	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	7	3.86
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	7	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	7	3.86
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	7	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	7	3.86
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	16	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	16	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	16	3.86
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	16	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	16	3.86
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	16	3.86
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	16	3.86
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	19	3.86
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	19	3.86
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	19	3.86
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	19	3.86
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	14	3.86
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	14	3.86
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	9	3.86
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	9	3.86
(4,414)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	10	3.86
(4,414)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	10	3.86
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	3	3.86
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	9	3.86
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	9	3.86
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	14	3.86
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	7	3.85
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	7	3.85
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	7	3.85
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	8	3.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	8	3.85
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	12	3.85
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	20	3.85
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	7	3.84
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	7	3.84
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	7	3.84
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	7	3.84
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	7	3.84
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	7	3.84
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	7	3.84
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	7	3.84
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	2	3.84
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	2	3.84
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	2	3.84
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	9	3.84
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	9	3.84
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	9	3.84
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	9	3.84
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	9	3.84
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.84
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.84
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.84
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	20	3.84
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.84
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.84
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.84
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	8	3.84
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	8	3.84
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	8	3.84
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	8	3.84
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	9	3.84
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	9	3.84
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	9	3.84
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	9	3.84
(4,704)	1:13:A:ALA:HB1	1:14:A:CYS:HB2	11	3.84
(4,704)	1:13:A:ALA:HB2	1:14:A:CYS:HB2	11	3.84
(4,704)	1:13:A:ALA:HB3	1:14:A:CYS:HB2	11	3.84
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	8	3.84
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	8	3.84
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	8	3.84
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	8	3.84
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	8	3.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	8	3.84
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	17	3.84
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	17	3.84
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	17	3.84
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	10	3.84
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	10	3.84
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	10	3.84
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	10	3.84
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	10	3.84
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	10	3.84
(4,7)	1:15:A:ARG:HB3	1:16:A:SER:H	18	3.84
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	19	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	19	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	19	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	19	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	20	3.83
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	20	3.83
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	9	3.83
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	9	3.83
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	9	3.83
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	17	3.83
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	17	3.83
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	17	3.83
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	9	3.83
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	9	3.83
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	9	3.83
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	9	3.83
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	13	3.83
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	10	3.83
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	10	3.83
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	10	3.83
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	10	3.83
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	10	3.83
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	10	3.83
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	10	3.83
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	5	3.83
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	5	3.83
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	5	3.83
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	12	3.83
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	12	3.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	12	3.83
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	13	3.83
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	13	3.83
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	19	3.83
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	19	3.83
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	19	3.83
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	2	3.83
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	1	3.82
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	1	3.82
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	7	3.82
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	9	3.82
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	13	3.82
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	13	3.82
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	13	3.82
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	13	3.82
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	8	3.82
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	8	3.82
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	8	3.82
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	8	3.82
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	8	3.82
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	8	3.82
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	8	3.82
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	8	3.82
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	8	3.82
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	8	3.82
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	8	3.82
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	8	3.82
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	8	3.82
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	20	3.82
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	3	3.82
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	3	3.82
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	18	3.82
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	18	3.82
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	9	3.82
(4,633)	1:55:A:PRO:HB2	1:56:A:ASP:HA	5	3.82
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	4	3.82
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	4	3.82
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	4	3.82
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	4	3.82
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	4	3.82
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	4	3.82
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	4	3.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	4	3.82
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	13	3.82
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	13	3.82
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	13	3.82
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	7	3.82
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	7	3.82
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	7	3.82
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	16	3.82
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	16	3.82
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	12	3.82
(4,486)	1:40:A:ASN:H	1:66:A:CYS:HB3	16	3.82
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	7	3.82
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	7	3.82
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	7	3.82
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	13	3.82
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	13	3.82
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	13	3.82
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	13	3.82
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	13	3.82
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	19	3.82
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	7	3.82
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	10	3.82
(4,265)	1:40:A:ASN:H	1:66:A:CYS:HB3	16	3.82
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	14	3.81
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	14	3.81
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	14	3.81
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	12	3.81
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	8	3.81
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	8	3.81
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	10	3.81
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	10	3.81
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	13	3.81
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	13	3.81
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	19	3.81
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	19	3.81
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	19	3.81
(4,484)	1:65:A:SER:HB2	1:66:A:CYS:HB3	1	3.81
(4,484)	1:65:A:SER:HB3	1:66:A:CYS:HB3	1	3.81
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	1	3.8
(4,1179)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	12	3.8
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	8	3.8
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	8	3.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	8	3.8
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	19	3.8
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	13	3.8
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	13	3.8
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	13	3.8
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	13	3.8
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	10	3.8
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	10	3.8
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	19	3.8
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	19	3.8
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	19	3.8
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	7	3.8
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	19	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	7	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	7	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	7	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	7	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	7	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	7	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	7	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	7	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	17	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	17	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	17	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	17	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	17	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	17	3.8
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	17	3.8
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	17	3.8
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	3	3.8
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	3	3.8
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	3	3.8
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	2	3.8
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	11	3.8
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	11	3.8
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	11	3.8
(4,452)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	3	3.8
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	16	3.8
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	16	3.8
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	16	3.8
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	16	3.8
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	7	3.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	7	3.8
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	17	3.8
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	8	3.8
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	8	3.8
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	3	3.8
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	12	3.8
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	12	3.8
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	19	3.79
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	20	3.79
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	14	3.79
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	14	3.79
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	14	3.79
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	14	3.79
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	14	3.79
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	14	3.79
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	14	3.79
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	14	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	10	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	10	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	10	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	10	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	15	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	15	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	15	3.79
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	15	3.79
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	9	3.79
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	9	3.79
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	13	3.79
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	13	3.79
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	12	3.79
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	12	3.79
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	20	3.79
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.79
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.79
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.79
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	20	3.79
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	20	3.79
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	20	3.79
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	20	3.79
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	20	3.79
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	2	3.79
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	2	3.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	2	3.79
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	5	3.79
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	4	3.79
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	4	3.79
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	11	3.79
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	11	3.79
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	19	3.78
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	19	3.78
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	19	3.78
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	16	3.78
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	16	3.78
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	16	3.78
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	2	3.78
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	2	3.78
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	2	3.78
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	2	3.78
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	2	3.78
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	2	3.78
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	2	3.78
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	2	3.78
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	12	3.78
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	12	3.78
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	12	3.78
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	12	3.78
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	19	3.78
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	9	3.78
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	15	3.78
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	15	3.78
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	15	3.78
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	12	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	12	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	12	3.78
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	12	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	12	3.78
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	12	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	12	3.78
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	19	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	19	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	19	3.78
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	19	3.78
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	19	3.78
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	19	3.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	19	3.78
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	18	3.78
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	2	3.78
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	6	3.78
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	6	3.78
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	6	3.78
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	18	3.78
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	5	3.78
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	5	3.78
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	5	3.78
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	13	3.78
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	13	3.78
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	13	3.78
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	13	3.78
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	4	3.78
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	4	3.78
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	4	3.78
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	16	3.78
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	16	3.78
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	4	3.78
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	4	3.78
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE2	1	3.77
(4,1193)	1:50:A:LYS:HB2	1:50:A:LYS:HE3	1	3.77
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	12	3.77
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	5	3.77
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	5	3.77
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE2	2	3.77
(4,1045)	1:9:A:LYS:HA	1:9:A:LYS:HE3	2	3.77
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	8	3.77
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	8	3.77
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	8	3.77
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	13	3.77
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	13	3.77
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	13	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	5	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	5	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	5	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	5	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	5	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	5	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	5	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	11	3.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	11	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	11	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	11	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	11	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	11	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	11	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	18	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	18	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	18	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	18	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	18	3.77
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	18	3.77
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	18	3.77
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	1	3.77
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	1	3.77
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	1	3.77
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	1	3.77
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	2	3.77
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	2	3.77
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	2	3.77
(4,158)	1:9:A:LYS:HD3	1:28:A:GLY:H	16	3.77
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	1	3.76
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	1	3.76
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	1	3.76
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	1	3.76
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	1	3.76
(4,1053)	1:33:A:CYS:H	1:37:A:LYS:HD2	19	3.76
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	14	3.76
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	14	3.76
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	17	3.76
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	17	3.76
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	20	3.76
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	20	3.76
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	6	3.76
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	6	3.76
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	6	3.76
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	6	3.76
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	6	3.76
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	6	3.76
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	6	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	8	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	8	3.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	8	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	8	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	8	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	8	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	8	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	8	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	10	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	10	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	10	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	10	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	10	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	10	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	10	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	10	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	13	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	13	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	13	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	13	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	13	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	13	3.76
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	13	3.76
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	13	3.76
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	14	3.76
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	14	3.76
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	14	3.76
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	4	3.76
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	4	3.76
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	4	3.76
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	18	3.76
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	18	3.76
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	17	3.76
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	19	3.76
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	1	3.76
(4,266)	1:39:A:CYS:HB3	1:40:A:ASN:H	8	3.76
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	8	3.75
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	8	3.75
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	8	3.75
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA2	20	3.75
(4,1186)	1:6:A:LYS:HD2	1:7:A:GLY:HA3	20	3.75
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA2	20	3.75
(4,1186)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	20	3.75
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	11	3.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	11	3.75
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	11	3.75
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	11	3.75
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	11	3.75
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	11	3.75
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	11	3.75
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	11	3.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	17	3.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	17	3.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	17	3.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	17	3.75
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	19	3.75
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	19	3.75
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	19	3.75
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	19	3.75
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	9	3.75
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	3	3.75
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	3	3.75
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	3	3.75
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	3	3.75
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	3	3.75
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	3	3.75
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	3	3.75
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	4	3.75
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	4	3.75
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	4	3.75
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	4	3.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	9	3.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	9	3.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	13	3.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	13	3.75
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	16	3.75
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	16	3.75
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	16	3.75
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	16	3.75
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	16	3.75
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	16	3.75
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	16	3.75
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	16	3.75
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	5	3.75
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	5	3.75
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	5	3.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	5	3.75
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	8	3.75
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	8	3.75
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	5	3.75
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	5	3.75
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	5	3.75
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	9	3.75
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	9	3.75
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	9	3.75
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	11	3.75
(4,1131)	1:13:A:ALA:HA	1:20:A:GLN:HG2	7	3.74
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	1	3.74
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	6	3.74
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	4	3.74
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	4	3.74
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	18	3.74
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	18	3.74
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	14	3.74
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	14	3.74
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	14	3.74
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	14	3.74
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	14	3.74
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	14	3.74
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	14	3.74
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	11	3.74
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	11	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	12	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	12	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	12	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	12	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	12	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	12	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	12	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	12	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	19	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	19	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	19	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	19	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	19	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	19	3.74
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	19	3.74
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	19	3.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	12	3.74
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	12	3.74
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	12	3.74
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	9	3.74
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	9	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	9	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	9	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	9	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	9	3.74
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	11	3.74
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	11	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	11	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	11	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	11	3.74
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	11	3.74
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	4	3.74
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	4	3.74
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	4	3.74
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	3	3.74
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	3	3.74
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	3.74
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	15	3.74
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	15	3.74
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	12	3.73
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	12	3.73
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	12	3.73
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	15	3.73
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	15	3.73
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	15	3.73
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	15	3.73
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	10	3.73
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	11	3.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	8	3.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	8	3.73
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	8	3.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	8	3.73
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	8	3.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	8	3.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	8	3.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	8	3.73
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	4	3.73
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	4	3.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	4	3.73
(4,608)	1:39:A:CYS:HB3	1:58:A:CYS:HB3	13	3.73
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	18	3.73
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	18	3.73
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	18	3.73
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	18	3.73
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	18	3.73
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	18	3.73
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.73
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	20	3.73
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.73
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	11	3.73
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	11	3.73
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	11	3.73
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	2	3.73
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	9	3.73
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	14	3.73
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	17	3.73
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	11	3.73
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	18	3.73
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	1	3.73
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	18	3.72
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	18	3.72
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	18	3.72
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	18	3.72
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	18	3.72
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	18	3.72
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	18	3.72
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	18	3.72
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	18	3.72
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	18	3.72
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	18	3.72
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	17	3.72
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	17	3.72
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	17	3.72
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	17	3.72
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	4	3.72
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	15	3.72
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	9	3.72
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	9	3.72
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	3.72
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	3.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	3.72
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	3.72
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	15	3.72
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	15	3.72
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	5	3.72
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	5	3.72
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	5	3.72
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	5	3.72
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	5	3.72
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	5	3.72
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	5	3.72
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	5	3.72
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	17	3.72
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	17	3.72
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	17	3.72
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	18	3.72
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	18	3.72
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	18	3.72
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	2	3.72
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	2	3.72
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	11	3.72
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	11	3.72
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	11	3.72
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	6	3.72
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	17	3.72
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	20	3.72
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	20	3.72
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	10	3.71
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	10	3.71
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	10	3.71
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	10	3.71
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	15	3.71
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	2	3.71
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	2	3.71
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	20	3.71
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	20	3.71
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	20	3.71
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	7	3.71
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	7	3.71
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	10	3.71
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	10	3.71
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	10	3.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	10	3.71
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	15	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	6	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	6	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	6	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	6	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	6	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	6	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	6	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	6	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	18	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	18	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	18	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	18	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	18	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	18	3.71
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	18	3.71
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	18	3.71
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	16	3.71
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	1	3.71
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	1	3.71
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	16	3.7
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	16	3.7
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	16	3.7
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	10	3.7
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	10	3.7
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	10	3.7
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	10	3.7
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	10	3.7
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	10	3.7
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	10	3.7
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	10	3.7
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	10	3.7
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	10	3.7
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	19	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	3.7
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	6	3.7
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	6	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	3.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	3.7
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	3.7
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	14	3.7
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	14	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	3	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	3	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	3	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	3	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	3	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	3	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	3	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	3	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	11	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	11	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	11	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	11	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	11	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	11	3.7
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	11	3.7
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	11	3.7
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	14	3.7
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	14	3.7
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	14	3.7
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	15	3.7
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	15	3.7
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	15	3.7
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	13	3.7
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	15	3.7
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	16	3.7
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	4	3.69
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	4	3.69
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	4	3.69
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	12	3.69
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	18	3.69
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	18	3.69
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	18	3.69
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	16	3.69
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	16	3.69
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	16	3.69
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	16	3.69
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	16	3.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	16	3.69
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	17	3.69
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	14	3.69
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	14	3.69
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	14	3.69
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	14	3.69
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	14	3.69
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	14	3.69
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	14	3.69
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	14	3.69
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	10	3.69
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	10	3.69
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	10	3.69
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	16	3.69
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	16	3.69
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	16	3.69
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	16	3.69
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	16	3.69
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	16	3.69
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	4	3.69
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	8	3.69
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	11	3.69
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	5	3.69
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	5	3.69
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	5	3.69
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	7	3.68
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	7	3.68
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	7	3.68
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	5	3.68
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	10	3.68
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	15	3.68
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	10	3.68
(4,920)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	13	3.68
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	9	3.68
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	9	3.68
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	9	3.68
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	8	3.68
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	8	3.68
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	4	3.68
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	10	3.68
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	2	3.68
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	2	3.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	2	3.68
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	2	3.68
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	2	3.68
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	6	3.68
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	4	3.68
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	16	3.68
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	16	3.68
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	14	3.67
(4,1127)	1:6:A:LYS:HG2	1:15:A:ARG:HA	6	3.67
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	4	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	8	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	8	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	8	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	8	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	8	3.67
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	8	3.67
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	8	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	8	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	17	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	17	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	17	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	17	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	17	3.67
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	17	3.67
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	17	3.67
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	17	3.67
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	13	3.67
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	13	3.67
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	13	3.67
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	13	3.67
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	4	3.67
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	7	3.67
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	16	3.67
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	2	3.67
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	2	3.67
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	2	3.67
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	2	3.67
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	2	3.67
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	2	3.67
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	2	3.67
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	16	3.67
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	15	3.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	1	3.67
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	7	3.67
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	20	3.66
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	20	3.66
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	20	3.66
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	12	3.66
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	15	3.66
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	12	3.66
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	3.66
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	3.66
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	3.66
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	3.66
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	7	3.66
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	7	3.66
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	20	3.66
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	20	3.66
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	3.66
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	20	3.66
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	20	3.66
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	20	3.66
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	20	3.66
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	20	3.66
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	19	3.66
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	19	3.66
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	19	3.66
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	19	3.66
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	19	3.66
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	19	3.66
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	10	3.66
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	10	3.66
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	10	3.66
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	15	3.66
(4,592)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	15	3.66
(4,592)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	15	3.66
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	19	3.66
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	19	3.66
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	3	3.66
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	10	3.66
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	17	3.66
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	17	3.66
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	2	3.65
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE2	2	3.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1141)	1:67:A:LYS:HA	1:67:A:LYS:HE3	2	3.65
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	20	3.65
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	19	3.65
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	11	3.65
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	11	3.65
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	4	3.65
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	4	3.65
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	12	3.65
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	12	3.65
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	12	3.65
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	12	3.65
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	9	3.65
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	13	3.65
(4,277)	1:55:A:PRO:HB3	1:56:A:ASP:H	2	3.65
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	15	3.65
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	15	3.65
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	1	3.65
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	14	3.65
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	14	3.65
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	2	3.65
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	2	3.65
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	2	3.65
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	2	3.65
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	18	3.65
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	18	3.65
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	16	3.64
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	20	3.64
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	20	3.64
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	1	3.64
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	1	3.64
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	1	3.64
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	1	3.64
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	1	3.64
(4,867)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	1	3.64
(4,867)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	1	3.64
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	11	3.64
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	3	3.64
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	3	3.64
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	3	3.64
(4,438)	1:13:A:ALA:HB1	1:21:A:CYS:HB3	17	3.64
(4,438)	1:13:A:ALA:HB2	1:21:A:CYS:HB3	17	3.64
(4,438)	1:13:A:ALA:HB3	1:21:A:CYS:HB3	17	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	20	3.64
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	9	3.64
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	11	3.63
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	11	3.63
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	11	3.63
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	7	3.63
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	7	3.63
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	20	3.63
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	20	3.63
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	20	3.63
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	20	3.63
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	20	3.63
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	20	3.63
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	20	3.63
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	20	3.63
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	16	3.63
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	20	3.63
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	1	3.63
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	1	3.63
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	1	3.63
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	15	3.63
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	15	3.63
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	15	3.63
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	15	3.63
(4,773)	1:6:A:LYS:HA	1:10:A:CYS:HB3	12	3.63
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	8	3.63
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	8	3.63
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	8	3.63
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	8	3.63
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	8	3.63
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	8	3.63
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	20	3.63
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	20	3.63
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	12	3.63
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	9	3.63
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	10	3.63
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	3	3.63
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	3	3.63
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	3	3.63
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	3	3.63
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	6	3.62
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	6	3.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	11	3.62
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	18	3.62
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	18	3.62
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	6	3.62
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	6	3.62
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	8	3.62
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	8	3.62
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	1	3.62
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	1	3.62
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	1	3.62
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	1	3.62
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	14	3.62
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	14	3.62
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	14	3.62
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	14	3.62
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	15	3.62
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	15	3.62
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	15	3.62
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	15	3.62
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	2	3.62
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	2	3.62
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	2	3.62
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	2	3.62
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	2	3.62
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	2	3.62
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	2	3.62
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	2	3.62
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	13	3.62
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	13	3.62
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	13	3.62
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	13	3.62
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	13	3.62
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	13	3.62
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	12	3.62
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	12	3.62
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	12	3.62
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	13	3.62
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	13	3.62
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	13	3.62
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	10	3.62
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	10	3.62
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	10	3.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	17	3.62
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	17	3.62
(4,365)	1:42:A:THR:H	1:42:A:THR:HB	1	3.62
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	1	3.62
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	8	3.62
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	4	3.62
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	17	3.61
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	17	3.61
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	17	3.61
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	16	3.61
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	16	3.61
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	16	3.61
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	16	3.61
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	16	3.61
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	16	3.61
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	16	3.61
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	16	3.61
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	17	3.61
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	17	3.61
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	19	3.61
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	19	3.61
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	19	3.61
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	19	3.61
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	19	3.61
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	19	3.61
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	2	3.61
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	2	3.61
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	12	3.61
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	12	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	5	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	5	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	5	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	5	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	9	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	9	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	9	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	9	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	10	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	10	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	10	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	10	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	11	3.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	11	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	11	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	11	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	12	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	12	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	12	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	12	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	18	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	18	3.61
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	18	3.61
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	18	3.61
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	19	3.61
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	19	3.61
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	19	3.61
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	19	3.61
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	9	3.61
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	9	3.61
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	9	3.61
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	7	3.61
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	7	3.61
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	7	3.61
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	7	3.61
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	7	3.61
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	7	3.61
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	4	3.61
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	4	3.61
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	4	3.61
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	4	3.61
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	15	3.61
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	15	3.61
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	15	3.61
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	15	3.61
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	18	3.61
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	18	3.61
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	18	3.61
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	17	3.61
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	17	3.61
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	17	3.61
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	5	3.61
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	20	3.61
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	14	3.61
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	14	3.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	17	3.6
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	18	3.6
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	18	3.6
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	18	3.6
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	18	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	7	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	7	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	7	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	7	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	8	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	8	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	8	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	8	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	20	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	20	3.6
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	20	3.6
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	20	3.6
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	17	3.6
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	13	3.6
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	13	3.6
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	13	3.6
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	13	3.6
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	1	3.6
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB2	1	3.6
(4,609)	1:55:A:PRO:HB3	1:58:A:CYS:HB3	1	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	5	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	5	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	5	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	5	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	5	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	5	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	12	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	12	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	12	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	17	3.6
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	17	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	17	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	17	3.6
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	17	3.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	17	3.6
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	2	3.6
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	12	3.6
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	13	3.6
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	15	3.6
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	2	3.6
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	2	3.6
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	20	3.59
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	12	3.59
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	16	3.59
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	16	3.59
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	16	3.59
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	16	3.59
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	4	3.59
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	4	3.59
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	4	3.59
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	4	3.59
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	4	3.59
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	4	3.59
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	4	3.59
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	13	3.59
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	13	3.59
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	13	3.59
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	13	3.59
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	19	3.59
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	19	3.59
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	19	3.59
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	19	3.59
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	1	3.59
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	1	3.59
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	1	3.59
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	3	3.59
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	3	3.59
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	3	3.59
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	3	3.59
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	3	3.59
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	3	3.59
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	13	3.59
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	13	3.59
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	13	3.59
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	13	3.59
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	13	3.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	13	3.59
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	14	3.59
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	14	3.59
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	14	3.59
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	14	3.59
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	17	3.58
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	17	3.58
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	17	3.58
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	17	3.58
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	17	3.58
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	7	3.58
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	19	3.58
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	19	3.58
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	19	3.58
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	19	3.58
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	19	3.58
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	19	3.58
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	19	3.58
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	16	3.58
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	16	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	2	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	2	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	2	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	2	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	3	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	3	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	3	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	3	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	6	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	6	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	6	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	6	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	16	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	16	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	16	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	16	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	17	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	17	3.58
(4,989)	1:49:A:GLY:HA3	1:50:A:LYS:HA	17	3.58
(4,989)	1:49:A:GLY:HA2	1:50:A:LYS:HA	17	3.58
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	2	3.58
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	2	3.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	2	3.58
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	2	3.58
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	10	3.58
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	10	3.58
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	7	3.58
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	1	3.58
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	1	3.58
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	1	3.58
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB2	1	3.58
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB3	1	3.58
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	1	3.58
(4,625)	1:30:A:GLY:HA2	1:31:A:CYS:HB2	1	3.58
(4,625)	1:30:A:GLY:HA3	1:31:A:CYS:HB3	1	3.58
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	7	3.58
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	7	3.58
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	7	3.58
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	7	3.58
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	9	3.58
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	9	3.58
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	9	3.58
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	9	3.58
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	6	3.58
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	6	3.58
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	6	3.58
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	11	3.58
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	11	3.58
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	11	3.58
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	11	3.58
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	13	3.58
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	13	3.58
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	13	3.58
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	8	3.58
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	12	3.58
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	16	3.58
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	20	3.58
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	19	3.58
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	19	3.58
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	19	3.58
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	1	3.58
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	19	3.58
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	2	3.57
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	2	3.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	2	3.57
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	2	3.57
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	4	3.57
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	4	3.57
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	11	3.57
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	11	3.57
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	11	3.57
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	11	3.57
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	18	3.57
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	18	3.57
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	7	3.57
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	7	3.57
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	7	3.57
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	7	3.57
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	4	3.57
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	4	3.57
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	3	3.57
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	3	3.57
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	3	3.57
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	3	3.57
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	3	3.57
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	3	3.57
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	6	3.57
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	6	3.57
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	6	3.57
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	6	3.57
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	6	3.57
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	6	3.57
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	5	3.57
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	10	3.57
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	17	3.57
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	17	3.57
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	17	3.57
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	17	3.57
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	7	3.57
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	7	3.57
(4,339)	1:51:A:GLU:HG2	1:52:A:CYS:H	7	3.57
(4,339)	1:51:A:GLU:HG3	1:52:A:CYS:H	7	3.57
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	20	3.57
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	20	3.57
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	10	3.57
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	10	3.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	10	3.57
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	4	3.56
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	4	3.56
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	4	3.56
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	4	3.56
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	6	3.56
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	6	3.56
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	6	3.56
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	6	3.56
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	19	3.56
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	19	3.56
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	17	3.56
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	17	3.56
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	17	3.56
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	17	3.56
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	17	3.56
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	17	3.56
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	14	3.56
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	14	3.56
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	14	3.56
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	14	3.56
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	2	3.56
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	2	3.56
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	2	3.56
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	2	3.56
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	2	3.56
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	2	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	8	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	8	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	8	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	8	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	10	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	10	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	10	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	10	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	11	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	11	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	11	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	11	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	16	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	16	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	16	3.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	16	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	18	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	18	3.56
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	18	3.56
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	18	3.56
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	16	3.56
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	16	3.56
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	16	3.56
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	6	3.56
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	1	3.56
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	20	3.56
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	8	3.56
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	1	3.56
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	1	3.56
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	8	3.56
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	8	3.56
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	7	3.55
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	7	3.55
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	7	3.55
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	7	3.55
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	7	3.55
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	7	3.55
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	7	3.55
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	7	3.55
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	16	3.55
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	16	3.55
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	2	3.55
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	2	3.55
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	2	3.55
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	2	3.55
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	20	3.55
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	16	3.55
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	16	3.55
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	16	3.55
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	16	3.55
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	11	3.55
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	11	3.55
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	4	3.55
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	4	3.55
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	4	3.55
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	4	3.55
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	4	3.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	4	3.55
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	3	3.55
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	3	3.55
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	3	3.55
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	3	3.55
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	9	3.55
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	9	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	9	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	9	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	9	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	9	3.54
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	9	3.54
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	9	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	9	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	12	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	12	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	12	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	12	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	12	3.54
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	12	3.54
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	12	3.54
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	12	3.54
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	12	3.54
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	12	3.54
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	12	3.54
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	12	3.54
(4,918)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	13	3.54
(4,918)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	13	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	1	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	1	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	1	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	1	3.54
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	1	3.54
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	1	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	13	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	13	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	13	3.54
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	13	3.54
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	13	3.54
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	13	3.54
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	17	3.54
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	17	3.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	17	3.54
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	17	3.54
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	19	3.54
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	19	3.54
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	19	3.54
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	19	3.54
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	17	3.54
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	3	3.54
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	19	3.54
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	17	3.54
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	17	3.54
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	13	3.53
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	13	3.53
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	13	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	1	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	1	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	1	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	1	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	1	3.53
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	1	3.53
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	1	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	1	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	4	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	4	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	4	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	4	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	4	3.53
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	4	3.53
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	4	3.53
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	4	3.53
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	13	3.53
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	13	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	5	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	5	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	5	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	5	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	18	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	18	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	18	3.53
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	18	3.53
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	1	3.53
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	1	3.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	1	3.53
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	1	3.53
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	20	3.53
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	20	3.53
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	20	3.53
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.53
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	20	3.53
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	20	3.53
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	9	3.53
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	9	3.53
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	9	3.53
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	5	3.53
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	5	3.53
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	5	3.53
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	5	3.53
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	6	3.53
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	6	3.53
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	6	3.53
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	6	3.53
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	7	3.53
(4,187)	1:21:A:CYS:H	1:36:A:CYS:HB3	20	3.53
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	4	3.53
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	7	3.53
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	7	3.53
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	10	3.53
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	10	3.53
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	6	3.53
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	6	3.53
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	16	3.52
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	16	3.52
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	16	3.52
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	16	3.52
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	20	3.52
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	20	3.52
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	3	3.52
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	3	3.52
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	3	3.52
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	3	3.52
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	3	3.52
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	3	3.52
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	3	3.52
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	3	3.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	10	3.52
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	10	3.52
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	10	3.52
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	10	3.52
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	5	3.52
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	5	3.52
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	5	3.52
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	5	3.52
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	5	3.52
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	5	3.52
(4,637)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	3	3.52
(4,637)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	3	3.52
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	1	3.52
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	1	3.52
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	1	3.52
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	1	3.52
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	14	3.52
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	14	3.52
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	14	3.52
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	14	3.52
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	20	3.52
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	20	3.52
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	20	3.52
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	20	3.52
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	6	3.52
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	6	3.52
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	6	3.52
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	13	3.52
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	9	3.52
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	8	3.52
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	8	3.52
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	9	3.52
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	9	3.52
(4,1116)	1:31:A:CYS:H	1:37:A:LYS:HD3	8	3.51
(4,1074)	1:37:A:LYS:HD3	1:55:A:PRO:HA	9	3.51
(4,1074)	1:37:A:LYS:HD2	1:55:A:PRO:HA	9	3.51
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	5	3.51
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	5	3.51
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	5	3.51
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	5	3.51
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	3	3.51
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	3	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	3	3.51
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	3	3.51
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	5	3.51
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	5	3.51
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	15	3.5
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	3.5
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	13	3.5
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	13	3.5
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	13	3.5
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	9	3.5
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	9	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	3	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	3	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	3	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	3	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	6	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	6	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	6	3.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	6	3.5
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	3	3.5
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	3	3.5
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	3	3.5
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	12	3.5
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	18	3.5
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	18	3.5
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	18	3.5
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	9	3.5
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	9	3.5
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	9	3.5
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	7	3.5
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	11	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	7	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	7	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	7	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	7	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	20	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	20	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	20	3.49
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	20	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	7	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	7	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	7	3.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	7	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	17	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	17	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	17	3.49
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	17	3.49
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	13	3.49
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	13	3.49
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	13	3.49
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	13	3.49
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	14	3.49
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	14	3.49
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	14	3.49
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	14	3.49
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	14	3.49
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	14	3.49
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	15	3.49
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	16	3.49
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	16	3.49
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	16	3.49
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	2	3.49
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	2	3.49
(4,480)	1:30:A:GLY:HA3	1:31:A:CYS:HA	2	3.49
(4,480)	1:30:A:GLY:HA2	1:31:A:CYS:HA	2	3.49
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	3.49
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	15	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	15	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	15	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	15	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	15	3.49
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	15	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	16	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	16	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	16	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	16	3.49
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	16	3.49
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	16	3.49
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	12	3.49
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	12	3.49
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	9	3.49
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	1	3.49
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	1	3.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	6	3.48
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD2	6	3.48
(4,1051)	1:33:A:CYS:H	1:37:A:LYS:HD3	6	3.48
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	4	3.48
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	4	3.48
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	4	3.48
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	4	3.48
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	4	3.48
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	4	3.48
(4,281)	1:39:A:CYS:HA	1:40:A:ASN:HD21	6	3.48
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	10	3.48
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	10	3.48
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	2	3.48
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	5	3.48
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	8	3.48
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	3	3.47
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	3	3.47
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	3	3.47
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	3	3.47
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	12	3.47
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	12	3.47
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	15	3.47
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	15	3.47
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	15	3.47
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	15	3.47
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	2	3.47
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	2	3.47
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	2	3.47
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	2	3.47
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	2	3.47
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	2	3.47
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	5	3.47
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	5	3.47
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	5	3.47
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	5	3.47
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	12	3.47
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	12	3.47
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	7	3.47
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	7	3.47
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	7	3.47
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	7	3.47
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	7	3.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	7	3.47
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	7	3.47
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	7	3.47
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	7	3.47
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	7	3.47
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	7	3.47
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	7	3.47
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	10	3.47
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	10	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	10	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	10	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	10	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	10	3.47
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA2	15	3.47
(4,594)	1:44:A:ASP:HB2	1:45:A:GLY:HA3	15	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	15	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	15	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA2	15	3.47
(4,594)	1:44:A:ASP:HB3	1:45:A:GLY:HA3	15	3.47
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	17	3.47
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	17	3.47
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	20	3.47
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	3.47
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	20	3.47
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	11	3.47
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	11	3.47
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	18	3.47
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	18	3.47
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	18	3.47
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	18	3.47
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	18	3.47
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	18	3.47
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	11	3.47
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	18	3.47
(4,63)	1:22:A:GLY:HA3	1:24:A:LYS:H	10	3.47
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	11	3.47
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	3	3.46
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	17	3.46
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	17	3.46
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	17	3.46
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	17	3.46
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	8	3.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1123)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	14	3.46
(4,1123)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	14	3.46
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	1	3.46
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	1	3.46
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	1	3.46
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	1	3.46
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	1	3.46
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	1	3.46
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	14	3.46
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	3	3.46
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	3	3.46
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	14	3.46
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	14	3.46
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	14	3.46
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	14	3.46
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	14	3.46
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	14	3.46
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	14	3.46
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	14	3.46
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	14	3.46
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	14	3.46
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	14	3.46
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	14	3.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	4	3.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	4	3.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	4	3.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	4	3.46
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	9	3.46
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	9	3.46
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	9	3.46
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	9	3.46
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	1	3.46
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	1	3.46
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	1	3.46
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	11	3.46
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	11	3.46
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	11	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	9	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	9	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	9	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	9	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	9	3.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	9	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	12	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	12	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	12	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	12	3.46
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	12	3.46
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	12	3.46
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	6	3.46
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	6	3.46
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	17	3.46
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	3	3.46
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	3	3.46
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	3	3.46
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	3	3.46
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	19	3.45
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	19	3.45
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	6	3.45
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	6	3.45
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	3	3.45
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	3	3.45
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	3	3.45
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	3	3.45
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	6	3.45
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	6	3.45
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	18	3.45
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	18	3.45
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	18	3.45
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	18	3.45
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	18	3.45
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	18	3.45
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	18	3.45
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	18	3.45
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	12	3.45
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	12	3.45
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	5	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	5	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	5	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	5	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	5	3.45
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	5	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	17	3.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	17	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	17	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	17	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	17	3.45
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	17	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	20	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	20	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	20	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	20	3.45
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	20	3.45
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	20	3.45
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	13	3.45
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	19	3.45
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	6	3.45
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	6	3.45
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	13	3.45
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	13	3.45
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	19	3.45
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	19	3.45
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	11	3.44
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	11	3.44
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	11	3.44
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	11	3.44
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	17	3.44
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	17	3.44
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	1	3.44
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	20	3.44
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	5	3.44
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	5	3.44
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	5	3.44
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	5	3.44
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	5	3.44
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	5	3.44
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	14	3.44
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	14	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	1	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	1	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	1	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	1	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	1	3.44
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	1	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	13	3.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	13	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	13	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	13	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	13	3.44
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	13	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	14	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	14	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	14	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	14	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	14	3.44
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	14	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	19	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	19	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	19	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	19	3.44
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	19	3.44
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	19	3.44
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	16	3.44
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	16	3.44
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	5	3.44
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	6	3.44
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	10	3.44
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	15	3.44
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	12	3.43
(4,1056)	1:33:A:CYS:H	1:37:A:LYS:HG3	13	3.43
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	3	3.43
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	3	3.43
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	3	3.43
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	10	3.43
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	10	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	7	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	7	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	7	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	7	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	7	3.43
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	7	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	10	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	10	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	10	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	10	3.43
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	10	3.43
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	10	3.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	8	3.43
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	8	3.43
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	8	3.43
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	12	3.43
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	12	3.43
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	11	3.42
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	11	3.42
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	11	3.42
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	11	3.42
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	15	3.42
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	15	3.42
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	15	3.42
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	15	3.42
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	15	3.42
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	15	3.42
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	15	3.42
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	15	3.42
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	6	3.42
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	6	3.42
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	12	3.42
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	12	3.42
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	12	3.42
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	12	3.42
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	5	3.42
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	5	3.42
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	11	3.42
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	15	3.42
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	20	3.42
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	13	3.42
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	13	3.42
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	11	3.41
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	11	3.41
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	11	3.41
(4,586)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	5	3.41
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	10	3.41
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	10	3.41
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	10	3.41
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	19	3.41
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	19	3.41
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	19	3.41
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	19	3.41
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	19	3.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	10	3.41
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	10	3.41
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	10	3.41
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	6	3.41
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	7	3.41
(4,40)	1:25:A:CYS:HB2	1:26:A:GLN:H	16	3.41
(4,40)	1:25:A:CYS:HB3	1:26:A:GLN:H	16	3.41
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	20	3.4
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	20	3.4
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	20	3.4
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	20	3.4
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	20	3.4
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	20	3.4
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	12	3.4
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	12	3.4
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	12	3.4
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	12	3.4
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	12	3.4
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	12	3.4
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	12	3.4
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	12	3.4
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	12	3.4
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	12	3.4
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	12	3.4
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	12	3.4
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	13	3.4
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	13	3.4
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	13	3.4
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	2	3.4
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	20	3.4
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	14	3.39
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	11	3.39
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	11	3.39
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	11	3.39
(4,975)	1:42:A:THR:HG21	1:54:A:GLY:HA2	19	3.39
(4,975)	1:42:A:THR:HG22	1:54:A:GLY:HA2	19	3.39
(4,975)	1:42:A:THR:HG23	1:54:A:GLY:HA2	19	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	15	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	15	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	15	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	15	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	15	3.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	15	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	15	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	15	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	15	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	15	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	15	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	15	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	19	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	19	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	19	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	19	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	19	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	19	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	19	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	19	3.39
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	19	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	19	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	19	3.39
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	19	3.39
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	2	3.39
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	2	3.39
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	2	3.39
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	2	3.39
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	20	3.39
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	20	3.39
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	20	3.39
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	6	3.39
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	6	3.39
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	13	3.39
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	13	3.39
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	16	3.39
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	12	3.39
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	4	3.39
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	4	3.39
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	20	3.38
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	20	3.38
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	20	3.38
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	20	3.38
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	6	3.38
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	6	3.38
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	6	3.38
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	6	3.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	6	3.38
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	6	3.38
(4,1085)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	6	3.38
(4,1085)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	6	3.38
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	1	3.38
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE2	1	3.38
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	1	3.38
(4,1044)	1:37:A:LYS:HA	1:37:A:LYS:HE3	1	3.38
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	6	3.38
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	6	3.38
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	6	3.38
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	6	3.38
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	6	3.38
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	6	3.38
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	9	3.38
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	9	3.38
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	9	3.38
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	9	3.38
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	9	3.38
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	9	3.38
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	9	3.38
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	9	3.38
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	3	3.38
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	3	3.38
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	3	3.38
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	3	3.38
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	3	3.38
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	3	3.38
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	3	3.38
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	3	3.38
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	3	3.38
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	3	3.38
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	3	3.38
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	3	3.38
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	12	3.38
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	12	3.38
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	14	3.38
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	14	3.38
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	14	3.38
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	11	3.38
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	11	3.38
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	2	3.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	12	3.37
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	12	3.37
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	12	3.37
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	11	3.37
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	11	3.37
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	11	3.37
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	11	3.37
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	10	3.37
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	10	3.37
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	10	3.37
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	10	3.37
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	15	3.37
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	15	3.37
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	13	3.37
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	13	3.37
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	13	3.37
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	9	3.37
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	9	3.37
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	9	3.37
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	14	3.37
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	7	3.37
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	7	3.37
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	12	3.36
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	11	3.36
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	10	3.36
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	16	3.36
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	16	3.36
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	16	3.36
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	11	3.36
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	4	3.36
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	4	3.36
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	4	3.36
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	4	3.36
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	4	3.36
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	4	3.36
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	4	3.36
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	4	3.36
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	4	3.36
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	4	3.36
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	4	3.36
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	4	3.36
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	15	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	15	3.36
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	6	3.35
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	15	3.35
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	15	3.35
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	15	3.35
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	11	3.35
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	11	3.35
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	11	3.35
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	11	3.35
(4,827)	1:33:A:CYS:H	1:37:A:LYS:HB2	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	2	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	2	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	2	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	2	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	2	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	2	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	2	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	2	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	2	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	2	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	2	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	2	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	11	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	11	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	11	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	11	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	11	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	11	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	11	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	16	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	16	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	16	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	16	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	16	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	16	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	16	3.35
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	16	3.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	16	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	16	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	16	3.35
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	16	3.35
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	5	3.35
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	3.35
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	5	3.35
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	19	3.35
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	19	3.35
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	19	3.35
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	15	3.35
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	16	3.35
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	20	3.35
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	20	3.35
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	16	3.34
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	16	3.34
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	16	3.34
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	16	3.34
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	9	3.34
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	9	3.34
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	9	3.34
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	19	3.34
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	19	3.34
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	19	3.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	20	3.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	20	3.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	20	3.34
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	20	3.34
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	7	3.34
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	7	3.34
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	16	3.34
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	16	3.34
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	16	3.34
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	15	3.34
(4,81)	1:46:A:CYS:H	1:53:A:THR:HA	8	3.34
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	11	3.33
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	17	3.33
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	16	3.33
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	16	3.33
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	16	3.33
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	16	3.33
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	19	3.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	19	3.33
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	19	3.33
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	5	3.33
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	5	3.33
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	5	3.33
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	5	3.33
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	20	3.33
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	20	3.33
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	20	3.33
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	20	3.33
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	20	3.33
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	20	3.33
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	20	3.33
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	20	3.33
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	20	3.33
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	20	3.33
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	20	3.33
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	20	3.33
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	18	3.33
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	17	3.33
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	17	3.33
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	17	3.33
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	17	3.33
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	9	3.33
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	9	3.33
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	9	3.33
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	3	3.33
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	14	3.33
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	1	3.32
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	7	3.32
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	7	3.32
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	7	3.32
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	2	3.32
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	2	3.32
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	2	3.32
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	2	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	6	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	6	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	6	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	6	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	6	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	6	3.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	6	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	6	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	6	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	6	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	6	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	6	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	10	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	10	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	10	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	10	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	10	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	10	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	10	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	10	3.32
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	10	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	10	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	10	3.32
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	10	3.32
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	1	3.32
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	1	3.32
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	14	3.32
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	14	3.32
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	11	3.32
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	11	3.32
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	11	3.32
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	11	3.32
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	10	3.32
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	10	3.32
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	10	3.32
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	20	3.32
(4,68)	1:39:A:CYS:H	1:39:A:CYS:HB2	1	3.32
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	3	3.31
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	2	3.31
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	2	3.31
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	3	3.31
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	3	3.31
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	15	3.3
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	15	3.3
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	15	3.3
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG2	1	3.3
(4,865)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	1	3.3
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG2	1	3.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,865)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	1	3.3
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	17	3.3
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	17	3.3
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	17	3.3
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	17	3.3
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	17	3.3
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	17	3.3
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	17	3.3
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	17	3.3
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	17	3.3
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	17	3.3
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	17	3.3
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	17	3.3
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	4	3.3
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	4	3.3
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	8	3.3
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	8	3.3
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	11	3.3
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	11	3.3
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	11	3.3
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	11	3.3
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	11	3.3
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	11	3.3
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	13	3.3
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	5	3.3
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	5	3.3
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	5	3.3
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	17	3.29
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	17	3.29
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	17	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	5	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	5	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	5	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	5	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	5	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	5	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	5	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	5	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	5	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	5	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	5	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	5	3.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	18	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	18	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	18	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	18	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	18	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	18	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	18	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	18	3.29
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	18	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	18	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	18	3.29
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	18	3.29
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	2	3.29
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	3.29
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	2	3.29
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	16	3.29
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	3.29
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	16	3.29
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	8	3.29
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	8	3.29
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	8	3.29
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	8	3.29
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	8	3.29
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	8	3.29
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	6	3.29
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB2	11	3.28
(4,1052)	1:33:A:CYS:H	1:37:A:LYS:HB3	11	3.28
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	11	3.28
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	3.28
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	3.28
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	3	3.28
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	18	3.28
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	18	3.28
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	18	3.28
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	2	3.28
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	2	3.28
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	2	3.28
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	2	3.28
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	2	3.28
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	2	3.28
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	2	3.28
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	7	3.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	4	3.27
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	4	3.27
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	4	3.27
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	4	3.27
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	14	3.27
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	14	3.27
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	14	3.27
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	10	3.27
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	8	3.27
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	9	3.26
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	9	3.26
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	9	3.26
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	9	3.26
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	16	3.26
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	16	3.26
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	1	3.26
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	1	3.26
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	1	3.26
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	1	3.26
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	1	3.26
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	1	3.26
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	1	3.26
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	1	3.26
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	1	3.26
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	1	3.26
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	1	3.26
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	1	3.26
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	13	3.26
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	19	3.26
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	19	3.26
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	19	3.26
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	19	3.26
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	19	3.26
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	19	3.26
(4,1124)	1:6:A:LYS:HG3	1:15:A:ARG:HA	1	3.25
(4,1014)	1:6:A:LYS:HG3	1:15:A:ARG:HA	1	3.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	12	3.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	12	3.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	12	3.25
(4,712)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	12	3.25
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	12	3.25
(4,712)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	12	3.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	18	3.25
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	18	3.25
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	18	3.25
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	18	3.25
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	14	3.25
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	14	3.25
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	14	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	3	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	3	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	3	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	3	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	3	3.25
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	3	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	6	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	6	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	6	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB3	6	3.25
(4,415)	1:45:A:GLY:HA2	1:46:A:CYS:HB2	6	3.25
(4,415)	1:45:A:GLY:HA3	1:46:A:CYS:HB2	6	3.25
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	11	3.25
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	18	3.24
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	18	3.24
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	18	3.24
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	18	3.24
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	10	3.24
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	7	3.24
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	7	3.24
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	13	3.24
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	13	3.24
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	13	3.24
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	13	3.24
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	13	3.24
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	13	3.24
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	13	3.24
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	13	3.24
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	13	3.24
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	13	3.24
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	13	3.24
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	13	3.24
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	14	3.24
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	14	3.24
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	14	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,394)	1:37:A:LYS:HD3	1:38:A:THR:H	13	3.24
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	15	3.24
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	16	3.24
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	16	3.24
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	2	3.24
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	2	3.24
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	5	3.24
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	5	3.24
(4,1155)	1:32:A:THR:HA	1:37:A:LYS:HG3	13	3.23
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	19	3.23
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	10	3.23
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	10	3.23
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	10	3.23
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	17	3.23
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	17	3.23
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	9	3.23
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	9	3.23
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	9	3.23
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	9	3.23
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	9	3.23
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	9	3.23
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	9	3.23
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	9	3.23
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	9	3.23
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	9	3.23
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	9	3.23
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	9	3.23
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	10	3.23
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	10	3.23
(4,585)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	11	3.23
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	12	3.23
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	12	3.23
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	12	3.23
(4,260)	1:37:A:LYS:HD2	1:38:A:THR:H	13	3.23
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	15	3.22
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	5	3.22
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	8	3.22
(4,992)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	1	3.22
(4,992)	1:39:A:CYS:HB2	1:54:A:GLY:HA2	1	3.22
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	3	3.22
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	3	3.22
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	18	3.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	18	3.22
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	1	3.22
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	1	3.22
(4,220)	1:8:A:GLU:HA	1:10:A:CYS:H	8	3.22
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	3	3.21
(4,1145)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	3	3.21
(4,1145)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	3	3.21
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	18	3.21
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	12	3.21
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	12	3.21
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB2	12	3.21
(4,1026)	1:23:A:SER:HB2	1:24:A:LYS:HB3	12	3.21
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB2	12	3.21
(4,1026)	1:23:A:SER:HB3	1:24:A:LYS:HB3	12	3.21
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	2	3.21
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	2	3.21
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	2	3.21
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	7	3.21
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	7	3.21
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	7	3.21
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	7	3.21
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	17	3.21
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	6	3.21
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	6	3.21
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	13	3.21
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	2	3.21
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	9	3.2
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	8	3.2
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	8	3.2
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	8	3.2
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	8	3.2
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	8	3.2
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	8	3.2
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB1	8	3.2
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB2	8	3.2
(4,638)	1:33:A:CYS:HB2	1:35:A:ALA:HB3	8	3.2
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB1	8	3.2
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB2	8	3.2
(4,638)	1:33:A:CYS:HB3	1:35:A:ALA:HB3	8	3.2
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	11	3.2
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	11	3.2
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	12	3.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	12	3.19
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	12	3.19
(4,1148)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	12	3.19
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	7	3.19
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	2	3.19
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	9	3.19
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	9	3.19
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	9	3.19
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	6	3.19
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	6	3.19
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	6	3.19
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	6	3.19
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	7	3.19
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	7	3.19
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	7	3.19
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	7	3.19
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	7	3.19
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	7	3.19
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	7	3.19
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	7	3.19
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	3.19
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	12	3.19
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	12	3.19
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	9	3.19
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	9	3.19
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	9	3.19
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	4	3.19
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	7	3.19
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	19	3.19
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	19	3.19
(4,1122)	1:6:A:LYS:HG2	1:15:A:ARG:HA	1	3.18
(4,1122)	1:6:A:LYS:HG3	1:15:A:ARG:HA	1	3.18
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	1	3.18
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	2	3.18
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	19	3.18
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	3	3.18
(4,820)	1:6:A:LYS:HG2	1:15:A:ARG:HA	1	3.18
(4,820)	1:6:A:LYS:HG3	1:15:A:ARG:HA	1	3.18
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	3	3.18
(4,731)	1:38:A:THR:HA	1:55:A:PRO:HB2	5	3.18
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	1	3.18
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	19	3.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	16	3.18
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	16	3.18
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	16	3.18
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	19	3.18
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	11	3.18
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	11	3.18
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	16	3.18
(4,1135)	1:37:A:LYS:HG3	1:38:A:THR:H	18	3.17
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	9	3.17
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	9	3.17
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	14	3.16
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	14	3.16
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	14	3.16
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	4	3.16
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	4	3.16
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	11	3.16
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	11	3.16
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	11	3.16
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	11	3.16
(4,1059)	1:34:A:ALA:HA	1:37:A:LYS:HD3	11	3.15
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	8	3.15
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	12	3.15
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	12	3.15
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	12	3.15
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	18	3.15
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	18	3.15
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	18	3.15
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	18	3.15
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	12	3.15
(4,424)	1:28:A:GLY:HA3	1:29:A:GLU:HG3	12	3.15
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	5	3.14
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG3	5	3.14
(4,1000)	1:58:A:CYS:HA	1:59:A:LYS:HG2	5	3.14
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	11	3.14
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	11	3.14
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE2	13	3.14
(4,587)	1:64:A:CYS:HB2	1:67:A:LYS:HE3	13	3.14
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	20	3.14
(4,425)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	20	3.14
(4,425)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	3.14
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	12	3.14
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	1	3.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	20	3.13
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	20	3.13
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	20	3.13
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	4	3.13
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	18	3.13
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	18	3.13
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	18	3.13
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	1	3.13
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	1	3.13
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA2	14	3.12
(4,1125)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	14	3.12
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA2	14	3.12
(4,1125)	1:6:A:LYS:HG3	1:7:A:GLY:HA3	14	3.12
(4,1073)	1:37:A:LYS:HB3	1:55:A:PRO:HA	13	3.12
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	8	3.12
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	4	3.12
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	16	3.12
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	16	3.12
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	16	3.12
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	16	3.12
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	16	3.12
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	16	3.12
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	16	3.12
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	16	3.12
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	3	3.12
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	10	3.12
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	10	3.12
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	10	3.12
(4,259)	1:37:A:LYS:HB3	1:38:A:THR:H	13	3.12
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	15	3.12
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	3.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	3.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	3.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	3.11
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	13	3.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	9	3.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	9	3.11
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	9	3.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	9	3.11
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	19	3.11
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	19	3.11
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	19	3.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	4	3.11
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	4	3.11
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	4	3.11
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	16	3.11
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	16	3.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	16	3.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	16	3.1
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	9	3.1
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	9	3.1
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	9	3.1
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	9	3.1
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	1	3.1
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	4	3.09
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	12	3.09
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	10	3.09
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	10	3.09
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	10	3.09
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	10	3.09
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	4	3.09
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	18	3.08
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	3.08
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	20	3.08
(4,423)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	20	3.08
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	12	3.08
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	18	3.07
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	4	3.07
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	4	3.07
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	5	3.07
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	8	3.07
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	12	3.07
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	7	3.07
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	19	3.07
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	19	3.07
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	19	3.07
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	19	3.07
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	11	3.07
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	11	3.07
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	11	3.07
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	15	3.07
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	15	3.07
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	15	3.07
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	16	3.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	16	3.07
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	16	3.07
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	1	3.06
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	20	3.06
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	20	3.06
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	20	3.06
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	11	3.06
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	17	3.06
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	18	3.06
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	18	3.06
(4,44)	1:26:A:GLN:H	1:26:A:GLN:HG3	18	3.06
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	18	3.05
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	4	3.05
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	4	3.05
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	4	3.05
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	4	3.05
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	17	3.05
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	7	3.05
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	15	3.05
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	5	3.05
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	5	3.05
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	5	3.05
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	14	3.05
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	3	3.05
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	3	3.05
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	6	3.04
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	19	3.04
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	8	3.04
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	1	3.03
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	2	3.03
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	8	3.03
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	19	3.03
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	2	3.03
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	11	3.03
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	15	3.03
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB2	15	3.03
(4,117)	1:22:A:GLY:H	1:25:A:CYS:HB3	15	3.03
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	5	3.02
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	6	3.02
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	11	3.02
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	16	3.02
(4,1178)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	16	3.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	10	3.02
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	10	3.02
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	10	3.02
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	10	3.02
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	6	3.02
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	6	3.02
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	6	3.02
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	13	3.02
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	13	3.02
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	13	3.02
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	13	3.02
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	12	3.02
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	3	3.02
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	18	3.02
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	18	3.02
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	8	3.02
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	8	3.02
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	8	3.02
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	8	3.02
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	16	3.01
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	16	3.01
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	16	3.01
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	1	3.01
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	1	3.01
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	1	3.01
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	4	3.01
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	4	3.01
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	17	3.01
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	17	3.01
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	17	3.01
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	17	3.01
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	8	3.01
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	8	3.01
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	14	3.01
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	14	3.01
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	10	3.01
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	10	3.01
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	16	3.0
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	10	3.0
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	12	3.0
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	12	3.0
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	12	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	12	3.0
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	14	3.0
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	14	3.0
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	14	3.0
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	14	3.0
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	16	2.99
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	17	2.99
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	20	2.99
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	12	2.99
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	12	2.99
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	13	2.99
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	13	2.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	7	2.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	7	2.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	7	2.99
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	7	2.99
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	14	2.99
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	18	2.99
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	3	2.99
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	3	2.99
(4,1200)	1:7:A:GLY:H	1:31:A:CYS:HA	11	2.98
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	2	2.98
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	13	2.98
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	3	2.98
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	3	2.98
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	3	2.98
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	7	2.98
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	7	2.98
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	7	2.98
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	5	2.98
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	5	2.98
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	18	2.97
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	18	2.97
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	18	2.97
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	4	2.97
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	4	2.97
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	4	2.97
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	4	2.97
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	2	2.97
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	2	2.97
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	2	2.97
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	16	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	13	2.96
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	14	2.96
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	15	2.96
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	15	2.96
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	15	2.96
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	15	2.96
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	5	2.96
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	5	2.96
(4,273)	1:55:A:PRO:HD2	1:56:A:ASP:H	9	2.96
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	4	2.95
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	4	2.95
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	4	2.95
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	17	2.95
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	3	2.94
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	3	2.94
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	19	2.94
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	3	2.94
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	15	2.94
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	15	2.94
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	15	2.94
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	15	2.94
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	15	2.94
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	15	2.94
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	15	2.94
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	15	2.94
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	18	2.94
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	18	2.94
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	18	2.94
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	5	2.93
(4,636)	1:60:A:CYS:HB2	1:67:A:LYS:HD3	16	2.93
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	17	2.93
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	20	2.92
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	6	2.92
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	6	2.92
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	6	2.92
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	6	2.92
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	3	2.92
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	9	2.92
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	15	2.92
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	15	2.92
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	16	2.92
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	16	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	15	2.92
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	18	2.92
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	14	2.92
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	14	2.92
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	17	2.92
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	17	2.92
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	13	2.91
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	4	2.91
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	4	2.91
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	4	2.91
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	19	2.91
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	19	2.91
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	18	2.9
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	7	2.9
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	2	2.9
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	2	2.9
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	2	2.9
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	6	2.9
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	6	2.9
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	6	2.9
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	8	2.9
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	10	2.9
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	19	2.9
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	12	2.89
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	14	2.89
(4,910)	1:20:A:GLN:HA	1:20:A:GLN:HG2	15	2.89
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	1	2.89
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	1	2.89
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	1	2.89
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	1	2.89
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	2	2.89
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	12	2.89
(4,453)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	1	2.88
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	1	2.88
(4,453)	1:9:A:LYS:HD3	1:28:A:GLY:HA2	1	2.88
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	14	2.88
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	4	2.87
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	4	2.87
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	4	2.87
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	4	2.87
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	4	2.87
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	4	2.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	4	2.87
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	6	2.87
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	15	2.87
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	1	2.87
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	1	2.87
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	5	2.86
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	5	2.86
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	5	2.86
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	1	2.86
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	7	2.86
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	14	2.86
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	14	2.86
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	9	2.85
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	9	2.85
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	13	2.85
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	1	2.84
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	1	2.84
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	18	2.84
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	18	2.84
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	2	2.84
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	2	2.84
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	2	2.84
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	2	2.84
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	1	2.84
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	1	2.84
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	6	2.84
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	6	2.84
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD3	6	2.84
(4,176)	1:31:A:CYS:H	1:37:A:LYS:HD2	6	2.84
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	5	2.83
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	5	2.83
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	4	2.83
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	4	2.83
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	4	2.83
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	4	2.83
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	4	2.83
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	4	2.83
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	4	2.83
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	4	2.83
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	20	2.83
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	9	2.83
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	9	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,192)	1:59:A:LYS:HB3	1:60:A:CYS:H	15	2.83
(4,192)	1:59:A:LYS:HB2	1:60:A:CYS:H	15	2.83
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	2	2.82
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	2	2.82
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	2	2.82
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	2	2.82
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	1	2.82
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	1	2.82
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	1	2.82
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	1	2.82
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	10	2.82
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	10	2.82
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	20	2.82
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	4	2.82
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	4	2.82
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	4	2.82
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	11	2.82
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	7	2.81
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	20	2.81
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	8	2.81
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	15	2.81
(4,588)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	15	2.81
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	6	2.81
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	6	2.81
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	3	2.81
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	2	2.8
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	2	2.8
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	2	2.8
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	7	2.8
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	7	2.8
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	7	2.8
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	7	2.8
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	17	2.8
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	17	2.8
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	17	2.8
(4,9)	1:15:A:ARG:HB2	1:16:A:SER:H	18	2.8
(4,9)	1:15:A:ARG:HB3	1:16:A:SER:H	18	2.8
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	3	2.79
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	3	2.79
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	3	2.79
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	12	2.79
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	12	2.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	12	2.79
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	12	2.79
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	7	2.79
(4,557)	1:6:A:LYS:HB3	1:10:A:CYS:HB3	7	2.79
(4,557)	1:6:A:LYS:HB2	1:10:A:CYS:HB3	7	2.79
(4,221)	1:7:A:GLY:HA2	1:10:A:CYS:H	14	2.79
(4,221)	1:7:A:GLY:HA3	1:10:A:CYS:H	14	2.79
(4,67)	1:39:A:CYS:H	1:55:A:PRO:HB3	5	2.79
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	10	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	10	2.78
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	10	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	10	2.78
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	10	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	10	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	10	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	10	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	17	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	17	2.78
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	17	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	17	2.78
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	17	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	17	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	17	2.78
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	17	2.78
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	3	2.78
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	3	2.78
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	3	2.78
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	3	2.78
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	19	2.78
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	19	2.78
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	4	2.77
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	4	2.77
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	14	2.77
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	14	2.77
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	9	2.77
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	9	2.77
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	18	2.77
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	18	2.77
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	18	2.77
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	14	2.76
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	14	2.76
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	14	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	14	2.76
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	7	2.76
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	7	2.76
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	16	2.76
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	16	2.76
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	16	2.76
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	16	2.76
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	16	2.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	16	2.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	16	2.75
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	16	2.75
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	16	2.75
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	16	2.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	2	2.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	2	2.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	6	2.75
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	6	2.75
(4,1007)	1:4:A:LYS:HG2	1:6:A:LYS:H	13	2.74
(4,1007)	1:4:A:LYS:HG3	1:6:A:LYS:H	13	2.74
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	3	2.74
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	3	2.74
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	3	2.74
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	3	2.74
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	4	2.74
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	1	2.74
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	1	2.74
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	1	2.74
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	9	2.73
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	10	2.73
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	13	2.73
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	13	2.73
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	12	2.72
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	12	2.72
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	12	2.72
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	12	2.72
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	12	2.72
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	12	2.72
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	12	2.72
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	12	2.72
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	19	2.72
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	19	2.72
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	1	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	1	2.72
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	1	2.72
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	1	2.72
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	7	2.72
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	13	2.71
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	13	2.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	5	2.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	5	2.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	17	2.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	17	2.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE21	20	2.71
(4,754)	1:26:A:GLN:HB3	1:26:A:GLN:HE22	20	2.71
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	6	2.7
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	6	2.7
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	6	2.7
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	6	2.7
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	6	2.7
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	16	2.7
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	16	2.7
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	16	2.7
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	16	2.7
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	5	2.7
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	5	2.7
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	5	2.7
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	13	2.7
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	13	2.7
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	13	2.7
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	10	2.69
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	10	2.69
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	10	2.69
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	10	2.69
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	13	2.69
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	13	2.69
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	13	2.69
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	13	2.69
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	13	2.69
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	13	2.69
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	13	2.69
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	13	2.69
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	2	2.69
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	6	2.68
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	6	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	16	2.68
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	16	2.68
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	16	2.68
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	16	2.68
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	17	2.68
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	12	2.67
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	12	2.67
(4,1177)	1:9:A:LYS:HB2	1:29:A:GLU:HG3	12	2.67
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	2.67
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	8	2.67
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	8	2.67
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	8	2.67
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	15	2.67
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	15	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	7	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	7	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	7	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	7	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	14	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	14	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	14	2.67
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	14	2.67
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	7	2.67
(4,559)	1:6:A:LYS:HB3	1:10:A:CYS:HB2	7	2.67
(4,559)	1:6:A:LYS:HB2	1:10:A:CYS:HB2	7	2.67
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	1	2.66
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	1	2.66
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	1	2.66
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	1	2.66
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	15	2.66
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	15	2.66
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	15	2.66
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	15	2.66
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	2	2.65
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	2	2.65
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	2	2.65
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	14	2.65
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	18	2.65
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	18	2.65
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	18	2.65
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	18	2.65
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	14	2.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	14	2.64
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	14	2.64
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	14	2.64
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	6	2.64
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	6	2.64
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	6	2.64
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	6	2.64
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	16	2.64
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	7	2.63
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	7	2.63
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	7	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	7	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	7	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	7	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	7	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	15	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	15	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	15	2.63
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	15	2.63
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	1	2.63
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	1	2.63
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	1	2.63
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	4	2.62
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	17	2.62
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	17	2.62
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	17	2.62
(4,467)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	17	2.62
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	14	2.61
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	14	2.61
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	14	2.61
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	14	2.61
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	14	2.61
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	14	2.61
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	14	2.61
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	14	2.61
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	17	2.61
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	13	2.61
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	13	2.61
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	13	2.61
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	8	2.61
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	8	2.61
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	15	2.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	15	2.61
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	4	2.6
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	14	2.6
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	14	2.6
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	14	2.6
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	14	2.6
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	6	2.6
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	18	2.6
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	14	2.6
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	14	2.6
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	14	2.6
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	14	2.6
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	18	2.6
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	16	2.6
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	16	2.6
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	12	2.59
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	19	2.59
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	19	2.59
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	19	2.59
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	19	2.59
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	10	2.59
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	10	2.59
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	16	2.59
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	1	2.58
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	1	2.58
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	9	2.58
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	20	2.57
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	9	2.57
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	9	2.57
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	9	2.57
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	9	2.57
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	6	2.56
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	6	2.56
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	6	2.56
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	6	2.56
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	6	2.56
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	6	2.56
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	6	2.56
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	6	2.56
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	6	2.56
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	12	2.56
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	12	2.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	12	2.56
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	12	2.56
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	6	2.56
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	17	2.56
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	17	2.56
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	17	2.56
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	17	2.56
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	3	2.56
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	7	2.56
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	11	2.56
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	10	2.56
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	10	2.56
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	10	2.56
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	14	2.55
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	18	2.55
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	17	2.55
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	17	2.55
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	17	2.55
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	17	2.55
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	19	2.55
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	19	2.55
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	19	2.55
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	19	2.55
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	17	2.55
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	12	2.55
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	12	2.55
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	12	2.55
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	12	2.55
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	9	2.55
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	8	2.55
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	8	2.55
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	8	2.55
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	8	2.55
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	18	2.55
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	18	2.55
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	7	2.54
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	14	2.54
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	1	2.54
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	18	2.54
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	18	2.54
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	9	2.54
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	9	2.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	14	2.54
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	10	2.54
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	14	2.54
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	17	2.54
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	17	2.54
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	10	2.53
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	18	2.53
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	18	2.53
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	18	2.53
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	18	2.53
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	17	2.53
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	6	2.53
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	3	2.53
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	10	2.53
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	19	2.53
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	14	2.52
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	10	2.52
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	10	2.52
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	20	2.52
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	20	2.52
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	20	2.52
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	20	2.52
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	20	2.52
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	7	2.52
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	18	2.52
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	7	2.52
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	7	2.52
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	2	2.52
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	2	2.52
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	20	2.52
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	9	2.51
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	9	2.51
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	9	2.51
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	9	2.51
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	9	2.51
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	9	2.51
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	9	2.51
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	9	2.51
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	9	2.51
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	9	2.51
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	6	2.51
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	6	2.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	6	2.51
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	6	2.51
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	9	2.51
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	15	2.51
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	15	2.51
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	15	2.51
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	15	2.51
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	2	2.51
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	15	2.51
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	8	2.51
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	14	2.51
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	20	2.51
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	7	2.51
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	7	2.51
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	3	2.51
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	5	2.5
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	5	2.5
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	5	2.5
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	7	2.5
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	18	2.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	9	2.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	9	2.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	9	2.5
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	9	2.5
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	18	2.5
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	13	2.5
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	11	2.5
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	11	2.5
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	18	2.49
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	5	2.49
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	3	2.49
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	3	2.49
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	11	2.49
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	12	2.49
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	9	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	9	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	9	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	9	2.49
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	10	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	10	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	10	2.49
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	10	2.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	11	2.49
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	12	2.49
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	16	2.49
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	18	2.49
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	4	2.49
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	4	2.49
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	20	2.49
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	20	2.49
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	12	2.48
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	12	2.48
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	12	2.48
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	12	2.48
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	6	2.48
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	6	2.48
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	12	2.48
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	17	2.48
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	17	2.48
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	7	2.48
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	7	2.48
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	7	2.48
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	7	2.48
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	13	2.48
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	19	2.48
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	15	2.48
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	6	2.48
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	8	2.48
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	8	2.48
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	3	2.48
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	3	2.48
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	12	2.48
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	12	2.48
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	17	2.47
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	1	2.47
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	7	2.47
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	8	2.47
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	9	2.47
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	10	2.47
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	14	2.47
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	4	2.47
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	5	2.47
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	12	2.47
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	2	2.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	8	2.47
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	17	2.47
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	17	2.47
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	5	2.46
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	5	2.46
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	5	2.46
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	5	2.46
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	1	2.46
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	6	2.46
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	6	2.46
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	8	2.46
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	8	2.46
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	20	2.46
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	20	2.46
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	13	2.46
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	13	2.46
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	12	2.46
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	11	2.46
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	16	2.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	14	2.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	14	2.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	14	2.46
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	14	2.46
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	17	2.46
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	17	2.46
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	6	2.46
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	6	2.46
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	15	2.46
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	15	2.46
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	3	2.45
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	9	2.45
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	15	2.45
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	8	2.45
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	8	2.45
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	4	2.45
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	4	2.45
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	11	2.45
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	1	2.45
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	10	2.45
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	10	2.45
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	13	2.45
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	13	2.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	18	2.45
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	18	2.45
(4,308)	1:62:A:SER:H	1:62:A:SER:HB2	4	2.45
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	15	2.44
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	15	2.44
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	4	2.44
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	4	2.44
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	4	2.44
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	4	2.44
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	3	2.44
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	5	2.44
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	20	2.44
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	9	2.44
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	9	2.44
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	7	2.44
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	7	2.44
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	7	2.44
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	7	2.44
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	11	2.43
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	11	2.43
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	11	2.43
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	11	2.43
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	11	2.43
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	11	2.43
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	11	2.43
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	11	2.43
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	11	2.43
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	11	2.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	17	2.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	17	2.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	17	2.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	18	2.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	18	2.43
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	18	2.43
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	18	2.43
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	4	2.43
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	4	2.43
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	18	2.43
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	18	2.43
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	19	2.43
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	19	2.43
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	12	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	12	2.43
(4,780)	1:50:A:LYS:HA	1:50:A:LYS:HB3	4	2.43
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	2	2.43
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	2	2.43
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	16	2.43
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	16	2.43
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	20	2.43
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	20	2.43
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	10	2.43
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	10	2.43
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	19	2.43
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	19	2.43
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	12	2.42
(4,1189)	1:24:A:LYS:HA	1:24:A:LYS:HB3	13	2.42
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	2.42
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	2.42
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	2.42
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	2.42
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	8	2.42
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	8	2.42
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	2.42
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	8	2.42
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	2.42
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	8	2.42
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	4	2.42
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	7	2.42
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	7	2.42
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	15	2.42
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	15	2.42
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	3	2.42
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	3	2.42
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	16	2.42
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	16	2.42
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	16	2.42
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	16	2.42
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	20	2.42
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	20	2.42
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	20	2.42
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	20	2.42
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	2	2.42
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	6	2.42
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	19	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	9	2.42
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	9	2.42
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	12	2.42
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	12	2.42
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	11	2.42
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	11	2.42
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	2	2.41
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	2	2.41
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	13	2.41
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	13	2.41
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	14	2.41
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	14	2.41
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	14	2.41
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	14	2.41
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	17	2.41
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	6	2.41
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	6	2.41
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	17	2.41
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	2	2.41
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	2	2.41
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	13	2.41
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	13	2.41
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	3	2.41
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	3	2.41
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	7	2.41
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	7	2.41
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	10	2.41
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	10	2.41
(4,1011)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	3	2.4
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	7	2.4
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	7	2.4
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	9	2.4
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	9	2.4
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	1	2.4
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	1	2.4
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	2	2.4
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	2	2.4
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	11	2.4
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	11	2.4
(4,656)	1:21:A:CYS:HA	1:21:A:CYS:HB3	17	2.4
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	3	2.4
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	3	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	6	2.4
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	6	2.4
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	5	2.4
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	5	2.4
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	14	2.4
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	14	2.4
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	1	2.39
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	1	2.39
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	10	2.39
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	10	2.39
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	12	2.39
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	12	2.39
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	12	2.39
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	12	2.39
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	18	2.39
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	18	2.39
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	1	2.39
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	1	2.39
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	5	2.39
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	5	2.39
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	15	2.39
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	15	2.39
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG21	7	2.39
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	11	2.38
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	11	2.38
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	11	2.38
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	1	2.38
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	1	2.38
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	18	2.38
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	18	2.38
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	5	2.38
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	2	2.38
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	2	2.38
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	19	2.38
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	19	2.38
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	19	2.38
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	19	2.38
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	20	2.38
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	20	2.38
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	5	2.37
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	3	2.37
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	3	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	3	2.37
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	3	2.37
(4,891)	1:51:A:GLU:HA	1:51:A:GLU:HG2	11	2.37
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	4	2.37
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	4	2.37
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	8	2.37
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	8	2.37
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	9	2.37
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	9	2.37
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	4	2.37
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	4	2.37
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	4	2.37
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	4	2.37
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	19	2.37
(4,610)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	11	2.37
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	20	2.37
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	20	2.37
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	3	2.37
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	3	2.37
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	8	2.36
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	8	2.36
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	8	2.36
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	8	2.36
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	5	2.36
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	5	2.36
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	5	2.36
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	5	2.36
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	14	2.36
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	14	2.36
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	12	2.36
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	12	2.36
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	11	2.36
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	11	2.36
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	11	2.36
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	11	2.36
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	15	2.36
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	15	2.36
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	15	2.36
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	15	2.36
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	6	2.36
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	6	2.36
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	3	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	3	2.35
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	3	2.35
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	3	2.35
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	9	2.35
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	9	2.35
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	9	2.35
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	9	2.35
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	19	2.35
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	19	2.35
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	14	2.35
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	13	2.35
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	13	2.35
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	16	2.35
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	16	2.35
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	17	2.35
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	17	2.35
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	14	2.35
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	4	2.35
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	4	2.35
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	4	2.35
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	8	2.35
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	8	2.35
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	8	2.35
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	8	2.35
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	14	2.35
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	14	2.35
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	11	2.35
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	11	2.35
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	7	2.35
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	7	2.35
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	7	2.35
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	7	2.35
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	7	2.35
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	7	2.35
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	9	2.35
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	9	2.35
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	9	2.35
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	9	2.35
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	10	2.35
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	10	2.35
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	10	2.35
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	10	2.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	16	2.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	16	2.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	16	2.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	16	2.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	16	2.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	16	2.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	16	2.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	16	2.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	16	2.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	16	2.34
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	14	2.34
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	14	2.34
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	14	2.34
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	14	2.34
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	16	2.34
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	16	2.34
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	16	2.34
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	16	2.34
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	19	2.34
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	19	2.34
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	19	2.34
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	19	2.34
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	3	2.34
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	3	2.34
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG2	11	2.34
(4,889)	1:51:A:GLU:HA	1:51:A:GLU:HG3	11	2.34
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	9	2.34
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	9	2.34
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	17	2.34
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	17	2.34
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	2	2.34
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	2	2.34
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	20	2.34
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	20	2.34
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	20	2.34
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	11	2.34
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	11	2.34
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	18	2.34
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	18	2.34
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	17	2.34
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	17	2.34
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	1	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	1	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	1	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	1	2.34
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	4	2.34
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	4	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	4	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	4	2.34
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	5	2.34
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	5	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	5	2.34
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	5	2.34
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	8	2.34
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	8	2.34
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	12	2.33
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	12	2.33
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	12	2.33
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	13	2.33
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	13	2.33
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	13	2.33
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	13	2.33
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	11	2.33
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	12	2.33
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	12	2.33
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	19	2.33
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	19	2.33
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	20	2.33
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	20	2.33
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	8	2.33
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	8	2.33
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	19	2.33
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	19	2.33
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	6	2.33
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	6	2.33
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	6	2.33
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	6	2.33
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG21	10	2.33
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	2	2.32
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	2	2.32
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	2	2.32
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	18	2.32
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	18	2.32
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	18	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	14	2.32
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	14	2.32
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	5	2.32
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	5	2.32
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	5	2.32
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	16	2.32
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	7	2.32
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	7	2.32
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB2	10	2.32
(4,818)	1:15:A:ARG:HA	1:15:A:ARG:HB3	10	2.32
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	16	2.32
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	10	2.32
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	10	2.32
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	10	2.32
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	2	2.32
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	2	2.32
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	15	2.31
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	15	2.31
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	20	2.31
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.31
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.31
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	2	2.31
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	2	2.31
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	2	2.31
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	2	2.31
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	15	2.31
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	15	2.31
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	15	2.31
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	15	2.31
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	18	2.31
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	18	2.31
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	18	2.31
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	18	2.31
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	1	2.31
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	1	2.31
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	1	2.31
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	15	2.31
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	15	2.31
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	15	2.31
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	13	2.31
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	13	2.31
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	13	2.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	13	2.31
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	14	2.31
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	14	2.31
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	14	2.31
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	16	2.31
(4,465)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	16	2.31
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	15	2.31
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	5	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	5	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	5	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	10	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	10	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	10	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	13	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	13	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	13	2.3
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	11	2.3
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	11	2.3
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	11	2.3
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	5	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	4	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	4	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	4	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	9	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	9	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	9	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	14	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	14	2.3
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	14	2.3
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	11	2.3
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	11	2.3
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG3	20	2.3
(4,885)	1:26:A:GLN:HA	1:26:A:GLN:HG2	20	2.3
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	2	2.3
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	2	2.3
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	2	2.3
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	2	2.3
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	6	2.3
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	6	2.3
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	6	2.3
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	6	2.3
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	7	2.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	7	2.3
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	7	2.3
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	18	2.3
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	18	2.3
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	18	2.3
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE2	16	2.3
(4,488)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	16	2.3
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	3	2.29
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	3	2.29
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	3	2.29
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	15	2.29
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	15	2.29
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	15	2.29
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	12	2.29
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	12	2.29
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	12	2.29
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	15	2.29
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	19	2.29
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	15	2.29
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	19	2.29
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	17	2.29
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	17	2.29
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	17	2.29
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	4	2.29
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	4	2.29
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	6	2.28
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	6	2.28
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	6	2.28
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	5	2.28
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	5	2.28
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	5	2.28
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	5	2.28
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	11	2.28
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	11	2.28
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	11	2.28
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	11	2.28
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	16	2.28
(4,1008)	1:6:A:LYS:H	1:6:A:LYS:HG3	2	2.28
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	17	2.28
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	17	2.28
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	17	2.28
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	18	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	18	2.28
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	18	2.28
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	3	2.28
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	3	2.28
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	3	2.28
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	9	2.28
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	9	2.28
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	9	2.28
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	3	2.28
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	3	2.28
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	3	2.28
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	3	2.28
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	7	2.27
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	7	2.27
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	7	2.27
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	19	2.27
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	19	2.27
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	19	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	6	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	6	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	6	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	11	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	11	2.27
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	11	2.27
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	13	2.27
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	13	2.27
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	13	2.27
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	13	2.27
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	15	2.27
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	15	2.27
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	15	2.27
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE2	15	2.27
(4,489)	1:50:A:LYS:HG3	1:50:A:LYS:HE3	15	2.27
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	2	2.26
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	2	2.26
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	2	2.26
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	2	2.26
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	2	2.26
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	2	2.26
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	2	2.26
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	2	2.26
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	18	2.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	18	2.26
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	20	2.26
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	20	2.26
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	20	2.26
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	8	2.26
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	8	2.26
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	8	2.26
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	8	2.26
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	13	2.26
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	13	2.26
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	13	2.26
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	16	2.26
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	18	2.26
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	18	2.26
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	18	2.26
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	18	2.26
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	9	2.26
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE2	2	2.25
(4,1140)	1:39:A:CYS:HA	1:67:A:LYS:HE3	2	2.25
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	2	2.25
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	2	2.25
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	2	2.25
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	2	2.25
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	7	2.25
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	7	2.25
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	7	2.25
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	7	2.25
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	7	2.25
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	7	2.25
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	8	2.25
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	8	2.25
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	8	2.25
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	8	2.25
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	1	2.25
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	5	2.25
(4,307)	1:62:A:SER:H	1:62:A:SER:HA	16	2.25
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	14	2.24
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	14	2.24
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	14	2.24
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	8	2.24
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	8	2.24
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	8	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	8	2.24
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	8	2.24
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	8	2.24
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	8	2.24
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	8	2.24
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	5	2.24
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	5	2.24
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	5	2.24
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	5	2.24
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	2	2.23
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	1	2.23
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	1	2.23
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	1	2.23
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	1	2.23
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	11	2.23
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	11	2.23
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	11	2.23
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	11	2.23
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	5	2.23
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	5	2.23
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	5	2.23
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	5	2.23
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	5	2.23
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	5	2.23
(4,1035)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	2	2.23
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	11	2.23
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	2	2.23
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	2	2.23
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	2	2.23
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	6	2.23
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	6	2.23
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	6	2.23
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	6	2.23
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	13	2.23
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	13	2.23
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	13	2.23
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	13	2.23
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	11	2.23
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	11	2.23
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	4	2.22
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	4	2.22
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	4	2.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	4	2.22
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	3	2.22
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	3	2.22
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	3	2.22
(4,800)	1:39:A:CYS:HB3	1:58:A:CYS:HB2	11	2.22
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	11	2.22
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB2	11	2.22
(4,800)	1:39:A:CYS:HB2	1:58:A:CYS:HB3	11	2.22
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	1	2.22
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	1	2.22
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	1	2.22
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	1	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	1	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	1	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	1	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	1	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	3	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	3	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	3	2.22
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	3	2.22
(4,451)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	17	2.22
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	8	2.21
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	8	2.21
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	8	2.21
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	8	2.21
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	8	2.21
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	8	2.21
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	8	2.21
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	17	2.21
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	17	2.21
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	17	2.21
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	20	2.21
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	20	2.21
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	20	2.21
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	20	2.21
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	20	2.21
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	20	2.21
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	20	2.21
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	20	2.21
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	16	2.21
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	16	2.21
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	16	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	9	2.21
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	9	2.21
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	9	2.21
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	9	2.21
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	16	2.21
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	16	2.21
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	16	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	3	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	3	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	3	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	3	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	11	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	11	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	11	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	11	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	20	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	20	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	20	2.21
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	20	2.21
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	10	2.2
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	10	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	4	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	4	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	4	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	4	2.2
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	4	2.2
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	4	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	4	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	4	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	2	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	2	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	2	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	8	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	8	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	8	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	19	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	19	2.2
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	19	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	5	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	5	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	5	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	5	2.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	6	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	6	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	6	2.2
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	6	2.2
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	13	2.2
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	13	2.2
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	13	2.2
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	13	2.2
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	5	2.2
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	11	2.19
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	11	2.19
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	11	2.19
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	11	2.19
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	11	2.19
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	11	2.19
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	11	2.19
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	11	2.19
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	10	2.19
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	10	2.19
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	10	2.19
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	13	2.19
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	13	2.19
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	13	2.19
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	5	2.19
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	17	2.19
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	17	2.19
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	17	2.19
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	17	2.19
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	8	2.19
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	8	2.19
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	8	2.19
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	19	2.19
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	19	2.19
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	19	2.19
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	19	2.19
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	4	2.19
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	14	2.19
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	14	2.19
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	14	2.19
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	14	2.19
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	16	2.19
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	16	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB2	16	2.19
(4,448)	1:28:A:GLY:HA2	1:62:A:SER:HB3	16	2.19
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	13	2.19
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	13	2.19
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	11	2.18
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	11	2.18
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	18	2.18
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	18	2.18
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	13	2.18
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	13	2.18
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	13	2.18
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	13	2.18
(4,1020)	1:12:A:SER:HA	1:15:A:ARG:HD3	18	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	11	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	11	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	11	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	11	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	19	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	19	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	19	2.18
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	19	2.18
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	8	2.17
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	8	2.17
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	20	2.17
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	20	2.17
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE2	20	2.17
(4,1065)	1:9:A:LYS:HB2	1:9:A:LYS:HE3	20	2.17
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.17
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	20	2.17
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	18	2.17
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	18	2.17
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	18	2.17
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	18	2.17
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	11	2.17
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	11	2.17
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	10	2.17
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	10	2.17
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	10	2.16
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	10	2.16
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	10	2.16
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	10	2.16
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	12	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	12	2.16
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	12	2.16
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	12	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	9	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	9	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	9	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	9	2.16
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	9	2.16
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	9	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	9	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	9	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	12	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	12	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	12	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	12	2.16
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	12	2.16
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	12	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	12	2.16
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	12	2.16
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	7	2.16
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB3	7	2.16
(4,890)	1:51:A:GLU:HA	1:51:A:GLU:HB2	7	2.16
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	2	2.16
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	2	2.16
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	2	2.16
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	2	2.16
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	19	2.16
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	19	2.16
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	19	2.16
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	8	2.16
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	8	2.16
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	16	2.16
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	16	2.16
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	16	2.16
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	16	2.16
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	11	2.16
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	11	2.16
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	11	2.16
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	11	2.16
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	8	2.16
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	8	2.16
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	8	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	8	2.16
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	4	2.15
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	4	2.15
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	5	2.15
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	5	2.15
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	14	2.15
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	14	2.15
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	9	2.15
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	9	2.15
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	9	2.15
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	9	2.15
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	1	2.15
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	1	2.15
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	1	2.15
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	14	2.15
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	14	2.15
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	14	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	10	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	10	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	10	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	10	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	16	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	16	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	16	2.15
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	16	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	1	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	1	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	1	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	2	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	2	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	2	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	5	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	5	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	5	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	11	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	11	2.15
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	11	2.15
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	15	2.15
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	15	2.15
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	15	2.15
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	15	2.15
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	12	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	12	2.15
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	12	2.15
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	12	2.15
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	20	2.15
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.15
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	20	2.15
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	20	2.15
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG23	2	2.15
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG21	6	2.15
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	12	2.15
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	9	2.14
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	9	2.14
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	1	2.14
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	1	2.14
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	1	2.14
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	20	2.14
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	20	2.14
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	20	2.14
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	20	2.14
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	8	2.14
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	8	2.14
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	8	2.14
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	8	2.14
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	6	2.14
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	6	2.14
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	6	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	4	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	4	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	4	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	4	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	12	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	12	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	12	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	12	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	18	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	18	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	18	2.14
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	18	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	5	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	5	2.14
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	5	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	5	2.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	14	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	14	2.14
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	14	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	14	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	15	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	15	2.14
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	15	2.14
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	15	2.14
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	12	2.14
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	12	2.14
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	12	2.14
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	12	2.14
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	1	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	1	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	1	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	1	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	5	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	5	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	5	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	5	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	15	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	15	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	15	2.13
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	15	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	4	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	4	2.13
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	4	2.13
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	4	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	10	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	10	2.13
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	10	2.13
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	10	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	17	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	17	2.13
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	17	2.13
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	17	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	7	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	7	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	7	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	7	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	20	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	20	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	20	2.13
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	20	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	2	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	2	2.13
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	2	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	2	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	3	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	3	2.13
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	3	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	3	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	6	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	6	2.13
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	6	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	6	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	10	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	10	2.13
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	10	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	10	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	18	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	18	2.13
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	18	2.13
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	18	2.13
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	14	2.13
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	14	2.13
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	14	2.13
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE2	6	2.12
(4,1068)	1:4:A:LYS:HG2	1:4:A:LYS:HE3	6	2.12
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE2	6	2.12
(4,1068)	1:4:A:LYS:HG3	1:4:A:LYS:HE3	6	2.12
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	12	2.12
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	12	2.12
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	12	2.12
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	12	2.12
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	5	2.12
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	5	2.12
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	5	2.12
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	5	2.12
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	11	2.11
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	11	2.11
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	11	2.11
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	19	2.11
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	19	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	3	2.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	3	2.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	3	2.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	3	2.11
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	13	2.11
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	13	2.11
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	13	2.11
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	13	2.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	7	2.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	7	2.11
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	7	2.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	7	2.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	17	2.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	17	2.11
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	17	2.11
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	17	2.11
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	17	2.11
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	17	2.11
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	17	2.11
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	17	2.11
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	7	2.1
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	7	2.1
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	7	2.1
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	7	2.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	4	2.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	4	2.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	4	2.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	8	2.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	8	2.1
(4,1069)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	8	2.1
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	18	2.1
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	20	2.1
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	10	2.1
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	10	2.1
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB2	10	2.1
(4,677)	1:52:A:CYS:HA	1:57:A:SER:HB3	10	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	9	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	9	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	9	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	9	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	19	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	19	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	19	2.1
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	19	2.1
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	1	2.1
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	1	2.1
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	1	2.1
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	1	2.1
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	12	2.09
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	12	2.09
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	14	2.09
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	17	2.09
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	17	2.09
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	17	2.09
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	17	2.09
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	14	2.09
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	14	2.09
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG2	14	2.09
(4,785)	1:24:A:LYS:HA	1:24:A:LYS:HG3	14	2.09
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	4	2.09
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	4	2.09
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	4	2.09
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	4	2.09
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE2	8	2.09
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	8	2.09
(4,490)	1:37:A:LYS:HG3	1:37:A:LYS:HE3	8	2.09
(4,490)	1:37:A:LYS:HG2	1:37:A:LYS:HE3	8	2.09
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE2	20	2.09
(4,464)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	20	2.09
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	20	2.09
(4,464)	1:6:A:LYS:HG3	1:6:A:LYS:HE3	20	2.09
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	6	2.09
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	6	2.09
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	6	2.09
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	20	2.08
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	20	2.08
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	12	2.08
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	12	2.08
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	12	2.08
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	12	2.08
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	12	2.08
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	12	2.08
(4,957)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	3	2.08
(4,957)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	3	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,280)	1:40:A:ASN:HD22	1:67:A:LYS:HA	5	2.08
(4,280)	1:40:A:ASN:HD21	1:67:A:LYS:HA	5	2.08
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	7	2.07
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	7	2.07
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	2.07
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	20	2.07
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	2.07
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	20	2.07
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	3	2.06
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	3	2.06
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	6	2.06
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	6	2.06
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	6	2.06
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	16	2.06
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	16	2.06
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	16	2.06
(4,1070)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	16	2.06
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	2	2.06
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	2	2.06
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	2	2.06
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	2	2.06
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	4	2.06
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	12	2.06
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	17	2.06
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	17	2.06
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	17	2.06
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	17	2.06
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	1	2.05
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	13	2.05
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	13	2.05
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	13	2.05
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	13	2.05
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	7	2.05
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	7	2.05
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	7	2.05
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	13	2.04
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	13	2.04
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	13	2.04
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	4	2.04
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	16	2.04
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	16	2.04
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	16	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	16	2.04
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	12	2.04
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB2	12	2.04
(4,781)	1:24:A:LYS:HA	1:24:A:LYS:HB3	12	2.04
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	2	2.04
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	2	2.04
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	2	2.04
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	2	2.04
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	10	2.04
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	17	2.03
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	17	2.03
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	18	2.03
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	18	2.03
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	18	2.03
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	18	2.03
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	18	2.03
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	18	2.03
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	18	2.03
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	18	2.03
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	11	2.03
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	11	2.03
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	11	2.03
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	11	2.03
(4,643)	1:9:A:LYS:HG2	1:29:A:GLU:HG3	11	2.03
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	11	2.03
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG2	11	2.03
(4,643)	1:9:A:LYS:HG3	1:29:A:GLU:HG3	11	2.03
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	2	2.02
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	2	2.02
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	8	2.02
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	8	2.02
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	8	2.02
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	16	2.02
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	10	2.02
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG2	10	2.02
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	10	2.02
(4,613)	1:47:A:LYS:HA	1:47:A:LYS:HG3	10	2.02
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	7	2.01
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	8	2.01
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	7	2.0
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	7	2.0
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	4	2.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	14	2.0
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	20	2.0
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	16	1.99
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	16	1.99
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	15	1.99
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	6	1.99
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	6	1.99
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	6	1.99
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	8	1.99
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	13	1.98
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	13	1.98
(4,1042)	1:32:A:THR:HA	1:37:A:LYS:HD2	19	1.98
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	6	1.98
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	13	1.98
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	18	1.97
(4,1110)	1:9:A:LYS:HD2	1:29:A:GLU:H	18	1.97
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	18	1.97
(4,1110)	1:9:A:LYS:HD3	1:29:A:GLU:H	18	1.97
(4,824)	1:39:A:CYS:HB2	1:55:A:PRO:HA	5	1.97
(4,797)	1:39:A:CYS:HB2	1:55:A:PRO:HA	5	1.97
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	13	1.96
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	1.96
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	5	1.96
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	5	1.96
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	5	1.96
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	10	1.95
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	9	1.94
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	9	1.94
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	9	1.94
(4,1119)	1:38:A:THR:HA	1:55:A:PRO:HG3	6	1.94
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	19	1.94
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD2	19	1.94
(4,1040)	1:32:A:THR:HA	1:37:A:LYS:HD3	19	1.94
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	19	1.94
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	19	1.94
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	19	1.94
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	19	1.94
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	19	1.94
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	19	1.94
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	19	1.94
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	19	1.94
(4,730)	1:38:A:THR:HA	1:55:A:PRO:HG3	6	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	12	1.94
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	12	1.94
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	12	1.94
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG21	18	1.94
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD2	6	1.93
(4,1190)	1:50:A:LYS:HA	1:50:A:LYS:HD3	6	1.93
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	17	1.93
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	17	1.93
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	17	1.93
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	17	1.93
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	17	1.93
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	17	1.93
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	17	1.93
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	17	1.93
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	12	1.93
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	3	1.93
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	5	1.93
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	10	1.92
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	10	1.92
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	10	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	13	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	13	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	13	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	13	1.92
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	13	1.92
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	13	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	13	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	13	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	16	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	16	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	16	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	16	1.92
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	16	1.92
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	16	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	16	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	16	1.92
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	14	1.92
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	14	1.92
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	14	1.92
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	14	1.92
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	3	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	3	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	3	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	3	1.91
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	3	1.91
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	3	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	3	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	3	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	10	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	10	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	10	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	10	1.91
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	10	1.91
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	10	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	10	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	10	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	15	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	15	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	15	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	15	1.91
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	15	1.91
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	15	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	15	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	15	1.91
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	4	1.91
(4,817)	1:6:A:LYS:HD2	1:15:A:ARG:HA	4	1.91
(4,817)	1:6:A:LYS:HD3	1:15:A:ARG:HA	4	1.91
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	11	1.91
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	4	1.91
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	4	1.91
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	4	1.91
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	4	1.91
(4,288)	1:8:A:GLU:HB2	1:9:A:LYS:H	3	1.91
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	3	1.91
(4,288)	1:8:A:GLU:HB3	1:9:A:LYS:H	3	1.91
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	1	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	1	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	1	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	1	1.9
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	1	1.9
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	1	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	1	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	1	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	7	1.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	7	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	7	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	7	1.9
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	7	1.9
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	7	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	7	1.9
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	7	1.9
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	3	1.9
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	18	1.9
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	18	1.9
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	18	1.9
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	18	1.9
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	18	1.9
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	4	1.89
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	4	1.89
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	4	1.89
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	4	1.89
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	2	1.89
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	8	1.89
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	8	1.88
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	8	1.88
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	8	1.88
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	8	1.88
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	9	1.88
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	17	1.88
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	13	1.88
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	13	1.88
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	13	1.88
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	13	1.88
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	10	1.88
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	10	1.88
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	10	1.88
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	10	1.88
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	6	1.87
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE2	6	1.87
(4,1192)	1:6:A:LYS:HB2	1:6:A:LYS:HE3	6	1.87
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	5	1.87
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	5	1.87
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	5	1.87
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	5	1.87
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE2	5	1.87
(4,1010)	1:9:A:LYS:HG2	1:9:A:LYS:HE3	5	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE2	5	1.87
(4,1010)	1:9:A:LYS:HG3	1:9:A:LYS:HE3	5	1.87
(4,825)	1:39:A:CYS:HB3	1:55:A:PRO:HD3	19	1.87
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	15	1.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	6	1.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	6	1.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD2	6	1.87
(4,620)	1:31:A:CYS:HB3	1:37:A:LYS:HD3	6	1.87
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	9	1.87
(4,882)	1:38:A:THR:HG21	1:39:A:CYS:H	8	1.86
(4,882)	1:38:A:THR:HG22	1:39:A:CYS:H	8	1.86
(4,882)	1:38:A:THR:HG23	1:39:A:CYS:H	8	1.86
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	19	1.86
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	19	1.86
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	19	1.86
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	19	1.86
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	14	1.85
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	14	1.85
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	14	1.85
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	14	1.85
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	1	1.85
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	1	1.85
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	1	1.85
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	1	1.85
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	1.85
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	3	1.85
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	3	1.85
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	3	1.85
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	12	1.84
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	17	1.84
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	17	1.84
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	17	1.84
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	1.84
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	16	1.84
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	16	1.84
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	16	1.84
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	18	1.83
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	18	1.83
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	18	1.83
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	14	1.83
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	14	1.83
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	14	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	14	1.82
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	14	1.82
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	14	1.82
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	17	1.81
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	17	1.81
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	1.79
(4,716)	1:9:A:LYS:HD2	1:28:A:GLY:HA3	2	1.79
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	1.79
(4,716)	1:9:A:LYS:HD3	1:28:A:GLY:HA3	2	1.79
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	4	1.78
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	4	1.78
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE2	4	1.78
(4,1066)	1:37:A:LYS:HB3	1:37:A:LYS:HE3	4	1.78
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	8	1.78
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	8	1.78
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	8	1.78
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	4	1.77
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	4	1.77
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	4	1.77
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	3	1.77
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	3	1.77
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	3	1.77
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	3	1.77
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	3	1.77
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	3	1.77
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	11	1.77
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	11	1.77
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	11	1.77
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	11	1.77
(4,451)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	7	1.77
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	9	1.77
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	9	1.77
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	9	1.77
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	16	1.76
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	2	1.76
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	2	1.76
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	2	1.76
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	16	1.76
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	16	1.76
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	16	1.76
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	16	1.76
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	14	1.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	14	1.75
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	14	1.75
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	17	1.73
(4,619)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	10	1.72
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	6	1.72
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	19	1.7
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	17	1.7
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	17	1.7
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	17	1.7
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	7	1.69
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	7	1.69
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	20	1.69
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	20	1.69
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	20	1.69
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	20	1.69
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	4	1.69
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	4	1.69
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	4	1.69
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	11	1.69
(1,884)	1:37:A:LYS:HE2	1:38:A:THR:HG23	1	1.67
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	10	1.65
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	10	1.65
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	10	1.65
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	10	1.65
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	16	1.65
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	16	1.65
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	16	1.65
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	16	1.65
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	16	1.65
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	7	1.64
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	14	1.64
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG2	14	1.64
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	14	1.64
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	15	1.64
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG2	15	1.64
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	15	1.64
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	10	1.64
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	10	1.64
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	10	1.64
(1,884)	1:37:A:LYS:HE3	1:38:A:THR:HG22	4	1.64
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	5	1.63
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	5	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	5	1.63
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	5	1.63
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	5	1.63
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	5	1.63
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	5	1.63
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	5	1.63
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	5	1.63
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	5	1.63
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	18	1.62
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	18	1.62
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	18	1.62
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	18	1.62
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	18	1.62
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	12	1.62
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	7	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	7	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	7	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	7	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	19	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	19	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	19	1.6
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	19	1.6
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	6	1.6
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	6	1.6
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	6	1.6
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	6	1.6
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	6	1.6
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	6	1.6
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	6	1.6
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	6	1.6
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	6	1.6
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	6	1.6
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	1	1.58
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	1	1.58
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	1	1.58
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	1	1.58
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	1	1.58
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	1	1.58
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	1	1.58
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	1	1.58
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	1	1.58
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	1	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	3	1.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	2	1.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	2	1.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	2	1.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	2	1.58
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	2	1.58
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	2	1.58
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	2	1.58
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	2	1.58
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	2	1.58
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	2	1.58
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	2	1.58
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	2	1.58
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	2	1.58
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	2	1.58
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	5	1.57
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	5	1.57
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	5	1.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	10	1.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	10	1.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	10	1.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	10	1.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	10	1.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	10	1.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	10	1.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	10	1.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	10	1.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	10	1.57
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	16	1.57
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	16	1.57
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	16	1.57
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	16	1.57
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	13	1.56
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	13	1.56
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	13	1.56
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	13	1.56
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	6	1.56
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	6	1.56
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	6	1.56
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	6	1.56
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	2	1.56
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	15	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	19	1.55
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	19	1.55
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	19	1.55
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	19	1.55
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	3	1.54
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG2	3	1.54
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	3	1.54
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	15	1.54
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	15	1.54
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	15	1.54
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	13	1.53
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	13	1.53
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	6	1.53
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	6	1.53
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	6	1.53
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	6	1.53
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	6	1.53
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	15	1.52
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	15	1.52
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	15	1.52
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	15	1.52
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	15	1.52
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	15	1.52
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	7	1.52
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	7	1.52
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	10	1.52
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG2	10	1.52
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	10	1.52
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	14	1.52
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	1	1.5
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	20	1.5
(1,425)	1:9:A:LYS:HB2	1:31:A:CYS:HA	1	1.5
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	18	1.49
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	18	1.49
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	18	1.49
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	9	1.49
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	9	1.49
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	9	1.49
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	9	1.49
(1,884)	1:32:A:THR:HG22	1:37:A:LYS:HE2	14	1.49
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	18	1.48
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	18	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	18	1.48
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	18	1.48
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	18	1.48
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	3	1.47
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	3	1.47
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	3	1.47
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	3	1.47
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	3	1.47
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	3	1.47
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	3	1.47
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	7	1.47
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	4	1.46
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	4	1.46
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	4	1.46
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	1.46
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	1.46
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	1.46
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	1.46
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	1.46
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	1.46
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	17	1.46
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	17	1.46
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	20	1.44
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	20	1.44
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	20	1.44
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	3	1.44
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	3	1.44
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	3	1.44
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	3	1.44
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	8	1.44
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	8	1.44
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	8	1.44
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	8	1.44
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	8	1.44
(1,896)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	5	1.44
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	8	1.43
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	8	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	8	1.43
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	8	1.43
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	5	1.41
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	5	1.41
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	8	1.41
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	8	1.41
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	8	1.41
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	8	1.41
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	8	1.41
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	20	1.39
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	20	1.39
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	20	1.39
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	9	1.38
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	9	1.38
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	9	1.38
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	9	1.38
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	9	1.38
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	9	1.38
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	9	1.38
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	9	1.38
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	9	1.38
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	9	1.38
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	7	1.38
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	7	1.38
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	7	1.38
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	19	1.36
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	19	1.36
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	19	1.36
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	19	1.36
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	19	1.36
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	19	1.36
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	19	1.36
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	19	1.36
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	19	1.36
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	19	1.36
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	1	1.36
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	3	1.36
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	3	1.36
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	3	1.36
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	19	1.35
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	19	1.35
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	19	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	15	1.35
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	12	1.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	12	1.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	12	1.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	12	1.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	12	1.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	12	1.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	12	1.34
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	12	1.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	12	1.34
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	12	1.34
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	7	1.34
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	7	1.34
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	7	1.34
(1,837)	1:42:A:THR:HG23	1:54:A:GLY:HA2	1	1.34
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	9	1.33
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	20	1.32
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	20	1.32
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	20	1.32
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	20	1.32
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	20	1.32
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	20	1.32
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	13	1.32
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	15	1.32
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	15	1.32
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	15	1.32
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	1.31
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	1.31
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	1.31
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	1.31
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	1.31
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	1.31
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	2	1.31
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	2	1.31
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	6	1.31
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	6	1.31
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	6	1.31
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	6	1.31
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	6	1.31
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	6	1.31
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	6	1.31
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	6	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,619)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	15	1.31
(4,590)	1:64:A:CYS:H	1:67:A:LYS:HE2	16	1.31
(4,590)	1:64:A:CYS:H	1:67:A:LYS:HE3	16	1.31
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	12	1.31
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	17	1.3
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	17	1.3
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	17	1.3
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	8	1.3
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	8	1.3
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	8	1.3
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	5	1.29
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	5	1.29
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	5	1.29
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	5	1.29
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	5	1.29
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	5	1.29
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	5	1.29
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	5	1.29
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	5	1.29
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	5	1.29
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	15	1.29
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	15	1.29
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	15	1.29
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	2	1.29
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	20	1.28
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	1	1.28
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	1	1.28
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	1	1.28
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	10	1.28
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	10	1.28
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	10	1.28
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	6	1.27
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	6	1.27
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	6	1.27
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	6	1.27
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	6	1.27
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	6	1.27
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	17	1.27
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	17	1.27
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	17	1.27
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	17	1.27
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	15	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG2	15	1.27
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	15	1.27
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	3	1.26
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	3	1.26
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	3	1.26
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	3	1.26
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	15	1.26
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	15	1.26
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	15	1.26
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	15	1.26
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	3	1.26
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG2	3	1.26
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	3	1.26
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	8	1.25
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	15	1.24
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	15	1.24
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	15	1.24
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	7	1.24
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	7	1.24
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	7	1.24
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	7	1.24
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	1.23
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	18	1.23
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	1.23
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	18	1.23
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	1.23
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	18	1.23
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	18	1.23
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	6	1.23
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	20	1.23
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	20	1.23
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	20	1.23
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	20	1.23
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	20	1.23
(1,865)	1:6:A:LYS:HG2	1:15:A:ARG:HA	3	1.23
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	8	1.22
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	8	1.22
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	8	1.22
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	8	1.22
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	10	1.22
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	10	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	10	1.22
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	10	1.22
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	10	1.22
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	10	1.22
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	12	1.22
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	12	1.22
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	4	1.22
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	4	1.22
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	4	1.22
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	4	1.22
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	4	1.22
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	12	1.22
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	12	1.22
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	12	1.22
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	12	1.22
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	12	1.22
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	10	1.21
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	10	1.21
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	10	1.21
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	10	1.21
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	20	1.21
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	20	1.21
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	9	1.2
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	9	1.2
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	9	1.2
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	7	1.2
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	11	1.2
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	7	1.2
(4,451)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	19	1.2
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	14	1.2
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	14	1.2
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	14	1.2
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	7	1.2
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	7	1.19
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	7	1.19
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	7	1.19
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	7	1.19
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	5	1.19
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	5	1.19
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	5	1.19
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	17	1.19
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	18	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	13	1.18
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	13	1.18
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	13	1.18
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	13	1.18
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	2	1.18
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	2	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	2	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	2	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	2	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	19	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	19	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	19	1.17
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	19	1.17
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	8	1.17
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	8	1.17
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	8	1.17
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	15	1.17
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	15	1.17
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	15	1.17
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	15	1.17
(1,897)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	5	1.17
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	16	1.16
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	16	1.16
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	16	1.16
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	16	1.16
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	20	1.16
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	20	1.16
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	20	1.16
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	20	1.16
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	20	1.16
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	20	1.16
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	20	1.16
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	20	1.16
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	15	1.16
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	19	1.16
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	19	1.16
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	19	1.16
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	19	1.16
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	19	1.16
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	7	1.16
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	7	1.16
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	7	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	20	1.16
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	20	1.16
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	20	1.16
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	20	1.16
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	6	1.15
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	6	1.15
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	6	1.15
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	14	1.15
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	14	1.15
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	14	1.15
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	5	1.15
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	16	1.15
(1,865)	1:6:A:LYS:HG2	1:15:A:ARG:HA	18	1.14
(4,1183)	1:29:A:GLU:HB2	1:61:A:GLY:HA2	13	1.13
(4,1183)	1:29:A:GLU:HB2	1:61:A:GLY:HA3	13	1.13
(4,1183)	1:29:A:GLU:HB3	1:61:A:GLY:HA3	13	1.13
(4,1183)	1:29:A:GLU:HB2	1:61:A:GLY:HA3	13	1.13
(4,1183)	1:29:A:GLU:HB3	1:61:A:GLY:HA2	13	1.13
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	17	1.13
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	17	1.13
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	17	1.13
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	18	1.13
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	18	1.13
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	18	1.13
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	18	1.13
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	6	1.13
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	6	1.13
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	6	1.13
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	6	1.13
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	15	1.13
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	15	1.13
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	15	1.13
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	15	1.13
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	10	1.12
(4,590)	1:64:A:CYS:H	1:67:A:LYS:HE2	2	1.12
(4,590)	1:64:A:CYS:H	1:67:A:LYS:HE3	2	1.12
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	16	1.12
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	16	1.12
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	16	1.12
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	16	1.12
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	20	1.12
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	20	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	20	1.12
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	20	1.12
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	3	1.11
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	2	1.11
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	2	1.11
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	2	1.11
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	2	1.11
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	2	1.11
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	2	1.11
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	2	1.11
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	10	1.11
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	17	1.11
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	11	1.1
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	11	1.1
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	11	1.1
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	11	1.1
(4,234)	1:33:A:CYS:HB3	1:37:A:LYS:H	11	1.1
(4,234)	1:33:A:CYS:HB2	1:37:A:LYS:H	11	1.1
(4,234)	1:33:A:CYS:HB3	1:37:A:LYS:H	11	1.1
(4,234)	1:33:A:CYS:HB2	1:37:A:LYS:H	11	1.1
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	19	1.1
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	16	1.1
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	14	1.09
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	17	1.09
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	17	1.09
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	17	1.09
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	8	1.09
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	9	1.09
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	8	1.08
(4,1176)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	8	1.08
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	8	1.08
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	8	1.08
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG3	8	1.08
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	2	1.08
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	2	1.08
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	2	1.08
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	5	1.08
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	7	1.08
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	15	1.08
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	10	1.08
(1,744)	1:5:A:GLY:HA2	1:6:A:LYS:HG3	18	1.08
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	2	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	5	1.08
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	17	1.07
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	17	1.07
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	17	1.07
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	17	1.07
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	12	1.07
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	12	1.07
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	12	1.07
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	1	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	5	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	5	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	5	1.07
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	5	1.07
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	5	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	7	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	7	1.07
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	7	1.07
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	7	1.07
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	7	1.07
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	1	1.07
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	1	1.07
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	1	1.07
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	6	1.07
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	6	1.07
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	6	1.07
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	3	1.07
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	3	1.07
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	3	1.07
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	19	1.07
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	19	1.07
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	19	1.07
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	19	1.07
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	6	1.07
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	3	1.06
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	3	1.06
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	3	1.06
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	1.06
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	20	1.06
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	1.06
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	20	1.06
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	4	1.06
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	4	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	4	1.06
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	8	1.06
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	1	1.06
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	1	1.06
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	1	1.06
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	1	1.06
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	4	1.06
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	4	1.06
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	4	1.06
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	4	1.06
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	9	1.06
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	9	1.06
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	3	1.06
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	18	1.06
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	2	1.05
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	2	1.05
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	2	1.05
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	14	1.05
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	14	1.05
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	14	1.05
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	14	1.05
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	10	1.05
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	10	1.05
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	10	1.05
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	10	1.05
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	17	1.05
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	17	1.05
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	17	1.05
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	17	1.05
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	16	1.05
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	7	1.05
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	8	1.04
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	10	1.04
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	10	1.04
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	10	1.04
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	17	1.04
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	17	1.04
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	17	1.04
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	17	1.04
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	17	1.04
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	17	1.04
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	17	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	17	1.04
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	8	1.04
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	8	1.04
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	8	1.04
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	8	1.04
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	1	1.04
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	1	1.04
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	1	1.04
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	2	1.04
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	2	1.04
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	2	1.04
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	2	1.04
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	13	1.04
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	13	1.04
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	13	1.04
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	13	1.04
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	14	1.04
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	14	1.04
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	14	1.04
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	17	1.04
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	17	1.04
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	17	1.04
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	17	1.04
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	13	1.04
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	13	1.03
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	19	1.03
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	19	1.03
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	19	1.03
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	19	1.03
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	10	1.03
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	15	1.03
(1,418)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	6	1.03
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	10	1.02
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	13	1.02
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	9	1.02
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	1	1.02
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	1	1.02
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	1	1.02
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	1	1.02
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	1	1.02
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	1	1.02
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	5	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	5	1.02
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	5	1.02
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	16	1.02
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	16	1.02
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	16	1.02
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	5	1.02
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	16	1.02
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	16	1.02
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE3	16	1.02
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	3	1.02
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	3	1.02
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	3	1.02
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	3	1.02
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	9	1.02
(1,923)	1:9:A:LYS:HB2	1:29:A:GLU:H	9	1.02
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	1	1.02
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	4	1.02
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	17	1.01
(4,619)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	14	1.01
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	15	1.01
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	15	1.01
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	15	1.01
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	15	1.01
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	18	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	18	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	18	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	18	1.0
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	8	1.0
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	8	1.0
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	8	1.0
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	8	1.0
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	19	1.0
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	7	1.0
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	7	1.0
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	10	1.0
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	10	1.0
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	10	1.0
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	17	1.0
(4,103)	1:31:A:CYS:H	1:33:A:CYS:H	11	1.0
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	14	1.0
(1,736)	1:11:A:THR:HG23	1:12:A:SER:HA	19	1.0
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	6	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	6	0.99
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	6	0.99
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	6	0.99
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	1	0.99
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	1	0.99
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	1	0.99
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	1	0.99
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	1	0.99
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	6	0.99
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	6	0.99
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	6	0.99
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	6	0.99
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	5	0.98
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	5	0.98
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	15	0.98
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	15	0.98
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	15	0.98
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	15	0.98
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	15	0.98
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG2	5	0.98
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.98
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	11	0.98
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	11	0.98
(1,736)	1:11:A:THR:HG21	1:62:A:SER:HB2	11	0.98
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	11	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	11	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	11	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	11	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	16	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	16	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	16	0.97
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	16	0.97
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	15	0.97
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	15	0.97
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	15	0.97
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	15	0.97
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	15	0.97
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	15	0.97
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	8	0.97
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	8	0.97
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	8	0.97
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	8	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:11:A:THR:HG21	1:12:A:SER:HA	12	0.97
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	0.96
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	0.96
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	0.96
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	0.96
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	0.96
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	0.96
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	8	0.96
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	8	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	11	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	11	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	11	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	11	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	16	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	16	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG2	16	0.96
(4,978)	1:58:A:CYS:HA	1:59:A:LYS:HG3	16	0.96
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	14	0.96
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	14	0.96
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	14	0.96
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	14	0.96
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	14	0.96
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG2	17	0.96
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG3	17	0.96
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	12	0.96
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	12	0.96
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	12	0.96
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	12	0.96
(1,736)	1:11:A:THR:HG22	1:12:A:SER:HA	20	0.96
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	17	0.95
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	17	0.95
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	17	0.95
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	17	0.95
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	17	0.95
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	17	0.95
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	17	0.95
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	17	0.95
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB2	3	0.95
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB2	3	0.95
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB3	3	0.95
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	14	0.95
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG2	14	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	14	0.95
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	20	0.95
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	20	0.95
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	20	0.95
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	20	0.95
(1,884)	1:32:A:THR:HG22	1:37:A:LYS:HE2	17	0.95
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	1	0.94
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	1	0.94
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	4	0.94
(1,744)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	17	0.94
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	4	0.93
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	12	0.93
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	12	0.93
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	10	0.93
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	10	0.93
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	10	0.93
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	2	0.92
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	2	0.92
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	2	0.92
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	2	0.92
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	8	0.92
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	8	0.92
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	8	0.92
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	8	0.92
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	8	0.92
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	8	0.92
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	8	0.92
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	8	0.92
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	8	0.92
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	8	0.92
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	8	0.92
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	17	0.92
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	17	0.92
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	17	0.92
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	10	0.92
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	10	0.92
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	10	0.92
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	10	0.92
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	10	0.92
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	10	0.92
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	10	0.92
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	10	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	18	0.92
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	18	0.92
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	18	0.92
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	18	0.92
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	18	0.92
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	18	0.92
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	18	0.92
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	18	0.92
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	9	0.92
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	9	0.92
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	9	0.92
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	9	0.92
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	9	0.92
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	14	0.92
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	14	0.92
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	14	0.92
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	14	0.92
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	9	0.92
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	9	0.92
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	9	0.92
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	9	0.92
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	9	0.92
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	9	0.92
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	9	0.92
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	9	0.92
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	2	0.92
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	15	0.92
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	15	0.92
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	15	0.92
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	15	0.92
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	9	0.92
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	9	0.92
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	9	0.92
(1,884)	1:32:A:THR:HG23	1:37:A:LYS:HE2	8	0.92
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	9	0.91
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	9	0.91
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	9	0.91
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	9	0.91
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	8	0.91
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	3	0.91
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	3	0.91
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	2	0.91
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	2	0.91
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	2	0.91
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	2	0.91
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	2	0.91
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	2	0.91
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	2	0.91
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	2	0.91
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	3	0.91
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	3	0.91
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	3	0.91
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	3	0.91
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	3	0.91
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	16	0.91
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	13	0.91
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	11	0.91
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	11	0.91
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	2	0.91
(1,884)	1:32:A:THR:HG21	1:37:A:LYS:HE2	19	0.91
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	2	0.91
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	2	0.91
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	2	0.91
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	2	0.91
(1,425)	1:9:A:LYS:HB2	1:31:A:CYS:HA	13	0.91
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	16	0.9
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	16	0.9
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	16	0.9
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	0.9
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	0.9
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	0.9
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	0.9
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	0.9
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	0.9
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	19	0.9
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	19	0.9
(4,619)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	3	0.9
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	10	0.9
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	10	0.9
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	10	0.9
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	16	0.9
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	16	0.9
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	16	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	16	0.9
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	5	0.89
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	5	0.89
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	5	0.89
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	5	0.89
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	5	0.89
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	5	0.89
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	5	0.89
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	5	0.89
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	5	0.89
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	5	0.89
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	2	0.89
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	0.89
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	0.89
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	0.89
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	0.89
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	0.89
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	0.89
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	0.89
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	0.89
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	19	0.89
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	19	0.89
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	10	0.89
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	6	0.89
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	6	0.89
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	6	0.89
(4,217)	1:7:A:GLY:HA2	1:10:A:CYS:H	12	0.89
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	8	0.89
(1,865)	1:7:A:GLY:HA3	1:9:A:LYS:HG3	2	0.89
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	19	0.88
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	19	0.88
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	19	0.88
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	19	0.88
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	19	0.88
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	19	0.88
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	19	0.88
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	19	0.88
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	19	0.88
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	19	0.88
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	15	0.88
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	15	0.88
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	15	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	15	0.88
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	15	0.88
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	15	0.88
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	15	0.88
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	15	0.88
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	15	0.88
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	15	0.88
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	10	0.88
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	10	0.88
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	10	0.88
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	10	0.88
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	12	0.88
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	20	0.88
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	20	0.88
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	20	0.88
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	5	0.88
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	5	0.88
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	5	0.88
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	6	0.88
(1,744)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	6	0.88
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	4	0.87
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	4	0.87
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	4	0.87
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	4	0.87
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	4	0.87
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	4	0.87
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	4	0.87
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	18	0.87
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	18	0.87
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	18	0.87
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	18	0.87
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	18	0.87
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	18	0.87
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	3	0.87
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	3	0.87
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	2	0.87
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	2	0.87
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	2	0.87
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	3	0.87
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	3	0.87
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	3	0.87
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	19	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	19	0.87
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	19	0.87
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	19	0.87
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	12	0.86
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA2	12	0.86
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	12	0.86
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA2	12	0.86
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	7	0.86
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.86
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	16	0.86
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	11	0.86
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	11	0.86
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	11	0.86
(1,748)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	12	0.86
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	18	0.85
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	18	0.85
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	18	0.85
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	18	0.85
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	17	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	0.85
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	16	0.85
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	16	0.85
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	7	0.85
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	4	0.85
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	4	0.85
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	19	0.85
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	19	0.85
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	19	0.85
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	19	0.85
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	11	0.85
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	18	0.85
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	18	0.85
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	18	0.85
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	18	0.85
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	3	0.85
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	16	0.85
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	16	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	16	0.85
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	16	0.85
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	1	0.85
(1,988)	1:6:A:LYS:HE2	1:15:A:ARG:HA	18	0.85
(1,988)	1:6:A:LYS:HE3	1:15:A:ARG:HA	18	0.85
(1,923)	1:9:A:LYS:HB2	1:29:A:GLU:H	17	0.85
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	3	0.85
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	0.84
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	0.84
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	6	0.84
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	6	0.84
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	12	0.84
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	10	0.84
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG2	10	0.84
(4,214)	1:15:A:ARG:H	1:15:A:ARG:HG3	10	0.84
(1,865)	1:6:A:LYS:HG2	1:15:A:ARG:HA	19	0.84
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	1	0.84
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	1	0.84
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	18	0.83
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	18	0.83
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	18	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	10	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	10	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	10	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	10	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	10	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	10	0.83
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	10	0.83
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	10	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	0.83
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	0.83
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	11	0.83
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	11	0.83
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	6	0.83
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	6	0.83
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	20	0.83
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	20	0.83
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	16	0.83
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	16	0.83
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	14	0.83
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	14	0.83
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	14	0.83
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	14	0.83
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	6	0.83
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	10	0.83
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.83
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.83
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.83
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	16	0.83
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	16	0.83
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	16	0.83
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	16	0.83
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	10	0.82
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	10	0.82
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	10	0.82
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	10	0.82
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	10	0.82
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	10	0.82
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	10	0.82
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	10	0.82
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	10	0.82
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	10	0.82
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	4	0.82
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	4	0.82
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	4	0.82
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	4	0.82
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	15	0.82
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	15	0.82
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	15	0.82
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	15	0.82
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	15	0.82
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	15	0.82
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	15	0.82
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	15	0.82
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	15	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	15	0.82
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	15	0.82
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	2	0.82
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	2	0.82
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	2	0.82
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	16	0.82
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	11	0.81
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	11	0.81
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	11	0.81
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	10	0.81
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	10	0.81
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	10	0.81
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	5	0.81
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	5	0.81
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	5	0.81
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	5	0.81
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	13	0.81
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	13	0.81
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	13	0.81
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	13	0.81
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	10	0.81
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	16	0.81
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	16	0.81
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	9	0.8
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	9	0.8
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	4	0.8
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	4	0.8
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	15	0.8
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	15	0.8
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	16	0.8
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	16	0.8
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	16	0.8
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	16	0.8
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	14	0.8
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	14	0.8
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	14	0.8
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	3	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	16	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	16	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	16	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	16	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	17	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	17	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	17	0.8
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	17	0.8
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	17	0.8
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	17	0.8
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	17	0.8
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	7	0.8
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	7	0.8
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	7	0.8
(4,100)	1:33:A:CYS:H	1:33:A:CYS:HB2	11	0.8
(4,100)	1:33:A:CYS:H	1:33:A:CYS:HB3	11	0.8
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	3	0.8
(1,837)	1:42:A:THR:HG23	1:54:A:GLY:HA2	6	0.8
(1,744)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	15	0.8
(1,358)	1:37:A:LYS:HD2	1:38:A:THR:H	7	0.8
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	15	0.79
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	15	0.79
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	15	0.79
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	15	0.79
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	15	0.79
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	15	0.79
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	15	0.79
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	15	0.79
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	15	0.79
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	15	0.79
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	13	0.79
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	13	0.79
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	13	0.79
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	13	0.79
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	13	0.79
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	13	0.79
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	19	0.79
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	19	0.79
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	4	0.79
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	4	0.79
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	4	0.79
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	4	0.79
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	4	0.79
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	4	0.79
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	4	0.79
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	4	0.79
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	4	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	17	0.79
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.79
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	9	0.79
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	9	0.79
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	9	0.79
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	9	0.79
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	16	0.79
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	16	0.79
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	16	0.79
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	16	0.79
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	10	0.79
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	10	0.79
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	10	0.79
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	10	0.79
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	3	0.79
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	7	0.79
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	7	0.79
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	7	0.79
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	1	0.79
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	15	0.79
(1,874)	1:23:A:SER:HB2	1:24:A:LYS:HB2	13	0.79
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	5	0.78
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	5	0.78
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	5	0.78
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	5	0.78
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	5	0.78
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	18	0.78
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	18	0.78
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	3	0.78
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	3	0.78
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	3	0.78
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	14	0.78
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	5	0.77
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	19	0.77
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	19	0.77
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	19	0.77
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	19	0.77
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	6	0.77
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	6	0.77
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	1	0.77
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	1	0.77
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	19	0.77
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	19	0.77
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	19	0.77
(1,923)	1:9:A:LYS:HB2	1:29:A:GLU:H	19	0.77
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB1	8	0.77
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	6	0.76
(4,1029)	1:25:A:CYS:HB3	1:26:A:GLN:HG2	5	0.76
(4,1029)	1:25:A:CYS:HB3	1:26:A:GLN:HG3	5	0.76
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	0.76
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	0.76
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	0.76
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	0.76
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	0.76
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	0.76
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	7	0.76
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	7	0.76
(4,698)	1:17:A:GLU:HG3	1:18:A:PRO:HD2	3	0.76
(4,698)	1:17:A:GLU:HG3	1:18:A:PRO:HD3	3	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	4	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	4	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	4	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	4	0.76
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	4	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	4	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	4	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	4	0.76
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	4	0.76
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.76
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	12	0.76
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.76
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	13	0.76
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	13	0.76
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	6	0.76
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	6	0.76
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	6	0.76
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	6	0.76
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	10	0.76
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	10	0.76
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	10	0.76
(1,608)	1:17:A:GLU:HG3	1:18:A:PRO:HD2	3	0.76
(1,143)	1:28:A:GLY:H	1:61:A:GLY:HA3	15	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	7	0.75
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	7	0.75
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	7	0.75
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	1	0.75
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	1	0.75
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	7	0.75
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	7	0.75
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	7	0.75
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	7	0.75
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	19	0.75
(1,930)	1:6:A:LYS:HG2	1:7:A:GLY:HA3	19	0.75
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	19	0.74
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	19	0.74
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	17	0.74
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	17	0.74
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	17	0.74
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	8	0.74
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	8	0.74
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	8	0.74
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	8	0.74
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	11	0.74
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	11	0.74
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	13	0.74
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	13	0.74
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	8	0.74
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	9	0.74
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	9	0.74
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	9	0.74
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	9	0.74
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	18	0.73
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	18	0.73
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	18	0.73
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	18	0.73
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	18	0.73
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	18	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	18	0.73
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	18	0.73
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	18	0.73
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	18	0.73
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	11	0.73
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	11	0.73
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	11	0.73
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	16	0.73
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	16	0.73
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	10	0.73
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	20	0.73
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	20	0.73
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	20	0.73
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	8	0.73
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	14	0.73
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	14	0.73
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	9	0.73
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	9	0.73
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	16	0.73
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	16	0.73
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	16	0.73
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	20	0.73
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	20	0.73
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	20	0.73
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	6	0.73
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	6	0.73
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB2	9	0.73
(1,744)	1:5:A:GLY:HA3	1:6:A:LYS:HG3	3	0.73
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	18	0.73
(1,143)	1:28:A:GLY:H	1:61:A:GLY:HA2	16	0.73
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	9	0.72
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	4	0.72
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	4	0.72
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	4	0.72
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	4	0.72
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	7	0.72
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	7	0.72
(4,116)	1:22:A:GLY:H	1:36:A:CYS:HB3	4	0.72
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	19	0.72
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	19	0.72
(1,484)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	11	0.72
(1,484)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	11	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	15	0.71
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	15	0.71
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	3	0.71
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	3	0.71
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	3	0.71
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	18	0.71
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	18	0.71
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	18	0.71
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	15	0.71
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	15	0.71
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	7	0.71
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	7	0.71
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	7	0.71
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	7	0.71
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	7	0.71
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	7	0.71
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	7	0.71
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	7	0.71
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	7	0.71
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	7	0.71
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	7	0.71
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	7	0.71
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	14	0.71
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	14	0.71
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	14	0.71
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	14	0.71
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	14	0.71
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	14	0.71
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	14	0.71
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	14	0.71
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	14	0.71
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	14	0.71
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	14	0.71
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	14	0.71
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	14	0.71
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	14	0.71
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	14	0.71
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	14	0.71
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	14	0.71
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	14	0.71
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	14	0.71
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	8	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,974)	1:49:A:GLY:HA3	1:50:A:LYS:HD3	1	0.71
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	15	0.71
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	14	0.71
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	8	0.71
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	2	0.7
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	2	0.7
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	2	0.7
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	2	0.7
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	2	0.7
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	2	0.7
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	2	0.7
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	2	0.7
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	2	0.7
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	2	0.7
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	3	0.7
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	3	0.7
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	3	0.7
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	3	0.7
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	3	0.7
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	3	0.7
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	3	0.7
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	3	0.7
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	3	0.7
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	14	0.7
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	14	0.7
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	14	0.7
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	14	0.7
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	14	0.7
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	14	0.7
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	14	0.7
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	14	0.7
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	18	0.7
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	18	0.7
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	18	0.7
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	18	0.7
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	18	0.7
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	18	0.7
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	18	0.7
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	18	0.7
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	18	0.7
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	18	0.7
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	15	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	16	0.7
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	16	0.7
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	17	0.7
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	17	0.7
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	17	0.7
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	17	0.7
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	16	0.7
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	16	0.7
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	16	0.7
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	16	0.7
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	17	0.7
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	17	0.7
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	17	0.7
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	17	0.7
(1,896)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	16	0.7
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	14	0.7
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	14	0.7
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	14	0.7
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	14	0.7
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	2	0.7
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	2	0.7
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	7	0.7
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	7	0.7
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	15	0.7
(1,425)	1:9:A:LYS:HB2	1:31:A:CYS:HA	16	0.7
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	3	0.69
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	3	0.69
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	3	0.69
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	3	0.69
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	15	0.69
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	15	0.69
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	15	0.69
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	15	0.69
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	15	0.69
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	15	0.69
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	15	0.69
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	15	0.69
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	13	0.69
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	13	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	2	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	2	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	2	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	17	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	17	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	17	0.69
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	17	0.69
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	4	0.69
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	4	0.69
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	4	0.69
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	4	0.69
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	4	0.69
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	2	0.69
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	2	0.69
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	2	0.69
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	2	0.69
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA3	1	0.69
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA2	1	0.69
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.69
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	10	0.69
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	10	0.69
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	14	0.69
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	14	0.69
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	14	0.69
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	4	0.69
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	17	0.69
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	6	0.69
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	6	0.69
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	6	0.69
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	2	0.69
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	18	0.69
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	15	0.69
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	15	0.69
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	15	0.69
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	15	0.69
(1,418)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	2	0.69
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	2	0.69
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	20	0.68
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	20	0.68
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	20	0.68
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	20	0.68
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	20	0.68
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	20	0.68
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	20	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	20	0.68
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	20	0.68
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	20	0.68
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	9	0.68
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	9	0.68
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	9	0.68
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	9	0.68
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	9	0.68
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	9	0.68
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	9	0.68
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	9	0.68
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.68
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG2	5	0.68
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.68
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	17	0.68
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	17	0.68
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	17	0.68
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	16	0.68
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	20	0.68
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	18	0.68
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	7	0.68
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	7	0.68
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	7	0.68
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	7	0.68
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	11	0.68
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	11	0.68
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	13	0.68
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	13	0.68
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	18	0.68
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	18	0.68
(1,668)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.68
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	16	0.67
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	16	0.67
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	16	0.67
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	19	0.67
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	19	0.67
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	1	0.67
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	1	0.67
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	1	0.67
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	1	0.67
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	1	0.67
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	1	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	1	0.67
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	1	0.67
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	1	0.67
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	1	0.67
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	1	0.67
(4,1029)	1:25:A:CYS:HB3	1:26:A:GLN:HG2	17	0.67
(4,1029)	1:25:A:CYS:HB3	1:26:A:GLN:HG3	17	0.67
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	18	0.67
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	18	0.67
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	18	0.67
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	18	0.67
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	18	0.67
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	18	0.67
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	18	0.67
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	18	0.67
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	9	0.67
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	17	0.67
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	17	0.67
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	17	0.67
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	17	0.67
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	17	0.67
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	17	0.67
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	17	0.67
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	17	0.67
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	17	0.67
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	17	0.67
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	5	0.67
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	5	0.67
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	5	0.67
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	19	0.67
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	19	0.67
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	19	0.67
(4,341)	1:50:A:LYS:HB3	1:52:A:CYS:H	11	0.67
(4,341)	1:50:A:LYS:HB2	1:52:A:CYS:H	11	0.67
(1,944)	1:46:A:CYS:HA	1:47:A:LYS:HG2	2	0.67
(1,944)	1:46:A:CYS:HA	1:47:A:LYS:HG3	2	0.67
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	19	0.67
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	4	0.67
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	7	0.67
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	18	0.67
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	18	0.67
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	18	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	18	0.67
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	8	0.67
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	8	0.67
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	7	0.66
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	7	0.66
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	5	0.66
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	5	0.66
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	10	0.66
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	10	0.66
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	16	0.66
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	16	0.66
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	16	0.66
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	16	0.66
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	16	0.66
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	16	0.66
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	16	0.66
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	16	0.66
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	16	0.66
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	17	0.66
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	17	0.66
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	17	0.66
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	17	0.66
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	7	0.66
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	7	0.66
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	7	0.66
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	7	0.66
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	7	0.66
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	7	0.66
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	7	0.66
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	7	0.66
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	7	0.66
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	7	0.66
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	7	0.66
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	7	0.66
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	7	0.66
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	7	0.66
(4,534)	1:37:A:LYS:HA	1:37:A:LYS:HE2	19	0.66
(4,534)	1:37:A:LYS:HA	1:37:A:LYS:HE3	19	0.66
(4,534)	1:37:A:LYS:HA	1:37:A:LYS:HE2	19	0.66
(4,534)	1:37:A:LYS:HA	1:37:A:LYS:HE3	19	0.66
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	12	0.66
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	15	0.66
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	15	0.66
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	16	0.66
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	16	0.66
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	16	0.66
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	7	0.66
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	4	0.66
(1,884)	1:32:A:THR:HG21	1:37:A:LYS:HE3	13	0.66
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	11	0.66
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	11	0.66
(1,163)	1:31:A:CYS:H	1:37:A:LYS:HD2	1	0.66
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	10	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	10	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	10	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	10	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	10	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	10	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	10	0.65
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	10	0.65
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	10	0.65
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	9	0.65
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	9	0.65
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	9	0.65
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	9	0.65
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	9	0.65
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	9	0.65
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	9	0.65
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	9	0.65
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	10	0.65
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	10	0.65
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	0.65
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	0.65
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	0.65
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	0.65
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	0.65
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	0.65
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	15	0.65
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	15	0.65
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	7	0.65
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	7	0.65
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	7	0.65
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	9	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	4	0.65
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	4	0.65
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	4	0.65
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	4	0.65
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	8	0.65
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	14	0.65
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	14	0.65
(1,968)	1:9:A:LYS:HB2	1:29:A:GLU:HG2	19	0.65
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	9	0.65
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	9	0.65
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	9	0.65
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	9	0.65
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	3	0.64
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	3	0.64
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	3	0.64
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	3	0.64
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	3	0.64
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	3	0.64
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	3	0.64
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	3	0.64
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	3	0.64
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	3	0.64
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	16	0.64
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	12	0.64
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	12	0.64
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	12	0.64
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	14	0.64
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	14	0.64
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	14	0.64
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	14	0.64
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	14	0.64
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	14	0.64
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	14	0.64
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	14	0.64
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	14	0.64
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	16	0.64
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	18	0.64
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	18	0.64
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	18	0.64
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	18	0.64
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	18	0.64
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	18	0.64
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	18	0.64
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	18	0.64
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	18	0.64
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	6	0.64
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	8	0.64
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	8	0.64
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	11	0.64
(1,896)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	12	0.64
(1,871)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	19	0.64
(1,871)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	19	0.64
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	10	0.64
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	10	0.64
(1,358)	1:32:A:THR:H	1:37:A:LYS:HD3	14	0.64
(1,229)	1:9:A:LYS:HE2	1:29:A:GLU:H	9	0.64
(1,229)	1:9:A:LYS:HE3	1:29:A:GLU:H	9	0.64
(1,229)	1:9:A:LYS:HE2	1:29:A:GLU:H	19	0.64
(1,229)	1:9:A:LYS:HE3	1:29:A:GLU:H	19	0.64
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	14	0.63
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	14	0.63
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	14	0.63
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	14	0.63
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	9	0.63
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	15	0.63
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	12	0.63
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	12	0.63
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	20	0.63
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	20	0.63
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	7	0.63
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	7	0.63
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	4	0.63
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	4	0.63
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	4	0.63
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	4	0.63
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	4	0.63
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	4	0.63
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	4	0.63
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	4	0.63
(4,881)	1:38:A:THR:H	1:38:A:THR:HG21	13	0.63
(4,881)	1:38:A:THR:H	1:38:A:THR:HG22	13	0.63
(4,881)	1:38:A:THR:H	1:38:A:THR:HG23	13	0.63
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	8	0.63
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	8	0.63
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	8	0.63
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	17	0.63
(4,619)	1:10:A:CYS:HB2	1:15:A:ARG:HG3	20	0.63
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	19	0.63
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	20	0.63
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	20	0.63
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	20	0.63
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	20	0.63
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	18	0.63
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	12	0.63
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	20	0.63
(1,673)	1:6:A:LYS:HA	1:6:A:LYS:HE2	8	0.63
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	10	0.63
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	5	0.62
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	17	0.62
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG2	17	0.62
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	17	0.62
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	6	0.62
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	6	0.62
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	6	0.62
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	6	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	7	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	7	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	7	0.62
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	7	0.62
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	9	0.62
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	9	0.62
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	9	0.62
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	15	0.62
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	15	0.62
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	20	0.62
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	20	0.62
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	20	0.62
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	20	0.62
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	5	0.62
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	5	0.62
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	5	0.62
(1,930)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	0.62
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	8	0.62
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	0.62
(1,668)	1:25:A:CYS:HA	1:26:A:GLN:HG3	17	0.62
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	7	0.62
(1,215)	1:33:A:CYS:HB2	1:37:A:LYS:H	11	0.62
(1,215)	1:33:A:CYS:HB3	1:37:A:LYS:H	11	0.62
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	13	0.61
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	13	0.61
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	17	0.61
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	17	0.61
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	10	0.61
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	10	0.61
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	10	0.61
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	10	0.61
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	10	0.61
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	10	0.61
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	10	0.61
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	10	0.61
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	10	0.61
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	19	0.61
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	19	0.61
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	19	0.61
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	19	0.61
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	19	0.61
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	19	0.61
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	11	0.61
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	11	0.61
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	11	0.61
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	2	0.61
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB2	12	0.61
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB3	12	0.61
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB2	5	0.61
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	6	0.61
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	2	0.61
(1,143)	1:28:A:GLY:H	1:61:A:GLY:HA3	11	0.61
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	1	0.6
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	1	0.6
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	1	0.6
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	1	0.6
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	15	0.6
(4,770)	1:33:A:CYS:HB3	1:36:A:CYS:H	11	0.6
(4,770)	1:33:A:CYS:HB2	1:36:A:CYS:H	11	0.6
(4,770)	1:33:A:CYS:HB2	1:36:A:CYS:H	11	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,770)	1:33:A:CYS:HB3	1:36:A:CYS:H	11	0.6
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	7	0.6
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	7	0.6
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	7	0.6
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	7	0.6
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	15	0.6
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	15	0.6
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	15	0.6
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	15	0.6
(4,595)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	4	0.6
(4,595)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	4	0.6
(4,595)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	4	0.6
(4,595)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	4	0.6
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	9	0.6
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	10	0.6
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	4	0.6
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	4	0.6
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	4	0.6
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	4	0.6
(1,988)	1:6:A:LYS:HE2	1:15:A:ARG:HA	1	0.6
(1,988)	1:6:A:LYS:HE3	1:15:A:ARG:HA	1	0.6
(1,923)	1:9:A:LYS:HB2	1:29:A:GLU:H	15	0.6
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	7	0.6
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	9	0.6
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	5	0.59
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	5	0.59
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	5	0.59
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	5	0.59
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	8	0.59
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	8	0.59
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	8	0.59
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	8	0.59
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	1	0.59
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	17	0.59
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	17	0.59
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	18	0.59
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	18	0.59
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	19	0.59
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	1	0.59
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	1	0.59
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	1	0.59
(4,723)	1:60:A:CYS:HB3	1:67:A:LYS:HE3	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	9	0.59
(4,341)	1:50:A:LYS:HB3	1:52:A:CYS:H	7	0.59
(4,341)	1:50:A:LYS:HB2	1:52:A:CYS:H	7	0.59
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	10	0.59
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	10	0.59
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	18	0.59
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	18	0.59
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	18	0.59
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	11	0.59
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	11	0.59
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	11	0.59
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	11	0.59
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	3	0.59
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	3	0.59
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	3	0.59
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	3	0.59
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	17	0.59
(1,287)	1:58:A:CYS:H	1:59:A:LYS:HG2	10	0.59
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	10	0.58
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	15	0.58
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	15	0.58
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	15	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	2	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	2	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	2	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	6	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	6	0.58
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	6	0.58
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	11	0.58
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	11	0.58
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	11	0.58
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	20	0.58
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	20	0.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	1	0.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	1	0.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	1	0.58
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	1	0.58
(4,899)	1:42:A:THR:HB	1:53:A:THR:HB	6	0.58
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	12	0.58
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	12	0.58
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	12	0.58
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	12	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	12	0.58
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	12	0.58
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	12	0.58
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	12	0.58
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	12	0.58
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	12	0.58
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	5	0.58
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	5	0.58
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	5	0.58
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	5	0.58
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	2	0.57
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	2	0.57
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	2	0.57
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	2	0.57
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	16	0.57
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	16	0.57
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	16	0.57
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	16	0.57
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	19	0.57
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	19	0.57
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	19	0.57
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	18	0.57
(4,866)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	20	0.57
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	19	0.57
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	19	0.57
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	19	0.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	9	0.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	9	0.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	9	0.57
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	9	0.57
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	9	0.57
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	18	0.57
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	18	0.57
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	18	0.57
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	18	0.57
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	10	0.57
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	12	0.57
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	12	0.57
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.57
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	4	0.57
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	4	0.57
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	14	0.57
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	14	0.57
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	14	0.57
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	14	0.57
(1,988)	1:6:A:LYS:HE2	1:15:A:ARG:HA	2	0.57
(1,988)	1:6:A:LYS:HE3	1:15:A:ARG:HA	2	0.57
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	16	0.57
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	16	0.57
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	3	0.57
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	19	0.57
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	19	0.57
(1,287)	1:58:A:CYS:H	1:59:A:LYS:HG2	4	0.57
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	3	0.56
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	3	0.56
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	3	0.56
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	6	0.56
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	10	0.56
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	10	0.56
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	7	0.56
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	7	0.56
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	7	0.56
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	6	0.56
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	6	0.56
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	6	0.56
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	3	0.56
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	3	0.56
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	3	0.56
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	3	0.56
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	3	0.56
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	3	0.56
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	3	0.56
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	3	0.56
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	17	0.56
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	17	0.56
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	20	0.56
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	20	0.56
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	17	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	15	0.56
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	15	0.56
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	15	0.56
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	15	0.56
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	15	0.56
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	15	0.56
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	15	0.56
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	15	0.56
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	20	0.56
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	19	0.56
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	5	0.56
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	5	0.56
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	19	0.56
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	19	0.56
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	19	0.56
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	8	0.56
(4,547)	1:33:A:CYS:HB2	1:36:A:CYS:HB3	8	0.56
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	8	0.56
(4,547)	1:33:A:CYS:HB3	1:36:A:CYS:HB3	8	0.56
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	12	0.56
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	12	0.56
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	1	0.56
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	1	0.56
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	4	0.56
(4,258)	1:37:A:LYS:HD2	1:38:A:THR:H	4	0.56
(4,258)	1:37:A:LYS:HD3	1:38:A:THR:H	4	0.56
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	1	0.56
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	1	0.56
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	1	0.56
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	1	0.56
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	10	0.56
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	6	0.56
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	6	0.56
(1,821)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	20	0.56
(1,358)	1:37:A:LYS:HD3	1:38:A:THR:H	16	0.56
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	13	0.55
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	13	0.55
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	13	0.55
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	13	0.55
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	2	0.55
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	9	0.55
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	9	0.55
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	9	0.55
(4,866)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	12	0.55
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	19	0.55
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	19	0.55
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	11	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	2	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	2	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	2	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	2	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	7	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	7	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	7	0.55
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	7	0.55
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	9	0.55
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	9	0.55
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	15	0.55
(1,870)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	19	0.55
(1,870)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	19	0.55
(1,425)	1:9:A:LYS:HB2	1:31:A:CYS:HA	11	0.55
(1,287)	1:37:A:LYS:HG2	1:58:A:CYS:H	14	0.55
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	19	0.54
(4,1176)	1:9:A:LYS:HD3	1:29:A:GLU:HG2	19	0.54
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	19	0.54
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	19	0.54
(4,1176)	1:9:A:LYS:HD2	1:29:A:GLU:HG3	19	0.54
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	13	0.54
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	13	0.54
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	13	0.54
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	14	0.54
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	14	0.54
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	14	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	1	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	1	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	1	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	2	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	2	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	2	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	5	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	5	0.54
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	5	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	1	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	1	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	1	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	1	0.54
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	1	0.54
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	1	0.54
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	1	0.54
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	8	0.54
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	8	0.54
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	8	0.54
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	18	0.54
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	20	0.54
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	11	0.54
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	11	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	1	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	1	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	2	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	2	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	5	0.54
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	5	0.54
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD2	12	0.54
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	13	0.54
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	13	0.54
(1,358)	1:37:A:LYS:HD3	1:38:A:THR:H	5	0.54
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	7	0.54
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	11	0.54
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	8	0.53
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	8	0.53
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	8	0.53
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	8	0.53
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	7	0.53
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	16	0.53
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	8	0.53
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	8	0.53
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	8	0.53
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	16	0.53
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	16	0.53
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	16	0.53
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	10	0.53
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	10	0.53
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	10	0.53
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	10	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	10	0.53
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	10	0.53
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	10	0.53
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	10	0.53
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	9	0.53
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	9	0.53
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	14	0.53
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	14	0.53
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	6	0.53
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	6	0.53
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	8	0.53
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	8	0.53
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	8	0.53
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	8	0.53
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	1	0.53
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	16	0.53
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	16	0.53
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	16	0.53
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	16	0.53
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	14	0.53
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	14	0.53
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	14	0.53
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	14	0.53
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	14	0.53
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	14	0.53
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	14	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	20	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	20	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	20	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	20	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	20	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	20	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	20	0.53
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	20	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	20	0.53
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	20	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	10	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	10	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	10	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	10	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	13	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	13	0.53
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	13	0.53
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	2	0.53
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	2	0.53
(4,341)	1:50:A:LYS:HB3	1:52:A:CYS:H	12	0.53
(4,341)	1:50:A:LYS:HB2	1:52:A:CYS:H	12	0.53
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	8	0.53
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	8	0.53
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	3	0.53
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	8	0.53
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	8	0.53
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	16	0.53
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	16	0.53
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	10	0.53
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	10	0.53
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	10	0.53
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	10	0.53
(1,687)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	1	0.53
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	19	0.52
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	19	0.52
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	19	0.52
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	19	0.52
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	4	0.52
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	4	0.52
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	11	0.52
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	11	0.52
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	11	0.52
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	12	0.52
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	12	0.52
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	9	0.52
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	9	0.52
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	9	0.52
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	9	0.52
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	9	0.52
(4,987)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	9	0.52
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	9	0.52
(4,987)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	9	0.52
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	0.52
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	0.52
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	0.52
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	1	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	1	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	6	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	6	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	6	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	9	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	9	0.52
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	9	0.52
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	5	0.52
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	17	0.52
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	20	0.52
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	20	0.52
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	3	0.52
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	3	0.52
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	3	0.52
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	3	0.52
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	3	0.52
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	3	0.52
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	3	0.52
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	3	0.52
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	12	0.52
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	12	0.52
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	4	0.52
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	11	0.52
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	11	0.52
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	17	0.52
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	12	0.52
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	16	0.51
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	16	0.51
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	8	0.51
(4,595)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	2	0.51
(4,595)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	0.51
(4,595)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	0.51
(4,595)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	2	0.51
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	2	0.51
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	2	0.51
(4,583)	1:67:A:LYS:HG2	1:67:A:LYS:HE3	2	0.51
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	17	0.51
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	9	0.51
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	9	0.51
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	9	0.51
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	19	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	19	0.51
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	19	0.51
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	19	0.51
(4,341)	1:50:A:LYS:HB3	1:52:A:CYS:H	1	0.51
(4,341)	1:50:A:LYS:HB2	1:52:A:CYS:H	1	0.51
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	11	0.51
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	6	0.51
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	16	0.51
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	16	0.51
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	8	0.51
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	14	0.51
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB2	12	0.51
(1,358)	1:37:A:LYS:HD2	1:38:A:THR:H	9	0.51
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	1	0.51
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	14	0.5
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	14	0.5
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	14	0.5
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	14	0.5
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	14	0.5
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	14	0.5
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	14	0.5
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	14	0.5
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	14	0.5
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	14	0.5
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	11	0.5
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	11	0.5
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	15	0.5
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	15	0.5
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	11	0.5
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	11	0.5
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	11	0.5
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	4	0.5
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	4	0.5
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	7	0.5
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	19	0.5
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	15	0.5
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	19	0.5
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	19	0.5
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	19	0.5
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	19	0.5
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB2	17	0.5
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB3	17	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:42:A:THR:HG23	1:54:A:GLY:HA2	20	0.5
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG2	3	0.5
(1,812)	1:50:A:LYS:H	1:51:A:GLU:HG3	3	0.5
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	16	0.5
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	16	0.5
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	3	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	3	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	3	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	3	0.49
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	7	0.49
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	7	0.49
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	2	0.49
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	2	0.49
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	2	0.49
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	12	0.49
(4,960)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	12	0.49
(4,960)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	12	0.49
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	14	0.49
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	14	0.49
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	14	0.49
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	14	0.49
(4,881)	1:38:A:THR:H	1:38:A:THR:HG21	8	0.49
(4,881)	1:38:A:THR:H	1:38:A:THR:HG22	8	0.49
(4,881)	1:38:A:THR:H	1:38:A:THR:HG23	8	0.49
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	7	0.49
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	7	0.49
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	7	0.49
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	20	0.49
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	20	0.49
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	17	0.49
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	17	0.49
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	14	0.49
(1,629)	1:62:A:SER:HA	1:67:A:LYS:HE2	2	0.49
(1,629)	1:62:A:SER:HA	1:67:A:LYS:HE3	2	0.49
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	1	0.49
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	20	0.49
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	11	0.48
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	11	0.48
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	11	0.48
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	11	0.48
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.48
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	8	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	4	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	4	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	4	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	17	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	17	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	17	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	20	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	20	0.48
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	20	0.48
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	11	0.48
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	11	0.48
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	11	0.48
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	11	0.48
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	2	0.48
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE2	2	0.48
(4,348)	1:64:A:CYS:H	1:67:A:LYS:HE3	2	0.48
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	16	0.48
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	16	0.48
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	16	0.48
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	16	0.48
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	4	0.48
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	4	0.48
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	5	0.47
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	5	0.47
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	5	0.47
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	14	0.47
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	14	0.47
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	14	0.47
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	14	0.47
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	14	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	8	0.47
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	8	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	8	0.47
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	8	0.47
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	8	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	8	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	8	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	8	0.47
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	8	0.47
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	19	0.47
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	10	0.47
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	3	0.47
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	3	0.47
(4,434)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	3	0.47
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	15	0.47
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	15	0.47
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	13	0.47
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	8	0.47
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	8	0.47
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	8	0.47
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	8	0.47
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	20	0.47
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	20	0.47
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	20	0.47
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	10	0.47
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	10	0.47
(1,886)	1:33:A:CYS:H	1:34:A:ALA:HB1	14	0.47
(1,443)	1:52:A:CYS:H	1:58:A:CYS:HB2	19	0.47
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	1	0.47
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	1	0.47
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	5	0.46
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	5	0.46
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	5	0.46
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	5	0.46
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	5	0.46
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	5	0.46
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	5	0.46
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	5	0.46
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	5	0.46
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	5	0.46
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	5	0.46
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	1	0.46
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	1	0.46
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	14	0.46
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	14	0.46
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	14	0.46
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	14	0.46
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	14	0.46
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	14	0.46
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	14	0.46
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	14	0.46
(4,866)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.46
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	2	0.46
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	15	0.46
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	15	0.46
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	5	0.46
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	8	0.46
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	20	0.46
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	7	0.46
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	7	0.46
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	20	0.46
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	5	0.46
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	5	0.46
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	5	0.46
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	5	0.46
(1,821)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	8	0.46
(1,365)	1:42:A:THR:HA	1:54:A:GLY:HA2	1	0.46
(1,217)	1:33:A:CYS:HB3	1:37:A:LYS:H	11	0.46
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	3	0.45
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	3	0.45
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	12	0.45
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	12	0.45
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	12	0.45
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	14	0.45
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	14	0.45
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	14	0.45
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	14	0.45
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	14	0.45
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	14	0.45
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	14	0.45
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	14	0.45
(4,980)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	6	0.45
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	10	0.45
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	10	0.45
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	10	0.45
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	6	0.45
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG2	6	0.45
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	6	0.45
(4,790)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	14	0.45
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	19	0.45
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE2	19	0.45
(4,721)	1:67:A:LYS:HG3	1:67:A:LYS:HE3	19	0.45
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	2	0.45
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	2	0.45
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	2	0.45
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	16	0.45
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	16	0.45
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	13	0.45
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	13	0.45
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	13	0.45
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	2	0.45
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	2	0.45
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	2	0.45
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	8	0.45
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	8	0.45
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG2	8	0.45
(4,360)	1:51:A:GLU:H	1:51:A:GLU:HG3	8	0.45
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	17	0.45
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	17	0.45
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	17	0.45
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	17	0.45
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	12	0.45
(4,58)	1:29:A:GLU:HB3	1:61:A:GLY:H	12	0.45
(4,58)	1:29:A:GLU:HB2	1:61:A:GLY:H	12	0.45
(1,923)	1:9:A:LYS:HD2	1:29:A:GLU:H	8	0.45
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	3	0.45
(1,843)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	6	0.45
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD3	6	0.45
(1,687)	1:47:A:LYS:HG2	1:66:A:CYS:HB3	14	0.45
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	2	0.44
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	2	0.44
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	2	0.44
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	2	0.44
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	2	0.44
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	2	0.44
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	2	0.44
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	2	0.44
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	2	0.44
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	2	0.44
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	4	0.44
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	4	0.44
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	4	0.44
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	4	0.44
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	4	0.44
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	4	0.44
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	4	0.44
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	12	0.44
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	12	0.44
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	10	0.44
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	10	0.44
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	10	0.44
(4,954)	1:16:A:SER:HB2	1:20:A:GLN:HE21	6	0.44
(4,954)	1:16:A:SER:HB3	1:20:A:GLN:HE21	6	0.44
(4,954)	1:16:A:SER:HB2	1:20:A:GLN:HE22	6	0.44
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	8	0.44
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	8	0.44
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	9	0.44
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	9	0.44
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	9	0.44
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	18	0.44
(4,584)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	16	0.44
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	8	0.44
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	4	0.44
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	4	0.44
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	4	0.44
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	4	0.44
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	6	0.44
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	6	0.44
(1,443)	1:6:A:LYS:H	1:10:A:CYS:HB2	4	0.44
(1,229)	1:9:A:LYS:HE2	1:29:A:GLU:H	8	0.44
(1,229)	1:9:A:LYS:HE3	1:29:A:GLU:H	8	0.44
(1,143)	1:28:A:GLY:H	1:61:A:GLY:HA3	18	0.44
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	9	0.43
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	9	0.43
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	9	0.43
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	11	0.43
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	11	0.43
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	9	0.43
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	9	0.43
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	9	0.43
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	9	0.43
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	9	0.43
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	9	0.43
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	9	0.43
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	9	0.43
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	9	0.43
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	4	0.43
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	4	0.43
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	4	0.43
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	4	0.43
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	13	0.43
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB3	1	0.43
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB2	1	0.43
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB3	1	0.43
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB2	1	0.43
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	5	0.43
(1,897)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	16	0.43
(1,287)	1:37:A:LYS:HG2	1:58:A:CYS:H	18	0.43
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	10	0.42
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	10	0.42
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	10	0.42
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	10	0.42
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	4	0.42
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	4	0.42
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	4	0.42
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	4	0.42
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	3	0.42
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	3	0.42
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	3	0.42
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	14	0.42
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	14	0.42
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	14	0.42
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	11	0.42
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	14	0.42
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	14	0.42
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	6	0.42
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	6	0.42
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	6	0.42
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	2	0.42
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	2	0.42
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	2	0.42
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	17	0.42
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	17	0.42
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	17	0.42
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	15	0.42
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	15	0.42
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	15	0.42
(4,99)	1:31:A:CYS:HB2	1:33:A:CYS:H	11	0.42
(4,99)	1:31:A:CYS:HB3	1:33:A:CYS:H	11	0.42
(4,99)	1:31:A:CYS:HB2	1:33:A:CYS:H	11	0.42
(4,99)	1:31:A:CYS:HB3	1:33:A:CYS:H	11	0.42
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	3	0.42
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	3	0.42
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	8	0.42
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	8	0.42
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB2	11	0.42
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	18	0.42
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	4	0.42
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	4	0.42
(1,865)	1:6:A:LYS:HG3	1:15:A:ARG:HA	9	0.42
(1,358)	1:37:A:LYS:HD3	1:38:A:THR:H	12	0.42
(1,236)	1:37:A:LYS:HE2	1:38:A:THR:H	9	0.42
(1,236)	1:37:A:LYS:HE3	1:38:A:THR:H	9	0.42
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	3	0.41
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	3	0.41
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	2	0.41
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	2	0.41
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	2	0.41
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	2	0.41
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	2	0.41
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	2	0.41
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	2	0.41
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	2	0.41
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	2	0.41
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	2	0.41
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	13	0.41
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	13	0.41
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	13	0.41
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	13	0.41
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	17	0.41
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	17	0.41
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	17	0.41
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB3	8	0.41
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB2	8	0.41
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB3	8	0.41
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB2	8	0.41
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA3	6	0.41
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA2	6	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	12	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	12	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	12	0.41
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	12	0.41
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	20	0.41
(4,79)	1:45:A:GLY:HA3	1:46:A:CYS:H	3	0.41
(4,79)	1:45:A:GLY:HA2	1:46:A:CYS:H	3	0.41
(4,69)	1:24:A:LYS:H	1:24:A:LYS:HB2	12	0.41
(4,69)	1:24:A:LYS:H	1:24:A:LYS:HB3	12	0.41
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB2	16	0.41
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	18	0.41
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	9	0.41
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	9	0.41
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	17	0.41
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	17	0.41
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	17	0.41
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	17	0.41
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	17	0.41
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	16	0.41
(1,204)	1:9:A:LYS:HB2	1:10:A:CYS:H	12	0.41
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	20	0.41
(1,52)	1:29:A:GLU:HB2	1:61:A:GLY:H	12	0.41
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	2	0.4
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	2	0.4
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	19	0.4
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	19	0.4
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	19	0.4
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	19	0.4
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	17	0.4
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	3	0.4
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	3	0.4
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	3	0.4
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	1	0.4
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	3	0.4
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	4	0.4
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	8	0.4
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	8	0.4
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	8	0.4
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	8	0.4
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	15	0.4
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	15	0.4
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	15	0.4
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	15	0.4
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	3	0.4
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	3	0.4
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	3	0.4
(4,106)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	3	0.4
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	13	0.4
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	13	0.4
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	19	0.4
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	19	0.4
(1,896)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	19	0.4
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG2	6	0.4
(1,418)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	8	0.4
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	19	0.39
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	19	0.39
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	19	0.39
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	15	0.39
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	15	0.39
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	15	0.39
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	1	0.39
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	1	0.39
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	16	0.39
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	16	0.39
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	15	0.39
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	10	0.39
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	6	0.39
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	15	0.39
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	20	0.39
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	10	0.39
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	10	0.39
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	10	0.39
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	10	0.39
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	4	0.39
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	4	0.39
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	4	0.39
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	4	0.39
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	4	0.39
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	4	0.39
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	4	0.39
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,79)	1:45:A:GLY:HA3	1:46:A:CYS:H	6	0.39
(4,79)	1:45:A:GLY:HA2	1:46:A:CYS:H	6	0.39
(1,837)	1:42:A:THR:HG21	1:54:A:GLY:HA2	8	0.39
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	4	0.39
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE3	16	0.39
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	6	0.39
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	5	0.38
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	5	0.38
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	20	0.38
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	13	0.38
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	13	0.38
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	13	0.38
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	13	0.38
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	13	0.38
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	13	0.38
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	13	0.38
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	13	0.38
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	13	0.38
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	13	0.38
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	8	0.38
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	8	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	12	0.38
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	12	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	12	0.38
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	12	0.38
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	12	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	12	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	12	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	12	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	12	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	20	0.38
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	20	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	20	0.38
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	20	0.38
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	20	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	20	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	20	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	20	0.38
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	20	0.38
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	7	0.38
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	15	0.38
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	9	0.38
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	9	0.38
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	9	0.38
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	9	0.38
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	9	0.38
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	9	0.38
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	9	0.38
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	9	0.38
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	9	0.38
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	9	0.38
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	9	0.38
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	9	0.38
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	19	0.38
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	19	0.38
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	19	0.38
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	19	0.38
(4,79)	1:45:A:GLY:HA3	1:46:A:CYS:H	2	0.38
(4,79)	1:45:A:GLY:HA2	1:46:A:CYS:H	2	0.38
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	5	0.38
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD2	16	0.38
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	19	0.38
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	2	0.38
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	8	0.38
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD2	3	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD3	3	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD2	3	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	0.37
(4,1180)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.37
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	11	0.37
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	11	0.37
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	11	0.37
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	11	0.37
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	14	0.37
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	14	0.37
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	14	0.37
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	14	0.37
(4,806)	1:62:A:SER:HA	1:64:A:CYS:HB2	10	0.37
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	12	0.37
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	16	0.37
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	16	0.37
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	16	0.37
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	16	0.37
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	16	0.37
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	1	0.37
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	12	0.37
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	12	0.37
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	19	0.37
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	19	0.37
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	19	0.37
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	5	0.37
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	5	0.37
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	5	0.37
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	5	0.37
(4,79)	1:45:A:GLY:HA3	1:46:A:CYS:H	8	0.37
(4,79)	1:45:A:GLY:HA2	1:46:A:CYS:H	8	0.37
(4,79)	1:45:A:GLY:HA3	1:46:A:CYS:H	11	0.37
(4,79)	1:45:A:GLY:HA2	1:46:A:CYS:H	11	0.37
(1,969)	1:12:A:SER:HA	1:15:A:ARG:HD2	3	0.37
(1,969)	1:12:A:SER:HA	1:15:A:ARG:HD3	3	0.37
(1,969)	1:12:A:SER:HA	1:15:A:ARG:HD2	15	0.37
(1,969)	1:12:A:SER:HA	1:15:A:ARG:HD3	15	0.37
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	2	0.37
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	2	0.37
(1,897)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	11	0.37
(1,897)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	12	0.37
(1,883)	1:9:A:LYS:HA	1:9:A:LYS:HE2	5	0.37
(1,730)	1:6:A:LYS:HD2	1:33:A:CYS:HA	14	0.37
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG21	16	0.37
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG22	16	0.37
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG23	16	0.37
(1,425)	1:9:A:LYS:HB2	1:31:A:CYS:HA	12	0.37
(1,418)	1:9:A:LYS:HG2	1:29:A:GLU:HG2	20	0.37
(1,358)	1:32:A:THR:H	1:37:A:LYS:HD2	3	0.37
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	15	0.36
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	15	0.36
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	15	0.36
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	15	0.36
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	5	0.36
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	5	0.36
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	5	0.36
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	5	0.36
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	12	0.36
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	12	0.36
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	12	0.36
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	12	0.36
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	16	0.36
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	16	0.36
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	16	0.36
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	16	0.36
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	16	0.36
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	16	0.36
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	16	0.36
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	16	0.36
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	4	0.36
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	4	0.36
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	4	0.36
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	4	0.36
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	10	0.36
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	10	0.36
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	10	0.36
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	4	0.36
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	4	0.36
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	4	0.36
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	4	0.36
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	3	0.36
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	3	0.36
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	3	0.36
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	3	0.36
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	7	0.36
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	7	0.36
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	7	0.36
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	15	0.36
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	15	0.36
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	15	0.36
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	15	0.36
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	13	0.36
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	13	0.36
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	10	0.36
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	10	0.36
(1,988)	1:6:A:LYS:HE2	1:15:A:ARG:HA	15	0.36
(1,988)	1:6:A:LYS:HE3	1:15:A:ARG:HA	15	0.36
(1,975)	1:6:A:LYS:HD3	1:7:A:GLY:HA3	1	0.36
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	12	0.36
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	10	0.36
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	10	0.36
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	10	0.36
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD3	20	0.36
(1,407)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	17	0.36
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	1	0.35
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	1	0.35
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	1	0.35
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	11	0.35
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	11	0.35
(4,1114)	1:22:A:GLY:HA3	1:25:A:CYS:HB2	11	0.35
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	11	0.35
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB3	11	0.35
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	19	0.35
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	19	0.35
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	19	0.35
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	19	0.35
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	16	0.35
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	16	0.35
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	16	0.35
(4,1024)	1:23:A:SER:HB2	1:24:A:LYS:HB2	13	0.35
(4,1024)	1:23:A:SER:HB3	1:24:A:LYS:HB2	13	0.35
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	13	0.35
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	13	0.35
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	13	0.35
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	16	0.35
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	16	0.35
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	6	0.35
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	6	0.35
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	6	0.35
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	6	0.35
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	4	0.35
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG2	4	0.35
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	4	0.35
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	18	0.35
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	6	0.35
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	6	0.35
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	6	0.35
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	11	0.35
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	11	0.35
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	3	0.35
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	3	0.35
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	3	0.35
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	3	0.35
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	3	0.35
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	3	0.35
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	19	0.35
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	19	0.35
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	5	0.35
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	15	0.34
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	15	0.34
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	18	0.34
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	18	0.34
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	7	0.34
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	7	0.34
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	7	0.34
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	7	0.34
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	20	0.34
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	20	0.34
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	20	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	3	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	3	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	3	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	3	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	5	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	5	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	5	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	5	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	20	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	20	0.34
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	0.34
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	16	0.34
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	11	0.34
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	11	0.34
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	11	0.34
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	11	0.34
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	11	0.34
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	11	0.34
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	11	0.34
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	11	0.34
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	0.34
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	2	0.34
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	2	0.34
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	2	0.34
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	15	0.34
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	12	0.34
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	12	0.34
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	12	0.34
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	12	0.34
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	14	0.34
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	15	0.34
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	12	0.34
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	12	0.34
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	2	0.34
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	16	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	6	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	6	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	6	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	6	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	20	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	20	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	20	0.34
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	20	0.34
(4,118)	1:21:A:CYS:HB2	1:22:A:GLY:H	4	0.34
(1,965)	1:37:A:LYS:HG3	1:55:A:PRO:HA	1	0.34
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	15	0.34
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	18	0.34
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	16	0.34
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	16	0.34
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	3	0.34
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	3	0.34
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	3	0.34
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	5	0.34
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	5	0.34
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	20	0.34
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	20	0.34
(1,884)	1:32:A:THR:HG22	1:37:A:LYS:HE2	9	0.34
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	14	0.34
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	14	0.34
(1,746)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	0.34
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	6	0.34
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,520)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	2	0.34
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	4	0.34
(1,163)	1:31:A:CYS:H	1:37:A:LYS:HD2	12	0.34
(1,107)	1:21:A:CYS:HB2	1:22:A:GLY:H	4	0.34
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	8	0.33
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	8	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	15	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	15	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	15	0.33
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	15	0.33
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	15	0.33
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	15	0.33
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	15	0.33
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	15	0.33
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	15	0.33
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	15	0.33
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	15	0.33
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	15	0.33
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	15	0.33
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	5	0.33
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	5	0.33
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	5	0.33
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	5	0.33
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	10	0.33
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	10	0.33
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	10	0.33
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	11	0.33
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	11	0.33
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	11	0.33
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	11	0.33
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	11	0.33
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	11	0.33
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	11	0.33
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	11	0.33
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	11	0.33
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	11	0.33
(4,584)	1:60:A:CYS:HB3	1:67:A:LYS:HE2	2	0.33
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	9	0.33
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	9	0.33
(4,503)	1:52:A:CYS:H	1:58:A:CYS:HB2	13	0.33
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	14	0.33
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	18	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	18	0.33
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	1	0.33
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	1	0.33
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	1	0.33
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	1	0.33
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	8	0.33
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	15	0.33
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	15	0.33
(1,883)	1:9:A:LYS:HA	1:9:A:LYS:HE3	12	0.33
(1,730)	1:6:A:LYS:HD2	1:33:A:CYS:HA	5	0.33
(1,210)	1:33:A:CYS:HB3	1:36:A:CYS:H	11	0.33
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	12	0.32
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	12	0.32
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	12	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	2	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	2	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	2	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	2	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	10	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	10	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	10	0.32
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	10	0.32
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE2	14	0.32
(4,1046)	1:32:A:THR:HG21	1:37:A:LYS:HE3	14	0.32
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE2	14	0.32
(4,1046)	1:32:A:THR:HG22	1:37:A:LYS:HE3	14	0.32
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE2	14	0.32
(4,1046)	1:32:A:THR:HG23	1:37:A:LYS:HE3	14	0.32
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	12	0.32
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	12	0.32
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	12	0.32
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	12	0.32
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	12	0.32
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	12	0.32
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	12	0.32
(4,1036)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	12	0.32
(4,1036)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	12	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	19	0.32
(4,1021)	1:18:A:PRO:HG3	1:20:A:GLN:HE21	19	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	19	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	19	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	19	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	19	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	19	0.32
(4,1021)	1:18:A:PRO:HG3	1:20:A:GLN:HE22	19	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE22	19	0.32
(4,1021)	1:18:A:PRO:HG2	1:20:A:GLN:HE21	19	0.32
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	7	0.32
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	7	0.32
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	7	0.32
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	7	0.32
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	7	0.32
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	7	0.32
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	7	0.32
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	7	0.32
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	4	0.32
(4,806)	1:62:A:SER:HA	1:64:A:CYS:HB2	7	0.32
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	5	0.32
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	5	0.32
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	5	0.32
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	2	0.32
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	2	0.32
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	2	0.32
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	2	0.32
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	2	0.32
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	2	0.32
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB2	15	0.32
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB2	15	0.32
(4,602)	1:52:A:CYS:HB2	1:57:A:SER:HB3	15	0.32
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	11	0.32
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA2	11	0.32
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	11	0.32
(4,601)	1:29:A:GLU:H	1:30:A:GLY:HA3	11	0.32
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	15	0.32
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	9	0.32
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	9	0.32
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	12	0.32
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	12	0.32
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	15	0.32
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	15	0.32
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	15	0.32
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	15	0.32
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	14	0.32
(4,252)	1:9:A:LYS:HG2	1:29:A:GLU:H	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,252)	1:9:A:LYS:HG3	1:29:A:GLU:H	14	0.32
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	11	0.32
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	11	0.32
(4,249)	1:9:A:LYS:HE2	1:29:A:GLU:H	11	0.32
(4,249)	1:9:A:LYS:HE3	1:29:A:GLU:H	11	0.32
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG21	8	0.32
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG22	8	0.32
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG23	8	0.32
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	14	0.32
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	2	0.32
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	2	0.32
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	10	0.32
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	10	0.32
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	7	0.32
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	7	0.32
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	7	0.32
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	7	0.32
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	2	0.32
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	2	0.32
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	5	0.32
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	5	0.32
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	6	0.32
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	7	0.32
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	7	0.32
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG21	8	0.32
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG22	8	0.32
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG23	8	0.32
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	14	0.32
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	4	0.31
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	4	0.31
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	17	0.31
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	17	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	5	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	5	0.31
(4,1114)	1:22:A:GLY:HA3	1:25:A:CYS:HB2	5	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	5	0.31
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB3	5	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	7	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	7	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	7	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	7	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	8	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	8	0.31
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	8	0.31
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	2	0.31
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	2	0.31
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	18	0.31
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	18	0.31
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	11	0.31
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA2	11	0.31
(4,864)	1:4:A:LYS:HG2	1:5:A:GLY:HA3	11	0.31
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA2	11	0.31
(4,864)	1:4:A:LYS:HG3	1:5:A:GLY:HA3	11	0.31
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	15	0.31
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	15	0.31
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	15	0.31
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	15	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	20	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	20	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	20	0.31
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	20	0.31
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	4	0.31
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	4	0.31
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	4	0.31
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	4	0.31
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	4	0.31
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	4	0.31
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	2	0.31
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	2	0.31
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	2	0.31
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	2	0.31
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	9	0.31
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	9	0.31
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	9	0.31
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	9	0.31
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	4	0.31
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	17	0.31
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	4	0.31
(1,896)	1:37:A:LYS:HB3	1:55:A:PRO:HG3	17	0.31
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	7	0.31
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	7	0.31
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	8	0.31
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	9	0.31
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	14	0.31
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	11	0.3
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	11	0.3
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	18	0.3
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	18	0.3
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	18	0.3
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	19	0.3
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	19	0.3
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	19	0.3
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	14	0.3
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	14	0.3
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	14	0.3
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	14	0.3
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	12	0.3
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	12	0.3
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	12	0.3
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	13	0.3
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	13	0.3
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	13	0.3
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	13	0.3
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	13	0.3
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	13	0.3
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	13	0.3
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	13	0.3
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	18	0.3
(4,980)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	2	0.3
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	12	0.3
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	12	0.3
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	12	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	17	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	17	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	17	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	17	0.3
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	17	0.3
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	17	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	17	0.3
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	17	0.3
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	16	0.3
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	16	0.3
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	4	0.3
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	4	0.3
(4,642)	1:8:A:GLU:HG2	1:9:A:LYS:HG3	6	0.3
(4,642)	1:8:A:GLU:HG3	1:9:A:LYS:HG3	6	0.3
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	7	0.3
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	7	0.3
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	7	0.3
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	7	0.3
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.3
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	8	0.3
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	8	0.3
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	10	0.3
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG2	10	0.3
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	10	0.3
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	3	0.3
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	3	0.3
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	3	0.3
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	2	0.3
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	2	0.3
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	11	0.3
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	14	0.3
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	14	0.3
(1,843)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	2	0.3
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	6	0.3
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	6	0.3
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG21	4	0.3
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG22	4	0.3
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG23	4	0.3
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	14	0.29
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	14	0.29
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	7	0.29
(4,1153)	1:32:A:THR:HA	1:37:A:LYS:HG2	18	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	6	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	6	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	6	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	6	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	11	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	11	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	11	0.29
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	11	0.29
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	4	0.29
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	4	0.29
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1022)	1:22:A:GLY:HA3	1:23:A:SER:HB2	12	0.29
(4,1022)	1:22:A:GLY:HA3	1:23:A:SER:HB3	12	0.29
(4,1022)	1:22:A:GLY:HA2	1:23:A:SER:HB2	12	0.29
(4,1022)	1:22:A:GLY:HA2	1:23:A:SER:HB3	12	0.29
(4,1022)	1:22:A:GLY:HA3	1:23:A:SER:HB2	12	0.29
(4,1022)	1:22:A:GLY:HA3	1:23:A:SER:HB3	12	0.29
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	5	0.29
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	3	0.29
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG2	3	0.29
(4,970)	1:14:A:CYS:HB3	1:15:A:ARG:HG3	3	0.29
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	19	0.29
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	19	0.29
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	19	0.29
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	19	0.29
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	19	0.29
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	19	0.29
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	19	0.29
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	19	0.29
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	10	0.29
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	17	0.29
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	17	0.29
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	17	0.29
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	17	0.29
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	20	0.29
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	1	0.29
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	1	0.29
(4,846)	1:6:A:LYS:HD2	1:33:A:CYS:HA	1	0.29
(4,846)	1:6:A:LYS:HD3	1:33:A:CYS:HA	1	0.29
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	9	0.29
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	9	0.29
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	9	0.29
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	3	0.29
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	3	0.29
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	3	0.29
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	17	0.29
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	13	0.29
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	13	0.29
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	10	0.29
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	10	0.29
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	10	0.29
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG21	13	0.29
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG22	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,240)	1:37:A:LYS:H	1:38:A:THR:HG23	13	0.29
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB3	13	0.29
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB2	13	0.29
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB3	13	0.29
(4,237)	1:37:A:LYS:H	1:37:A:LYS:HB2	13	0.29
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	9	0.29
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	9	0.29
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	9	0.29
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	9	0.29
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	9	0.29
(4,116)	1:22:A:GLY:H	1:36:A:CYS:HB3	11	0.29
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	14	0.29
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	7	0.29
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	5	0.29
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	6	0.29
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	6	0.29
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	11	0.29
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	11	0.29
(1,883)	1:9:A:LYS:HA	1:9:A:LYS:HE2	20	0.29
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	3	0.29
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	3	0.29
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	18	0.29
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	18	0.29
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG21	2	0.29
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG22	2	0.29
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG23	2	0.29
(1,407)	1:9:A:LYS:HB2	1:28:A:GLY:HA2	7	0.29
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG21	13	0.29
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG22	13	0.29
(1,220)	1:37:A:LYS:H	1:38:A:THR:HG23	13	0.29
(1,106)	1:22:A:GLY:H	1:36:A:CYS:HB3	11	0.29
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	10	0.28
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	10	0.28
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	5	0.28
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	18	0.28
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	18	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	9	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	9	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	9	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	9	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	20	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	20	0.28
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	20	0.28
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	7	0.28
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	4	0.28
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	14	0.28
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	3	0.28
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	3	0.28
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	3	0.28
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	3	0.28
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	5	0.28
(4,850)	1:33:A:CYS:HA	1:34:A:ALA:H	11	0.28
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	4	0.28
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	9	0.28
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	17	0.28
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	17	0.28
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	17	0.28
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	17	0.28
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	17	0.28
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	17	0.28
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	7	0.28
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	7	0.28
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	6	0.28
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	6	0.28
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	6	0.28
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	6	0.28
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	4	0.28
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	10	0.28
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.28
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	17	0.28
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.28
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	17	0.28
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	10	0.28
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG2	11	0.28
(1,961)	1:50:A:LYS:HA	1:51:A:GLU:HG3	11	0.28
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	10	0.28
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	18	0.28
(1,732)	1:33:A:CYS:HA	1:34:A:ALA:H	11	0.28
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	20	0.28
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	17	0.28
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	5	0.28
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	2	0.28
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	4	0.28
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	10	0.28
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	4	0.27
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	4	0.27
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	4	0.27
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	4	0.27
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	4	0.27
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	4	0.27
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	4	0.27
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	4	0.27
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	4	0.27
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	4	0.27
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	4	0.27
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	13	0.27
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	13	0.27
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	13	0.27
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	13	0.27
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	13	0.27
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	13	0.27
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	13	0.27
(4,1156)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	13	0.27
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	13	0.27
(4,1156)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	13	0.27
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	6	0.27
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	6	0.27
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	3	0.27
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	3	0.27
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	3	0.27
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	3	0.27
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	3	0.27
(4,1005)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	3	0.27
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	3	0.27
(4,1005)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	3	0.27
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	18	0.27
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	18	0.27
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	18	0.27
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	18	0.27
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	12	0.27
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	12	0.27
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	12	0.27
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	12	0.27
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	4	0.27
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	4	0.27
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	5	0.27
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	5	0.27
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	5	0.27
(4,806)	1:62:A:SER:HA	1:64:A:CYS:HB2	12	0.27
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	5	0.27
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	15	0.27
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	15	0.27
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	15	0.27
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	15	0.27
(4,709)	1:14:A:CYS:H	1:15:A:ARG:HG2	11	0.27
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	14	0.27
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB2	14	0.27
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	14	0.27
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	15	0.27
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB2	15	0.27
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	15	0.27
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	16	0.27
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	16	0.27
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	16	0.27
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	16	0.27
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	16	0.27
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	19	0.27
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	19	0.27
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	19	0.27
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	19	0.27
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	19	0.27
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	19	0.27
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	7	0.27
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	14	0.27
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	14	0.27
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	18	0.27
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	18	0.27
(4,173)	1:31:A:CYS:H	1:32:A:THR:HB	12	0.27
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	14	0.27
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	15	0.27
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE2	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:5:A:GLY:HA2	1:6:A:LYS:HE3	3	0.27
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE2	3	0.27
(1,862)	1:5:A:GLY:HA3	1:6:A:LYS:HE3	3	0.27
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	4	0.27
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	4	0.27
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	4	0.27
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	5	0.27
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	5	0.27
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	5	0.27
(1,730)	1:6:A:LYS:HD3	1:33:A:CYS:HA	4	0.27
(1,179)	1:19:A:CYS:H	1:21:A:CYS:H	15	0.27
(1,161)	1:31:A:CYS:H	1:32:A:THR:HB	12	0.27
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	11	0.26
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	11	0.26
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	11	0.26
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	11	0.26
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	19	0.26
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	19	0.26
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	19	0.26
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	19	0.26
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	18	0.26
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	18	0.26
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD3	18	0.26
(4,1063)	1:37:A:LYS:HA	1:37:A:LYS:HD2	18	0.26
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	20	0.26
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	20	0.26
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	10	0.26
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	14	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	3	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB2	3	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	3	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	4	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB2	4	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	4	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	7	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB2	7	0.26
(4,645)	1:57:A:SER:HA	1:57:A:SER:HB3	7	0.26
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	17	0.26
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	17	0.26
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	17	0.26
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	17	0.26
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	1	0.26
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	1	0.26
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	9	0.26
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	7	0.26
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	11	0.26
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	11	0.26
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	11	0.26
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	11	0.26
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	5	0.26
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	5	0.26
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	12	0.26
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	12	0.26
(4,161)	1:16:A:SER:HB2	1:20:A:GLN:H	12	0.26
(4,161)	1:16:A:SER:HB3	1:20:A:GLN:H	12	0.26
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	1	0.26
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	1	0.26
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	6	0.26
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	6	0.26
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	17	0.26
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	17	0.26
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD2	18	0.26
(1,891)	1:37:A:LYS:HA	1:37:A:LYS:HD3	18	0.26
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	20	0.26
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	20	0.26
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	9	0.26
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	9	0.26
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	14	0.26
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	16	0.25
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	16	0.25
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB3	16	0.25
(4,1163)	1:46:A:CYS:HB3	1:51:A:GLU:HB2	16	0.25
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	20	0.25
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	20	0.25
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	20	0.25
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	14	0.25
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	14	0.25
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	13	0.25
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	8	0.25
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	8	0.25
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	8	0.25
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	8	0.25
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	8	0.25
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	8	0.25
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	8	0.25
(4,899)	1:42:A:THR:HB	1:53:A:THR:HB	2	0.25
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	8	0.25
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	8	0.25
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	8	0.25
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	13	0.25
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	17	0.25
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	11	0.25
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	11	0.25
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	11	0.25
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	19	0.25
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	20	0.25
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	20	0.25
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	20	0.25
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB2	20	0.25
(4,644)	1:56:A:ASP:HB2	1:57:A:SER:HB3	20	0.25
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	20	0.25
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	20	0.25
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB2	20	0.25
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	20	0.25
(4,644)	1:56:A:ASP:HB3	1:57:A:SER:HB3	20	0.25
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	6	0.25
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	6	0.25
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	6	0.25
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	6	0.25
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	10	0.25
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	10	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	3	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	3	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	3	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	4	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	4	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	4	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	6	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	6	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	6	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	12	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	12	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	12	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	17	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	17	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	19	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB2	19	0.25
(4,527)	1:16:A:SER:HA	1:16:A:SER:HB3	19	0.25
(4,422)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	5	0.25
(4,422)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	5	0.25
(4,422)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	5	0.25
(4,422)	1:28:A:GLY:HA3	1:29:A:GLU:HG2	5	0.25
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	18	0.25
(4,392)	1:37:A:LYS:HD2	1:38:A:THR:H	18	0.25
(4,392)	1:37:A:LYS:HD3	1:38:A:THR:H	18	0.25
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.25
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	7	0.25
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.25
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	7	0.25
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	11	0.25
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	11	0.25
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	18	0.25
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	18	0.25
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	14	0.25
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	20	0.25
(1,883)	1:32:A:THR:HA	1:37:A:LYS:HE2	18	0.25
(1,881)	1:29:A:GLU:HG2	1:61:A:GLY:HA2	10	0.25
(1,881)	1:29:A:GLU:HG2	1:61:A:GLY:HA3	10	0.25
(1,881)	1:29:A:GLU:HG3	1:61:A:GLY:HA2	10	0.25
(1,881)	1:29:A:GLU:HG3	1:61:A:GLY:HA3	10	0.25
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	18	0.25
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	18	0.25
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	8	0.25
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	8	0.25
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	8	0.25
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE2	17	0.25
(1,689)	1:34:A:ALA:HA	1:37:A:LYS:HE3	17	0.25
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	7	0.25
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	19	0.25
(1,497)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	6	0.25
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	3	0.25
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	3	0.25
(4,1075)	1:37:A:LYS:HD2	1:55:A:PRO:HG2	19	0.24
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	19	0.24
(4,1075)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	8	0.24
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	12	0.24
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	0.24
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	0.24
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	0.24
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	0.24
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	20	0.24
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	20	0.24
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	20	0.24
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	20	0.24
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	12	0.24
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	12	0.24
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	12	0.24
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	12	0.24
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	11	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	9	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	9	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	9	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	9	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	16	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	16	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	16	0.24
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	16	0.24
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	15	0.24
(4,899)	1:42:A:THR:HB	1:53:A:THR:HB	1	0.24
(4,866)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	11	0.24
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	9	0.24
(4,808)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	9	0.24
(4,808)	1:61:A:GLY:HA3	1:64:A:CYS:HB2	9	0.24
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	19	0.24
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	7	0.24
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	7	0.24
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	7	0.24
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	7	0.24
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	7	0.24
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	7	0.24
(4,612)	1:46:A:CYS:HA	1:47:A:LYS:HG2	8	0.24
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	3	0.24
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	3	0.24
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	3	0.24
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	3	0.24
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	12	0.24
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	4	0.24
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	3	0.24
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	9	0.24
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	17	0.24
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	17	0.24
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	17	0.24
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	17	0.24
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	15	0.24
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	15	0.24
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	17	0.24
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	4	0.24
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	4	0.24
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	12	0.24
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB2	11	0.24
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB3	11	0.24
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	4	0.24
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG21	7	0.24
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG22	7	0.24
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG23	7	0.24
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	4	0.24
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB3	13	0.24
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	2	0.24
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	8	0.24
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	1	0.23
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	1	0.23
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	1	0.23
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	1	0.23
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	1	0.23
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	1	0.23
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	1	0.23
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	1	0.23
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	1	0.23
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	1	0.23
(4,1083)	1:42:A:THR:HG21	1:44:A:ASP:HB2	1	0.23
(4,1083)	1:42:A:THR:HG21	1:44:A:ASP:HB3	1	0.23
(4,1083)	1:42:A:THR:HG22	1:44:A:ASP:HB2	1	0.23
(4,1083)	1:42:A:THR:HG22	1:44:A:ASP:HB3	1	0.23
(4,1083)	1:42:A:THR:HG23	1:44:A:ASP:HB2	1	0.23
(4,1083)	1:42:A:THR:HG23	1:44:A:ASP:HB3	1	0.23
(4,1083)	1:42:A:THR:HG21	1:44:A:ASP:HB2	1	0.23
(4,1083)	1:42:A:THR:HG22	1:44:A:ASP:HB2	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1083)	1:42:A:THR:HG23	1:44:A:ASP:HB2	1	0.23
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	16	0.23
(4,1077)	1:37:A:LYS:HD2	1:55:A:PRO:HG3	16	0.23
(4,1077)	1:37:A:LYS:HD3	1:55:A:PRO:HG3	16	0.23
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	0.23
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	20	0.23
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	20	0.23
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	7	0.23
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	7	0.23
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	7	0.23
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	19	0.23
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA2	19	0.23
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	19	0.23
(4,870)	1:9:A:LYS:HB2	1:30:A:GLY:HA2	19	0.23
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	7	0.23
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	7	0.23
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	7	0.23
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	7	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	2	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	2	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	2	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	9	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	9	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	9	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	14	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	14	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	14	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	15	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	15	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	15	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	18	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	18	0.23
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	18	0.23
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	18	0.23
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	18	0.23
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	18	0.23
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	18	0.23
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	18	0.23
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	15	0.23
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	15	0.23
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	15	0.23
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	20	0.23
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	20	0.23
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	17	0.23
(4,391)	1:47:A:LYS:H	1:47:A:LYS:HD2	17	0.23
(4,391)	1:47:A:LYS:H	1:47:A:LYS:HD3	17	0.23
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	14	0.23
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG2	14	0.23
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	14	0.23
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	1	0.23
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	17	0.23
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	17	0.23
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	17	0.23
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	17	0.23
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	19	0.23
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	3	0.23
(4,103)	1:31:A:CYS:H	1:33:A:CYS:H	13	0.23
(4,53)	1:39:A:CYS:HA	1:40:A:ASN:HD21	15	0.23
(1,974)	1:49:A:GLY:HA3	1:50:A:LYS:HD2	20	0.23
(1,968)	1:9:A:LYS:HD2	1:29:A:GLU:HG2	9	0.23
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	5	0.23
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	5	0.23
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	8	0.23
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	8	0.23
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	8	0.23
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	8	0.23
(1,899)	1:42:A:THR:HG21	1:44:A:ASP:HB2	1	0.23
(1,899)	1:42:A:THR:HG21	1:44:A:ASP:HB3	1	0.23
(1,899)	1:42:A:THR:HG22	1:44:A:ASP:HB2	1	0.23
(1,899)	1:42:A:THR:HG22	1:44:A:ASP:HB3	1	0.23
(1,899)	1:42:A:THR:HG23	1:44:A:ASP:HB2	1	0.23
(1,899)	1:42:A:THR:HG23	1:44:A:ASP:HB3	1	0.23
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	14	0.23
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	14	0.23
(1,748)	1:9:A:LYS:HB2	1:30:A:GLY:HA3	19	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	2	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	2	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	2	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	9	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	9	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	9	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	14	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	14	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	15	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	15	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	15	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	18	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	18	0.23
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	18	0.23
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	17	0.23
(1,443)	1:39:A:CYS:H	1:58:A:CYS:HB2	11	0.23
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG2	6	0.23
(1,379)	1:28:A:GLY:HA2	1:29:A:GLU:HG3	6	0.23
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	17	0.23
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	14	0.23
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	14	0.23
(1,47)	1:39:A:CYS:HA	1:40:A:ASN:HD21	15	0.23
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	1	0.22
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	1	0.22
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	11	0.22
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.22
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	4	0.22
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	4	0.22
(4,1115)	1:15:A:ARG:HG3	1:16:A:SER:H	3	0.22
(4,1057)	1:33:A:CYS:HB3	1:37:A:LYS:HB2	11	0.22
(4,1057)	1:33:A:CYS:HB3	1:37:A:LYS:HB3	11	0.22
(4,1057)	1:33:A:CYS:HB3	1:37:A:LYS:HB2	11	0.22
(4,1057)	1:33:A:CYS:HB3	1:37:A:LYS:HB3	11	0.22
(4,1057)	1:33:A:CYS:HB2	1:37:A:LYS:HB2	11	0.22
(4,1057)	1:33:A:CYS:HB3	1:37:A:LYS:HB2	11	0.22
(4,1057)	1:33:A:CYS:HB2	1:37:A:LYS:HB2	11	0.22
(4,980)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	3	0.22
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	8	0.22
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	8	0.22
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	8	0.22
(4,916)	1:61:A:GLY:HA2	1:64:A:CYS:HB2	12	0.22
(4,844)	1:22:A:GLY:HA3	1:24:A:LYS:H	17	0.22
(4,844)	1:22:A:GLY:HA2	1:24:A:LYS:H	17	0.22
(4,844)	1:22:A:GLY:HA2	1:24:A:LYS:H	17	0.22
(4,844)	1:22:A:GLY:HA3	1:24:A:LYS:H	17	0.22
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	14	0.22
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	14	0.22
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	11	0.22
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	11	0.22
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	11	0.22
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	1	0.22
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	1	0.22
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	1	0.22
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	1	0.22
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	1	0.22
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	1	0.22
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	16	0.22
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	16	0.22
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	16	0.22
(4,399)	1:56:A:ASP:HB3	1:57:A:SER:HA	9	0.22
(4,399)	1:56:A:ASP:HB3	1:57:A:SER:HA	18	0.22
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA3	13	0.22
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA2	13	0.22
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA3	13	0.22
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA2	13	0.22
(4,341)	1:50:A:LYS:HB3	1:52:A:CYS:H	14	0.22
(4,341)	1:50:A:LYS:HB2	1:52:A:CYS:H	14	0.22
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	8	0.22
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	8	0.22
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	10	0.22
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	10	0.22
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE2	10	0.22
(4,206)	1:50:A:LYS:H	1:50:A:LYS:HE3	10	0.22
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	8	0.22
(4,156)	1:28:A:GLY:H	1:31:A:CYS:HB2	11	0.22
(4,156)	1:28:A:GLY:H	1:31:A:CYS:HB2	11	0.22
(4,156)	1:28:A:GLY:H	1:31:A:CYS:HB3	11	0.22
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	12	0.22
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	12	0.22
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	19	0.22
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	19	0.22
(4,6)	1:15:A:ARG:HG3	1:16:A:SER:H	3	0.22
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	1	0.22
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	11	0.22
(1,951)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	14	0.22
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	14	0.22
(1,874)	1:23:A:SER:HB2	1:24:A:LYS:HB2	7	0.22
(1,843)	1:48:A:CYS:HB2	1:64:A:CYS:HB3	3	0.22
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	11	0.22
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:33:A:CYS:HA	1:37:A:LYS:HD3	15	0.22
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG21	1	0.22
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG22	1	0.22
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG23	1	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG21	3	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG22	3	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG23	3	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG21	17	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG22	17	0.22
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG23	17	0.22
(4,1182)	1:16:A:SER:HB2	1:17:A:GLU:H	17	0.21
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	17	0.21
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	17	0.21
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	14	0.21
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	10	0.21
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	10	0.21
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD2	10	0.21
(4,915)	1:47:A:LYS:HA	1:47:A:LYS:HD3	10	0.21
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	8	0.21
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	16	0.21
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	8	0.21
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	8	0.21
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	8	0.21
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	20	0.21
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	20	0.21
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	20	0.21
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	13	0.21
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	8	0.21
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	8	0.21
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	8	0.21
(4,709)	1:14:A:CYS:H	1:15:A:ARG:HG2	18	0.21
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	9	0.21
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG2	9	0.21
(4,702)	1:14:A:CYS:HB2	1:15:A:ARG:HG3	9	0.21
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	13	0.21
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	5	0.21
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	5	0.21
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	5	0.21
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	10	0.21
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG2	3	0.21
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG3	3	0.21
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG3	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG2	3	0.21
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	1	0.21
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	1	0.21
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG2	5	0.21
(4,419)	1:38:A:THR:HA	1:55:A:PRO:HG3	5	0.21
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	15	0.21
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	15	0.21
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	2	0.21
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	6	0.21
(4,80)	1:46:A:CYS:H	1:51:A:GLU:HA	11	0.21
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	10	0.21
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	10	0.21
(1,971)	1:16:A:SER:HB2	1:17:A:GLU:H	17	0.21
(1,971)	1:16:A:SER:HB3	1:17:A:GLU:H	17	0.21
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	14	0.21
(1,952)	1:14:A:CYS:HA	1:36:A:CYS:HB2	20	0.21
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	6	0.21
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	6	0.21
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG2	16	0.21
(1,841)	1:58:A:CYS:HA	1:59:A:LYS:HG3	16	0.21
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	19	0.21
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	13	0.21
(1,497)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	14	0.21
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	6	0.21
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	13	0.2
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	12	0.2
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	12	0.2
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	12	0.2
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	12	0.2
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	9	0.2
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	9	0.2
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	9	0.2
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	3	0.2
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	3	0.2
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	10	0.2
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	10	0.2
(4,806)	1:62:A:SER:HA	1:64:A:CYS:HB2	5	0.2
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	10	0.2
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	3	0.2
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	12	0.2
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	12	0.2
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	6	0.2
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	6	0.2
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	14	0.2
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA3	2	0.2
(4,406)	1:42:A:THR:HA	1:54:A:GLY:HA2	2	0.2
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	20	0.2
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	20	0.2
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	10	0.2
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA2	10	0.2
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	10	0.2
(4,247)	1:29:A:GLU:H	1:61:A:GLY:HA3	10	0.2
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	5	0.2
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	5	0.2
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	13	0.2
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	7	0.2
(1,837)	1:42:A:THR:HG21	1:54:A:GLY:HA2	2	0.2
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	8	0.2
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	3	0.2
(1,561)	1:9:A:LYS:HB2	1:10:A:CYS:HA	13	0.2
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	12	0.2
(1,232)	1:9:A:LYS:HG2	1:29:A:GLU:H	6	0.2
(1,232)	1:9:A:LYS:HG3	1:29:A:GLU:H	6	0.2
(1,189)	1:50:A:LYS:H	1:50:A:LYS:HE2	16	0.2
(1,189)	1:50:A:LYS:H	1:50:A:LYS:HE3	16	0.2
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	1	0.19
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	3	0.19
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	3	0.19
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	4	0.19
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	4	0.19
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	4	0.19
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	4	0.19
(4,1120)	1:8:A:GLU:HA	1:9:A:LYS:HG2	20	0.19
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	11	0.19
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	11	0.19
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	8	0.19
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	8	0.19
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	17	0.19
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	17	0.19
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG2	17	0.19
(4,946)	1:50:A:LYS:H	1:51:A:GLU:HG3	17	0.19
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	18	0.19
(4,873)	1:22:A:GLY:HA2	1:24:A:LYS:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,873)	1:22:A:GLY:HA3	1:24:A:LYS:H	17	0.19
(4,873)	1:22:A:GLY:HA2	1:24:A:LYS:H	17	0.19
(4,873)	1:22:A:GLY:HA3	1:24:A:LYS:H	17	0.19
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	13	0.19
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	13	0.19
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	13	0.19
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	13	0.19
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	12	0.19
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	2	0.19
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	2	0.19
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	2	0.19
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	2	0.19
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	13	0.19
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	15	0.19
(4,635)	1:6:A:LYS:HG3	1:33:A:CYS:HB2	20	0.19
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	18	0.19
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	17	0.19
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	17	0.19
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	4	0.19
(4,284)	1:18:A:PRO:HD2	1:20:A:GLN:HE22	15	0.19
(4,284)	1:18:A:PRO:HD2	1:20:A:GLN:HE21	15	0.19
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	1	0.19
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	1	0.19
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	1	0.19
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	1	0.19
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	7	0.19
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	1	0.19
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	3	0.19
(1,930)	1:8:A:GLU:HA	1:9:A:LYS:HG2	20	0.19
(1,709)	1:38:A:THR:HG23	1:39:A:CYS:HB2	13	0.19
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	16	0.19
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	13	0.19
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	15	0.19
(1,497)	1:60:A:CYS:HB3	1:67:A:LYS:HD2	1	0.19
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	18	0.19
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	4	0.19
(1,358)	1:32:A:THR:H	1:37:A:LYS:HD2	15	0.19
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	9	0.19
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	9	0.19
(1,219)	1:35:A:ALA:HB1	1:37:A:LYS:H	8	0.19
(1,179)	1:19:A:CYS:H	1:21:A:CYS:H	14	0.19
(4,1182)	1:16:A:SER:HB2	1:17:A:GLU:H	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	6	0.18
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	6	0.18
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	15	0.18
(4,1171)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	13	0.18
(4,1171)	1:40:A:ASN:HB3	1:48:A:CYS:HB3	13	0.18
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	11	0.18
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG2	11	0.18
(4,1150)	1:46:A:CYS:HA	1:47:A:LYS:HG3	11	0.18
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	14	0.18
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB2	14	0.18
(4,1132)	1:23:A:SER:HA	1:25:A:CYS:HB3	14	0.18
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	20	0.18
(4,1024)	1:23:A:SER:HB2	1:24:A:LYS:HB2	15	0.18
(4,1024)	1:23:A:SER:HB3	1:24:A:LYS:HB2	15	0.18
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	19	0.18
(4,1012)	1:6:A:LYS:HG3	1:15:A:ARG:HA	19	0.18
(4,1012)	1:6:A:LYS:HG2	1:15:A:ARG:HA	19	0.18
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	15	0.18
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.18
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	11	0.18
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.18
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA2	11	0.18
(4,959)	1:6:A:LYS:HB2	1:7:A:GLY:HA3	11	0.18
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	11	0.18
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.18
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA2	11	0.18
(4,959)	1:6:A:LYS:HB3	1:7:A:GLY:HA3	11	0.18
(4,954)	1:16:A:SER:HB2	1:20:A:GLN:HE21	12	0.18
(4,954)	1:16:A:SER:HB3	1:20:A:GLN:HE21	12	0.18
(4,954)	1:16:A:SER:HB2	1:20:A:GLN:HE22	12	0.18
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	12	0.18
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	12	0.18
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	5	0.18
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	8	0.18
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	8	0.18
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	8	0.18
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	8	0.18
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	13	0.18
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	13	0.18
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	13	0.18
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	20	0.18
(4,529)	1:16:A:SER:HA	1:17:A:GLU:HG2	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,524)	1:11:A:THR:HA	1:26:A:GLN:HB2	5	0.18
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG2	8	0.18
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG3	8	0.18
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG3	8	0.18
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG2	8	0.18
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	1	0.18
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	7	0.18
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	10	0.18
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	3	0.18
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG2	3	0.18
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	3	0.18
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	13	0.18
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	13	0.18
(4,342)	1:50:A:LYS:HG3	1:52:A:CYS:H	18	0.18
(4,342)	1:50:A:LYS:HG2	1:52:A:CYS:H	18	0.18
(4,279)	1:39:A:CYS:HA	1:40:A:ASN:HD22	2	0.18
(4,202)	1:42:A:THR:HG21	1:45:A:GLY:H	3	0.18
(4,202)	1:42:A:THR:HG22	1:45:A:GLY:H	3	0.18
(4,202)	1:42:A:THR:HG23	1:45:A:GLY:H	3	0.18
(4,202)	1:42:A:THR:HG21	1:45:A:GLY:H	8	0.18
(4,202)	1:42:A:THR:HG22	1:45:A:GLY:H	8	0.18
(4,202)	1:42:A:THR:HG23	1:45:A:GLY:H	8	0.18
(4,105)	1:16:A:SER:HB3	1:20:A:GLN:HE21	16	0.18
(4,105)	1:16:A:SER:HB2	1:20:A:GLN:HE21	16	0.18
(4,105)	1:16:A:SER:HB2	1:20:A:GLN:HE21	16	0.18
(4,105)	1:16:A:SER:HB3	1:20:A:GLN:HE21	16	0.18
(4,105)	1:16:A:SER:HB3	1:20:A:GLN:HE22	16	0.18
(4,105)	1:16:A:SER:HB2	1:20:A:GLN:HE21	16	0.18
(4,105)	1:16:A:SER:HB2	1:20:A:GLN:HE22	16	0.18
(4,105)	1:16:A:SER:HB3	1:20:A:GLN:HE21	16	0.18
(4,105)	1:16:A:SER:HB3	1:20:A:GLN:HE22	16	0.18
(1,971)	1:16:A:SER:HB2	1:17:A:GLU:H	6	0.18
(1,971)	1:16:A:SER:HB3	1:17:A:GLU:H	6	0.18
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	15	0.18
(1,962)	1:40:A:ASN:HB2	1:48:A:CYS:HB3	13	0.18
(1,796)	1:29:A:GLU:HA	1:31:A:CYS:HB2	12	0.18
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	5	0.18
(1,497)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	20	0.18
(1,465)	1:16:A:SER:HA	1:17:A:GLU:HG2	3	0.18
(1,460)	1:11:A:THR:HA	1:26:A:GLN:HB2	5	0.18
(1,443)	1:6:A:LYS:H	1:10:A:CYS:HB2	6	0.18
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	7	0.18
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	10	0.18
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	4	0.18
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	4	0.18
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	18	0.18
(1,305)	1:50:A:LYS:HG2	1:52:A:CYS:H	2	0.18
(1,287)	1:37:A:LYS:HG2	1:58:A:CYS:H	16	0.18
(1,185)	1:42:A:THR:HG21	1:45:A:GLY:H	3	0.18
(1,185)	1:42:A:THR:HG22	1:45:A:GLY:H	3	0.18
(1,185)	1:42:A:THR:HG23	1:45:A:GLY:H	3	0.18
(1,185)	1:42:A:THR:HG21	1:45:A:GLY:H	8	0.18
(1,185)	1:42:A:THR:HG22	1:45:A:GLY:H	8	0.18
(1,185)	1:42:A:THR:HG23	1:45:A:GLY:H	8	0.18
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	7	0.17
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	10	0.17
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	10	0.17
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	10	0.17
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	5	0.17
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	5	0.17
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	5	0.17
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	5	0.17
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG2	5	0.17
(4,1016)	1:7:A:GLY:HA2	1:8:A:GLU:HG3	5	0.17
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG2	5	0.17
(4,1016)	1:7:A:GLY:HA3	1:8:A:GLU:HG3	5	0.17
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA3	9	0.17
(4,993)	1:41:A:CYS:HB2	1:54:A:GLY:HA2	9	0.17
(4,963)	1:67:A:LYS:HA	1:67:A:LYS:HD3	16	0.17
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	11	0.17
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	11	0.17
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	11	0.17
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	11	0.17
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	5	0.17
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	5	0.17
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	20	0.17
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	20	0.17
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE2	20	0.17
(4,793)	1:34:A:ALA:HA	1:37:A:LYS:HE3	20	0.17
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	14	0.17
(4,482)	1:39:A:CYS:HB3	1:52:A:CYS:HB2	4	0.17
(4,482)	1:39:A:CYS:HB2	1:52:A:CYS:HB2	4	0.17
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	8	0.17
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG2	11	0.17
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG3	11	0.17
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG3	11	0.17
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG2	11	0.17
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	6	0.17
(4,367)	1:42:A:THR:H	1:53:A:THR:HA	10	0.17
(4,315)	1:56:A:ASP:HB2	1:58:A:CYS:H	3	0.17
(4,315)	1:56:A:ASP:HB2	1:58:A:CYS:H	3	0.17
(4,315)	1:56:A:ASP:HB3	1:58:A:CYS:H	3	0.17
(4,315)	1:56:A:ASP:HB3	1:58:A:CYS:H	3	0.17
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	7	0.17
(1,828)	1:67:A:LYS:HA	1:67:A:LYS:HD3	16	0.17
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	16	0.17
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	11	0.17
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	11	0.17
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	11	0.17
(1,715)	1:19:A:CYS:HB2	1:35:A:ALA:HA	9	0.17
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	14	0.17
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	6	0.17
(1,331)	1:42:A:THR:H	1:53:A:THR:HA	10	0.17
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	8	0.17
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	8	0.17
(1,179)	1:19:A:CYS:H	1:21:A:CYS:H	9	0.17
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	8	0.16
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	8	0.16
(4,1208)	1:6:A:LYS:HE2	1:15:A:ARG:HA	8	0.16
(4,1208)	1:6:A:LYS:HE3	1:15:A:ARG:HA	8	0.16
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	5	0.16
(4,1115)	1:15:A:ARG:HG3	1:16:A:SER:H	15	0.16
(4,1109)	1:9:A:LYS:HB2	1:29:A:GLU:H	7	0.16
(4,1096)	1:21:A:CYS:HB3	1:25:A:CYS:H	6	0.16
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	15	0.16
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG3	15	0.16
(4,1054)	1:33:A:CYS:H	1:37:A:LYS:HG2	15	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	2	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	2	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	2	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	2	0.16
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	2	0.16
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	2	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	2	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	7	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	7	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	7	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	7	0.16
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	7	0.16
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	7	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	7	0.16
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	7	0.16
(4,869)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	0.16
(4,869)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	0.16
(4,869)	1:29:A:GLU:HB2	1:30:A:GLY:HA3	18	0.16
(4,869)	1:29:A:GLU:HB2	1:30:A:GLY:HA2	18	0.16
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	7	0.16
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	15	0.16
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG2	15	0.16
(4,783)	1:9:A:LYS:HA	1:9:A:LYS:HG3	15	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	4	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	4	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	4	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	4	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	6	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	6	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	6	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	6	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	14	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	14	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	14	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	14	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	16	0.16
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	16	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	16	0.16
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	16	0.16
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	16	0.16
(4,751)	1:16:A:SER:HB2	1:20:A:GLN:HB3	16	0.16
(4,751)	1:16:A:SER:HB3	1:20:A:GLN:HB3	16	0.16
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	15	0.16
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	7	0.16
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	7	0.16
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	11	0.16
(4,315)	1:56:A:ASP:HB2	1:58:A:CYS:H	8	0.16
(4,315)	1:56:A:ASP:HB2	1:58:A:CYS:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,315)	1:56:A:ASP:HB3	1:58:A:CYS:H	8	0.16
(4,315)	1:56:A:ASP:HB3	1:58:A:CYS:H	8	0.16
(4,121)	1:11:A:THR:H	1:12:A:SER:HA	19	0.16
(4,26)	1:21:A:CYS:HA	1:25:A:CYS:H	14	0.16
(4,6)	1:15:A:ARG:HG3	1:16:A:SER:H	15	0.16
(1,988)	1:6:A:LYS:HE2	1:15:A:ARG:HA	8	0.16
(1,988)	1:6:A:LYS:HE3	1:15:A:ARG:HA	8	0.16
(1,965)	1:37:A:LYS:HG3	1:55:A:PRO:HA	13	0.16
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	5	0.16
(1,947)	1:37:A:LYS:HG3	1:38:A:THR:HA	18	0.16
(1,928)	1:15:A:ARG:HG3	1:16:A:SER:H	15	0.16
(1,923)	1:9:A:LYS:HB2	1:29:A:GLU:H	7	0.16
(1,910)	1:21:A:CYS:HB3	1:25:A:CYS:H	6	0.16
(1,883)	1:9:A:LYS:HA	1:9:A:LYS:HE3	3	0.16
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	5	0.16
(1,687)	1:66:A:CYS:HB3	1:67:A:LYS:HD3	9	0.16
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	11	0.16
(1,325)	1:51:A:GLU:H	1:51:A:GLU:HG2	16	0.16
(1,325)	1:51:A:GLU:H	1:51:A:GLU:HG3	16	0.16
(1,287)	1:58:A:CYS:H	1:59:A:LYS:HG3	1	0.16
(1,110)	1:11:A:THR:H	1:12:A:SER:HA	19	0.16
(1,24)	1:21:A:CYS:HA	1:25:A:CYS:H	14	0.16
(4,1209)	1:23:A:SER:HB2	1:24:A:LYS:HG2	11	0.15
(4,1209)	1:23:A:SER:HB2	1:24:A:LYS:HG3	11	0.15
(4,1209)	1:23:A:SER:HB3	1:24:A:LYS:HG2	11	0.15
(4,1209)	1:23:A:SER:HB3	1:24:A:LYS:HG3	11	0.15
(4,1209)	1:23:A:SER:HB2	1:24:A:LYS:HG2	11	0.15
(4,1209)	1:23:A:SER:HB2	1:24:A:LYS:HG2	11	0.15
(4,1209)	1:23:A:SER:HB3	1:24:A:LYS:HG2	11	0.15
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	4	0.15
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	11	0.15
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	18	0.15
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	1	0.15
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	1	0.15
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	1	0.15
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	1	0.15
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	13	0.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	6	0.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	6	0.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	6	0.15
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	6	0.15
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD2	6	0.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	6	0.15
(4,1159)	1:33:A:CYS:HB2	1:37:A:LYS:HD3	6	0.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	6	0.15
(4,1159)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	6	0.15
(4,1027)	1:23:A:SER:HB2	1:24:A:LYS:HG2	11	0.15
(4,1027)	1:23:A:SER:HB2	1:24:A:LYS:HG3	11	0.15
(4,1027)	1:23:A:SER:HB3	1:24:A:LYS:HG2	11	0.15
(4,1027)	1:23:A:SER:HB3	1:24:A:LYS:HG3	11	0.15
(4,1027)	1:23:A:SER:HB3	1:24:A:LYS:HG2	11	0.15
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA3	6	0.15
(4,995)	1:39:A:CYS:HB3	1:54:A:GLY:HA2	6	0.15
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	6	0.15
(4,935)	1:40:A:ASN:H	1:66:A:CYS:HA	13	0.15
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	16	0.15
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	16	0.15
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	16	0.15
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	17	0.15
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	17	0.15
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	17	0.15
(4,799)	1:39:A:CYS:HB3	1:41:A:CYS:HB2	20	0.15
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	18	0.15
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	18	0.15
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	18	0.15
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	5	0.15
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	5	0.15
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	5	0.15
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	5	0.15
(4,686)	1:21:A:CYS:H	1:36:A:CYS:HB2	19	0.15
(4,669)	1:41:A:CYS:H	1:46:A:CYS:HA	1	0.15
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	4	0.15
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	1	0.15
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	1	0.15
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE2	1	0.15
(4,631)	1:4:A:LYS:HA	1:4:A:LYS:HE3	1	0.15
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	1	0.15
(4,562)	1:64:A:CYS:HB2	1:67:A:LYS:HD2	13	0.15
(4,524)	1:11:A:THR:HA	1:26:A:GLN:HB2	17	0.15
(4,479)	1:7:A:GLY:HA2	1:31:A:CYS:HA	3	0.15
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG2	19	0.15
(4,421)	1:39:A:CYS:H	1:55:A:PRO:HG3	19	0.15
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	12	0.15
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	12	0.15
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	12	0.15
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	16	0.15
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	16	0.15
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	16	0.15
(4,279)	1:39:A:CYS:HA	1:40:A:ASN:HD22	15	0.15
(4,257)	1:38:A:THR:H	1:55:A:PRO:HB3	14	0.15
(4,257)	1:38:A:THR:H	1:55:A:PRO:HB2	14	0.15
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	2	0.15
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	2	0.15
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	2	0.15
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	2	0.15
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	4	0.15
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	4	0.15
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	8	0.15
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	8	0.15
(4,217)	1:7:A:GLY:HA2	1:10:A:CYS:H	20	0.15
(4,202)	1:42:A:THR:HG21	1:45:A:GLY:H	2	0.15
(4,202)	1:42:A:THR:HG22	1:45:A:GLY:H	2	0.15
(4,202)	1:42:A:THR:HG23	1:45:A:GLY:H	2	0.15
(4,202)	1:42:A:THR:HG21	1:45:A:GLY:H	11	0.15
(4,202)	1:42:A:THR:HG22	1:45:A:GLY:H	11	0.15
(4,202)	1:42:A:THR:HG23	1:45:A:GLY:H	11	0.15
(4,175)	1:9:A:LYS:HB2	1:31:A:CYS:H	20	0.15
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB2	2	0.15
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB2	2	0.15
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB3	2	0.15
(4,65)	1:21:A:CYS:HB2	1:24:A:LYS:H	7	0.15
(4,37)	1:42:A:THR:H	1:54:A:GLY:H	2	0.15
(4,37)	1:42:A:THR:H	1:54:A:GLY:H	14	0.15
(4,14)	1:18:A:PRO:HD3	1:19:A:CYS:H	16	0.15
(4,14)	1:18:A:PRO:HD2	1:19:A:CYS:H	16	0.15
(4,2)	1:14:A:CYS:HB3	1:16:A:SER:H	10	0.15
(1,989)	1:23:A:SER:HB2	1:24:A:LYS:HG2	11	0.15
(1,989)	1:23:A:SER:HB2	1:24:A:LYS:HG3	11	0.15
(1,989)	1:23:A:SER:HB3	1:24:A:LYS:HG2	11	0.15
(1,989)	1:23:A:SER:HB3	1:24:A:LYS:HG3	11	0.15
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	4	0.15
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	11	0.15
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	18	0.15
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,877)	1:25:A:CYS:HB3	1:26:A:GLN:HG3	20	0.15
(1,875)	1:23:A:SER:HB2	1:24:A:LYS:HG2	11	0.15
(1,875)	1:23:A:SER:HB2	1:24:A:LYS:HG3	11	0.15
(1,875)	1:23:A:SER:HB3	1:24:A:LYS:HG2	11	0.15
(1,875)	1:23:A:SER:HB3	1:24:A:LYS:HG3	11	0.15
(1,837)	1:42:A:THR:HG21	1:54:A:GLY:HA2	12	0.15
(1,813)	1:18:A:PRO:HB2	1:19:A:CYS:HB2	10	0.15
(1,803)	1:40:A:ASN:H	1:66:A:CYS:HA	13	0.15
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	14	0.15
(1,766)	1:39:A:CYS:HB3	1:55:A:PRO:HD2	2	0.15
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	16	0.15
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	16	0.15
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	16	0.15
(1,730)	1:6:A:LYS:HD3	1:33:A:CYS:HA	17	0.15
(1,595)	1:21:A:CYS:H	1:36:A:CYS:HB2	19	0.15
(1,579)	1:41:A:CYS:H	1:46:A:CYS:HA	1	0.15
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	4	0.15
(1,460)	1:11:A:THR:HA	1:26:A:GLN:HB2	17	0.15
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	5	0.15
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE2	17	0.15
(1,312)	1:64:A:CYS:H	1:67:A:LYS:HE3	17	0.15
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	17	0.15
(1,237)	1:38:A:THR:H	1:55:A:PRO:HB3	14	0.15
(1,185)	1:42:A:THR:HG21	1:45:A:GLY:H	2	0.15
(1,185)	1:42:A:THR:HG22	1:45:A:GLY:H	2	0.15
(1,185)	1:42:A:THR:HG23	1:45:A:GLY:H	2	0.15
(1,185)	1:42:A:THR:HG21	1:45:A:GLY:H	11	0.15
(1,185)	1:42:A:THR:HG22	1:45:A:GLY:H	11	0.15
(1,185)	1:42:A:THR:HG23	1:45:A:GLY:H	11	0.15
(1,179)	1:19:A:CYS:H	1:21:A:CYS:H	16	0.15
(1,58)	1:21:A:CYS:HB2	1:24:A:LYS:H	7	0.15
(1,35)	1:42:A:THR:H	1:54:A:GLY:H	2	0.15
(1,35)	1:42:A:THR:H	1:54:A:GLY:H	14	0.15
(1,2)	1:14:A:CYS:HB3	1:16:A:SER:H	10	0.15
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD2	8	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD3	8	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD2	8	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD3	8	0.14
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	2	0.14
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	12	0.14
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	4	0.14
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG2	4	0.14
(4,1170)	1:50:A:LYS:HA	1:51:A:GLU:HG3	4	0.14
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	2	0.14
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	3	0.14
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	7	0.14
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	7	0.14
(4,1114)	1:22:A:GLY:HA3	1:25:A:CYS:HB2	7	0.14
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB2	7	0.14
(4,1114)	1:22:A:GLY:HA2	1:25:A:CYS:HB3	7	0.14
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB3	2	0.14
(4,1108)	1:37:A:LYS:H	1:55:A:PRO:HB2	2	0.14
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	10	0.14
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	10	0.14
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	14	0.14
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	14	0.14
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	14	0.14
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	9	0.14
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA3	3	0.14
(4,868)	1:29:A:GLU:HG3	1:30:A:GLY:HA2	3	0.14
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA2	3	0.14
(4,868)	1:29:A:GLU:HG2	1:30:A:GLY:HA3	3	0.14
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	5	0.14
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	5	0.14
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	5	0.14
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	6	0.14
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	6	0.14
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	6	0.14
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	16	0.14
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	16	0.14
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	16	0.14
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	1	0.14
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	0.14
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	7	0.14
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	7	0.14
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	7	0.14
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	13	0.14
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	13	0.14
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	15	0.14
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	15	0.14
(4,709)	1:14:A:CYS:H	1:15:A:ARG:HG2	1	0.14
(4,686)	1:21:A:CYS:H	1:36:A:CYS:HB2	7	0.14
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	12	0.14
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG2	12	0.14
(4,569)	1:41:A:CYS:HB3	1:47:A:LYS:HG3	12	0.14
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	14	0.14
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	14	0.14
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	14	0.14
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	14	0.14
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	3	0.14
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	12	0.14
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	15	0.14
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG2	15	0.14
(4,390)	1:15:A:ARG:HA	1:15:A:ARG:HG3	15	0.14
(4,367)	1:42:A:THR:H	1:53:A:THR:HA	1	0.14
(4,311)	1:55:A:PRO:HA	1:58:A:CYS:H	2	0.14
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	7	0.14
(4,173)	1:31:A:CYS:H	1:32:A:THR:HB	4	0.14
(4,153)	1:28:A:GLY:H	1:31:A:CYS:HA	19	0.14
(4,150)	1:41:A:CYS:H	1:66:A:CYS:HA	5	0.14
(4,144)	1:41:A:CYS:H	1:54:A:GLY:HA2	13	0.14
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	1	0.14
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	1	0.14
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	1	0.14
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	1	0.14
(4,128)	1:11:A:THR:H	1:28:A:GLY:H	4	0.14
(4,128)	1:11:A:THR:H	1:28:A:GLY:H	17	0.14
(4,116)	1:22:A:GLY:H	1:36:A:CYS:HB3	5	0.14
(4,80)	1:46:A:CYS:H	1:51:A:GLU:HA	2	0.14
(4,37)	1:42:A:THR:H	1:54:A:GLY:H	18	0.14
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	2	0.14
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	12	0.14
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	2	0.14
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	3	0.14
(1,922)	1:37:A:LYS:H	1:55:A:PRO:HB3	2	0.14
(1,837)	1:42:A:THR:HG22	1:54:A:GLY:HA2	10	0.14
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	12	0.14
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	12	0.14
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	12	0.14
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	17	0.14
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	19	0.14
(1,715)	1:19:A:CYS:HB2	1:35:A:ALA:HA	5	0.14
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	1	0.14
(1,632)	1:67:A:LYS:H	1:67:A:LYS:HE2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,595)	1:21:A:CYS:H	1:36:A:CYS:HB2	7	0.14
(1,425)	1:31:A:CYS:HA	1:37:A:LYS:HD2	20	0.14
(1,418)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	14	0.14
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	3	0.14
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	12	0.14
(1,331)	1:42:A:THR:H	1:53:A:THR:HA	1	0.14
(1,287)	1:37:A:LYS:HG2	1:58:A:CYS:H	20	0.14
(1,282)	1:55:A:PRO:HA	1:58:A:CYS:H	2	0.14
(1,161)	1:31:A:CYS:H	1:32:A:THR:HB	4	0.14
(1,143)	1:28:A:GLY:H	1:31:A:CYS:HA	19	0.14
(1,140)	1:41:A:CYS:H	1:66:A:CYS:HA	5	0.14
(1,134)	1:41:A:CYS:H	1:54:A:GLY:HA2	13	0.14
(1,117)	1:11:A:THR:H	1:28:A:GLY:H	4	0.14
(1,117)	1:11:A:THR:H	1:28:A:GLY:H	17	0.14
(1,106)	1:22:A:GLY:H	1:36:A:CYS:HB3	5	0.14
(1,35)	1:42:A:THR:H	1:54:A:GLY:H	18	0.14
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	0.13
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	0.13
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD2	20	0.13
(4,1211)	1:47:A:LYS:HA	1:47:A:LYS:HD3	20	0.13
(4,1196)	1:6:A:LYS:HA	1:7:A:GLY:H	13	0.13
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	3	0.13
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	20	0.13
(4,1172)	1:38:A:THR:HG21	1:67:A:LYS:HA	8	0.13
(4,1172)	1:38:A:THR:HG22	1:67:A:LYS:HA	8	0.13
(4,1172)	1:38:A:THR:HG23	1:67:A:LYS:HA	8	0.13
(4,1143)	1:6:A:LYS:HG2	1:33:A:CYS:HB2	17	0.13
(4,1129)	1:52:A:CYS:HB2	1:60:A:CYS:H	8	0.13
(4,1096)	1:21:A:CYS:HB3	1:25:A:CYS:H	17	0.13
(4,1096)	1:21:A:CYS:HB3	1:25:A:CYS:H	19	0.13
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	20	0.13
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG3	20	0.13
(4,1023)	1:23:A:SER:HA	1:24:A:LYS:HG2	20	0.13
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	11	0.13
(4,973)	1:42:A:THR:HG21	1:54:A:GLY:HA3	11	0.13
(4,973)	1:42:A:THR:HG22	1:54:A:GLY:HA3	11	0.13
(4,973)	1:42:A:THR:HG23	1:54:A:GLY:HA3	11	0.13
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	6	0.13
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	6	0.13
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	6	0.13
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	6	0.13
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,958)	1:7:A:GLY:HA2	1:8:A:GLU:HB3	6	0.13
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB2	6	0.13
(4,958)	1:7:A:GLY:HA3	1:8:A:GLU:HB3	6	0.13
(4,866)	1:7:A:GLY:HA2	1:10:A:CYS:HB2	5	0.13
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	9	0.13
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	9	0.13
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	9	0.13
(4,787)	1:14:A:CYS:HA	1:20:A:GLN:HB2	15	0.13
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	5	0.13
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD2	5	0.13
(4,782)	1:9:A:LYS:HA	1:9:A:LYS:HD3	5	0.13
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	6	0.13
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	16	0.13
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	2	0.13
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	2	0.13
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE2	2	0.13
(4,772)	1:6:A:LYS:HA	1:6:A:LYS:HE3	2	0.13
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG2	11	0.13
(4,766)	1:25:A:CYS:HA	1:26:A:GLN:HG3	11	0.13
(4,686)	1:21:A:CYS:H	1:36:A:CYS:HB2	4	0.13
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	6	0.13
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB2	6	0.13
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	6	0.13
(4,675)	1:52:A:CYS:HA	1:57:A:SER:HB3	6	0.13
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	18	0.13
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	6	0.13
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	6	0.13
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	6	0.13
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	6	0.13
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	6	0.13
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	6	0.13
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	12	0.13
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	12	0.13
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	12	0.13
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	12	0.13
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	12	0.13
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	12	0.13
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	13	0.13
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	13	0.13
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	13	0.13
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	13	0.13
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB2	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	13	0.13
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	13	0.13
(4,603)	1:56:A:ASP:HB3	1:57:A:SER:HB3	13	0.13
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB2	13	0.13
(4,603)	1:56:A:ASP:HB2	1:57:A:SER:HB3	13	0.13
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	18	0.13
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	18	0.13
(4,566)	1:67:A:LYS:H	1:67:A:LYS:HD2	7	0.13
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	11	0.13
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	18	0.13
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	4	0.13
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	11	0.13
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	20	0.13
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	12	0.13
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	12	0.13
(4,466)	1:8:A:GLU:HG2	1:9:A:LYS:HG2	12	0.13
(4,466)	1:8:A:GLU:HG3	1:9:A:LYS:HG2	12	0.13
(4,279)	1:39:A:CYS:HA	1:40:A:ASN:HD22	16	0.13
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	5	0.13
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	5	0.13
(4,256)	1:37:A:LYS:HE2	1:38:A:THR:H	5	0.13
(4,256)	1:37:A:LYS:HE3	1:38:A:THR:H	5	0.13
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	16	0.13
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	16	0.13
(4,225)	1:9:A:LYS:H	1:10:A:CYS:H	12	0.13
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	2	0.13
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	2	0.13
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE2	2	0.13
(4,140)	1:67:A:LYS:H	1:67:A:LYS:HE3	2	0.13
(4,128)	1:11:A:THR:H	1:28:A:GLY:H	18	0.13
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	6	0.13
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	6	0.13
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	6	0.13
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	9	0.13
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG2	9	0.13
(4,94)	1:14:A:CYS:H	1:15:A:ARG:HG3	9	0.13
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB2	13	0.13
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB2	13	0.13
(4,75)	1:57:A:SER:H	1:58:A:CYS:HB3	13	0.13
(1,980)	1:6:A:LYS:HA	1:7:A:GLY:H	13	0.13
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	3	0.13
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,963)	1:38:A:THR:HG21	1:67:A:LYS:HA	8	0.13
(1,963)	1:38:A:THR:HG22	1:67:A:LYS:HA	8	0.13
(1,963)	1:38:A:THR:HG23	1:67:A:LYS:HA	8	0.13
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB2	6	0.13
(1,934)	1:23:A:SER:HA	1:25:A:CYS:HB3	6	0.13
(1,932)	1:52:A:CYS:HB2	1:60:A:CYS:H	8	0.13
(1,910)	1:21:A:CYS:HB3	1:25:A:CYS:H	17	0.13
(1,910)	1:21:A:CYS:HB3	1:25:A:CYS:H	19	0.13
(1,897)	1:37:A:LYS:HD3	1:55:A:PRO:HG2	19	0.13
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG2	20	0.13
(1,873)	1:23:A:SER:HA	1:24:A:LYS:HG3	20	0.13
(1,813)	1:18:A:PRO:HB2	1:19:A:CYS:HB2	6	0.13
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	13	0.13
(1,766)	1:39:A:CYS:HB3	1:55:A:PRO:HD2	5	0.13
(1,766)	1:39:A:CYS:HB3	1:55:A:PRO:HD2	14	0.13
(1,755)	1:25:A:CYS:HA	1:26:A:GLN:HG2	5	0.13
(1,755)	1:25:A:CYS:HA	1:26:A:GLN:HG3	5	0.13
(1,715)	1:19:A:CYS:HB2	1:35:A:ALA:HA	13	0.13
(1,684)	1:14:A:CYS:HA	1:20:A:GLN:HB2	15	0.13
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	6	0.13
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	16	0.13
(1,595)	1:21:A:CYS:H	1:36:A:CYS:HB2	4	0.13
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	18	0.13
(1,499)	1:67:A:LYS:H	1:67:A:LYS:HD2	7	0.13
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	11	0.13
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	4	0.13
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	11	0.13
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	20	0.13
(1,390)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	10	0.13
(1,390)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	10	0.13
(1,333)	1:41:A:CYS:HB2	1:42:A:THR:H	4	0.13
(1,232)	1:9:A:LYS:HG2	1:29:A:GLU:H	20	0.13
(1,232)	1:9:A:LYS:HG3	1:29:A:GLU:H	20	0.13
(1,207)	1:9:A:LYS:H	1:10:A:CYS:H	12	0.13
(1,117)	1:11:A:THR:H	1:28:A:GLY:H	18	0.13
(4,1182)	1:16:A:SER:HB2	1:17:A:GLU:H	1	0.12
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	1	0.12
(4,1182)	1:16:A:SER:HB3	1:17:A:GLU:H	1	0.12
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	19	0.12
(4,1100)	1:11:A:THR:HG21	1:28:A:GLY:H	13	0.12
(4,1100)	1:11:A:THR:HG22	1:28:A:GLY:H	13	0.12
(4,1100)	1:11:A:THR:HG23	1:28:A:GLY:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE2	4	0.12
(4,1043)	1:32:A:THR:HA	1:37:A:LYS:HE3	4	0.12
(4,1032)	1:26:A:GLN:HA	1:62:A:SER:HB2	2	0.12
(4,1032)	1:26:A:GLN:HA	1:62:A:SER:HB3	2	0.12
(4,1032)	1:26:A:GLN:HA	1:62:A:SER:HB2	2	0.12
(4,1032)	1:26:A:GLN:HA	1:62:A:SER:HB3	2	0.12
(4,1003)	1:5:A:GLY:HA2	1:6:A:LYS:HB2	8	0.12
(4,1003)	1:5:A:GLY:HA3	1:6:A:LYS:HB2	8	0.12
(4,1003)	1:5:A:GLY:HA2	1:6:A:LYS:HB2	8	0.12
(4,1003)	1:5:A:GLY:HA2	1:6:A:LYS:HB3	8	0.12
(4,1003)	1:5:A:GLY:HA3	1:6:A:LYS:HB2	8	0.12
(4,1003)	1:5:A:GLY:HA3	1:6:A:LYS:HB3	8	0.12
(4,990)	1:39:A:CYS:HB2	1:54:A:GLY:HA3	15	0.12
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	12	0.12
(4,937)	1:55:A:PRO:HD3	1:58:A:CYS:HB3	16	0.12
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB2	20	0.12
(4,929)	1:29:A:GLU:HA	1:31:A:CYS:HB3	20	0.12
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	16	0.12
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG2	16	0.12
(4,878)	1:25:A:CYS:HA	1:26:A:GLN:HG3	16	0.12
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	12	0.12
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	12	0.12
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	12	0.12
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	5	0.12
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	5	0.12
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	5	0.12
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	5	0.12
(4,787)	1:14:A:CYS:HA	1:20:A:GLN:HB2	20	0.12
(4,775)	1:9:A:LYS:HA	1:28:A:GLY:HA3	20	0.12
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB3	10	0.12
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB2	10	0.12
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB3	10	0.12
(4,769)	1:31:A:CYS:HA	1:33:A:CYS:HB2	10	0.12
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	2	0.12
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	2	0.12
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	2	0.12
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	2	0.12
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	11	0.12
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	11	0.12
(4,724)	1:60:A:CYS:H	1:67:A:LYS:HE3	1	0.12
(4,724)	1:60:A:CYS:H	1:67:A:LYS:HE2	1	0.12
(4,709)	1:14:A:CYS:H	1:15:A:ARG:HG2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	14	0.12
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	14	0.12
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	14	0.12
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	14	0.12
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	14	0.12
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	14	0.12
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	19	0.12
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	19	0.12
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	19	0.12
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	19	0.12
(4,567)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	13	0.12
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	2	0.12
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	12	0.12
(4,475)	1:9:A:LYS:HB2	1:31:A:CYS:HA	2	0.12
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	10	0.12
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	19	0.12
(4,451)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	3	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	16	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	16	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	16	0.12
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	16	0.12
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG2	13	0.12
(4,420)	1:39:A:CYS:HB2	1:55:A:PRO:HG3	13	0.12
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG3	13	0.12
(4,420)	1:39:A:CYS:HB3	1:55:A:PRO:HG2	13	0.12
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	6	0.12
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG2	13	0.12
(4,320)	1:58:A:CYS:H	1:59:A:LYS:HG3	13	0.12
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	18	0.12
(4,305)	1:61:A:GLY:HA2	1:62:A:SER:H	18	0.12
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	18	0.12
(4,305)	1:61:A:GLY:HA3	1:62:A:SER:H	18	0.12
(4,279)	1:39:A:CYS:HA	1:40:A:ASN:HD22	14	0.12
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	1	0.12
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	1	0.12
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	14	0.12
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	14	0.12
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	14	0.12
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	14	0.12
(4,219)	1:7:A:GLY:HA3	1:10:A:CYS:H	9	0.12
(4,202)	1:42:A:THR:HG21	1:45:A:GLY:H	6	0.12
(4,202)	1:42:A:THR:HG22	1:45:A:GLY:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,202)	1:42:A:THR:HG23	1:45:A:GLY:H	6	0.12
(4,173)	1:31:A:CYS:H	1:32:A:THR:HB	15	0.12
(4,160)	1:10:A:CYS:H	1:28:A:GLY:H	10	0.12
(4,150)	1:41:A:CYS:H	1:66:A:CYS:HA	3	0.12
(4,144)	1:41:A:CYS:H	1:54:A:GLY:HA2	19	0.12
(4,121)	1:11:A:THR:H	1:12:A:SER:HA	5	0.12
(4,56)	1:61:A:GLY:H	1:64:A:CYS:HB3	1	0.12
(4,37)	1:42:A:THR:H	1:54:A:GLY:H	5	0.12
(4,37)	1:42:A:THR:H	1:54:A:GLY:H	17	0.12
(4,17)	1:19:A:CYS:H	1:35:A:ALA:HB1	13	0.12
(4,17)	1:19:A:CYS:H	1:35:A:ALA:HB2	13	0.12
(4,17)	1:19:A:CYS:H	1:35:A:ALA:HB3	13	0.12
(1,971)	1:16:A:SER:HB2	1:17:A:GLU:H	1	0.12
(1,971)	1:16:A:SER:HB3	1:17:A:GLU:H	1	0.12
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	19	0.12
(1,928)	1:31:A:CYS:H	1:37:A:LYS:HD3	3	0.12
(1,914)	1:11:A:THR:HG21	1:28:A:GLY:H	13	0.12
(1,914)	1:11:A:THR:HG22	1:28:A:GLY:H	13	0.12
(1,914)	1:11:A:THR:HG23	1:28:A:GLY:H	13	0.12
(1,886)	1:33:A:CYS:H	1:37:A:LYS:HG3	9	0.12
(1,879)	1:26:A:GLN:HA	1:62:A:SER:HB2	2	0.12
(1,879)	1:26:A:GLN:HA	1:62:A:SER:HB3	2	0.12
(1,824)	1:7:A:GLY:HA2	1:9:A:LYS:HB2	10	0.12
(1,824)	1:7:A:GLY:HA3	1:9:A:LYS:HB2	10	0.12
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	8	0.12
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	9	0.12
(1,771)	1:41:A:CYS:HB2	1:53:A:THR:HB	18	0.12
(1,766)	1:39:A:CYS:HB3	1:55:A:PRO:HD2	6	0.12
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	12	0.12
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	12	0.12
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	12	0.12
(1,684)	1:14:A:CYS:HA	1:20:A:GLN:HB2	20	0.12
(1,675)	1:9:A:LYS:HA	1:28:A:GLY:HA3	20	0.12
(1,671)	1:33:A:CYS:HB2	1:36:A:CYS:H	11	0.12
(1,671)	1:33:A:CYS:HB3	1:36:A:CYS:H	11	0.12
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG21	14	0.12
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG22	14	0.12
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG23	14	0.12
(1,500)	1:9:A:LYS:HB2	1:27:A:CYS:HB3	13	0.12
(1,497)	1:39:A:CYS:HB2	1:67:A:LYS:HD2	19	0.12
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	2	0.12
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	10	0.12
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	19	0.12
(1,333)	1:41:A:CYS:HB2	1:42:A:THR:H	10	0.12
(1,185)	1:42:A:THR:HG21	1:45:A:GLY:H	6	0.12
(1,185)	1:42:A:THR:HG22	1:45:A:GLY:H	6	0.12
(1,185)	1:42:A:THR:HG23	1:45:A:GLY:H	6	0.12
(1,161)	1:31:A:CYS:H	1:32:A:THR:HB	15	0.12
(1,149)	1:10:A:CYS:H	1:28:A:GLY:H	10	0.12
(1,140)	1:41:A:CYS:H	1:66:A:CYS:HA	3	0.12
(1,134)	1:41:A:CYS:H	1:54:A:GLY:HA2	19	0.12
(1,110)	1:11:A:THR:H	1:12:A:SER:HA	5	0.12
(1,50)	1:61:A:GLY:H	1:64:A:CYS:HB3	1	0.12
(1,35)	1:42:A:THR:H	1:54:A:GLY:H	5	0.12
(1,35)	1:42:A:THR:H	1:54:A:GLY:H	17	0.12
(1,15)	1:19:A:CYS:H	1:35:A:ALA:HB1	13	0.12
(1,15)	1:19:A:CYS:H	1:35:A:ALA:HB2	13	0.12
(1,15)	1:19:A:CYS:H	1:35:A:ALA:HB3	13	0.12
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	6	0.11
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	8	0.11
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	16	0.11
(4,1168)	1:33:A:CYS:H	1:37:A:LYS:HB3	13	0.11
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	15	0.11
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	15	0.11
(4,1157)	1:62:A:SER:HB2	1:67:A:LYS:HD2	15	0.11
(4,1157)	1:62:A:SER:HB3	1:67:A:LYS:HD2	15	0.11
(4,982)	1:47:A:LYS:HB2	1:48:A:CYS:HB2	20	0.11
(4,969)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	10	0.11
(4,969)	1:14:A:CYS:HB3	1:15:A:ARG:HB2	10	0.11
(4,969)	1:14:A:CYS:HB3	1:15:A:ARG:HB3	10	0.11
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	2	0.11
(4,953)	1:16:A:SER:HB2	1:20:A:GLN:HB2	1	0.11
(4,953)	1:16:A:SER:HB3	1:20:A:GLN:HB2	1	0.11
(4,953)	1:16:A:SER:HB2	1:20:A:GLN:HB2	1	0.11
(4,953)	1:16:A:SER:HB3	1:20:A:GLN:HB2	1	0.11
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	2	0.11
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	2	0.11
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	2	0.11
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	8	0.11
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	8	0.11
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	8	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	3	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	3	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	3	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	7	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	7	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA2	7	0.11
(4,840)	1:21:A:CYS:HB2	1:22:A:GLY:HA3	7	0.11
(4,836)	1:46:A:CYS:HB3	1:53:A:THR:HG21	3	0.11
(4,836)	1:46:A:CYS:HB3	1:53:A:THR:HG22	3	0.11
(4,836)	1:46:A:CYS:HB3	1:53:A:THR:HG23	3	0.11
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	1	0.11
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	2	0.11
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	8	0.11
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	19	0.11
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	0.11
(4,764)	1:56:A:ASP:HB2	1:57:A:SER:HA	10	0.11
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	10	0.11
(4,764)	1:56:A:ASP:HB3	1:57:A:SER:HA	10	0.11
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	5	0.11
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	5	0.11
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE3	10	0.11
(4,725)	1:67:A:LYS:H	1:67:A:LYS:HE2	10	0.11
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	7	0.11
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE2	7	0.11
(4,722)	1:62:A:SER:HA	1:67:A:LYS:HE3	7	0.11
(4,686)	1:21:A:CYS:H	1:36:A:CYS:HB2	1	0.11
(4,663)	1:46:A:CYS:HA	1:53:A:THR:HA	7	0.11
(4,580)	1:16:A:SER:H	1:16:A:SER:HB3	16	0.11
(4,580)	1:16:A:SER:H	1:16:A:SER:HB2	16	0.11
(4,579)	1:16:A:SER:HB3	1:20:A:GLN:H	8	0.11
(4,579)	1:16:A:SER:HB2	1:20:A:GLN:H	8	0.11
(4,578)	1:16:A:SER:HB3	1:20:A:GLN:HB2	10	0.11
(4,578)	1:16:A:SER:HB2	1:20:A:GLN:HB2	10	0.11
(4,528)	1:16:A:SER:HA	1:20:A:GLN:HG3	7	0.11
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	1	0.11
(4,522)	1:11:A:THR:HA	1:26:A:GLN:HB3	15	0.11
(4,498)	1:23:A:SER:HA	1:24:A:LYS:HB2	13	0.11
(4,497)	1:63:A:SER:HA	1:64:A:CYS:HB2	20	0.11
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	12	0.11
(4,470)	1:25:A:CYS:HA	1:26:A:GLN:HB3	14	0.11
(4,451)	1:9:A:LYS:HD2	1:28:A:GLY:HA2	11	0.11
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	17	0.11
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB2	17	0.11
(4,441)	1:42:A:THR:HB	1:43:A:SER:HB3	17	0.11
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA3	12	0.11
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA2	12	0.11
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA3	12	0.11
(4,396)	1:29:A:GLU:H	1:61:A:GLY:HA2	12	0.11
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	5	0.11
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG2	5	0.11
(4,375)	1:47:A:LYS:H	1:47:A:LYS:HG3	5	0.11
(4,328)	1:47:A:LYS:HB2	1:49:A:GLY:H	14	0.11
(4,311)	1:55:A:PRO:HA	1:58:A:CYS:H	3	0.11
(4,311)	1:55:A:PRO:HA	1:58:A:CYS:H	6	0.11
(4,286)	1:9:A:LYS:H	1:10:A:CYS:HB2	12	0.11
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	7	0.11
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	7	0.11
(4,236)	1:33:A:CYS:HB2	1:37:A:LYS:H	20	0.11
(4,236)	1:33:A:CYS:HB3	1:37:A:LYS:H	20	0.11
(4,228)	1:33:A:CYS:HB2	1:36:A:CYS:H	3	0.11
(4,228)	1:33:A:CYS:HB3	1:36:A:CYS:H	3	0.11
(4,195)	1:21:A:CYS:H	1:24:A:LYS:H	4	0.11
(4,173)	1:31:A:CYS:H	1:32:A:THR:HB	9	0.11
(4,150)	1:41:A:CYS:H	1:66:A:CYS:HA	2	0.11
(4,144)	1:41:A:CYS:H	1:54:A:GLY:HA2	5	0.11
(4,128)	1:11:A:THR:H	1:28:A:GLY:H	15	0.11
(4,121)	1:11:A:THR:H	1:12:A:SER:HA	7	0.11
(4,73)	1:55:A:PRO:HA	1:57:A:SER:H	5	0.11
(4,26)	1:21:A:CYS:HA	1:25:A:CYS:H	19	0.11
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	6	0.11
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	8	0.11
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	16	0.11
(1,959)	1:33:A:CYS:H	1:37:A:LYS:HB3	13	0.11
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD2	12	0.11
(1,951)	1:33:A:CYS:HB3	1:37:A:LYS:HD3	12	0.11
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG2	9	0.11
(1,948)	1:9:A:LYS:HE2	1:29:A:GLU:HG3	9	0.11
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG2	9	0.11
(1,948)	1:9:A:LYS:HE3	1:29:A:GLU:HG3	9	0.11
(1,889)	1:35:A:ALA:H	1:37:A:LYS:HB3	8	0.11
(1,814)	1:18:A:PRO:HB2	1:19:A:CYS:HB3	17	0.11
(1,766)	1:39:A:CYS:HB3	1:55:A:PRO:HD2	18	0.11
(1,730)	1:6:A:LYS:HD3	1:33:A:CYS:HA	1	0.11
(1,721)	1:46:A:CYS:HB3	1:53:A:THR:HG21	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:46:A:CYS:HB3	1:53:A:THR:HG22	3	0.11
(1,721)	1:46:A:CYS:HB3	1:53:A:THR:HG23	3	0.11
(1,681)	1:9:A:LYS:HA	1:9:A:LYS:HG2	9	0.11
(1,681)	1:9:A:LYS:HA	1:9:A:LYS:HG3	9	0.11
(1,595)	1:21:A:CYS:H	1:36:A:CYS:HB2	1	0.11
(1,572)	1:46:A:CYS:HA	1:53:A:THR:HA	7	0.11
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG21	19	0.11
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG22	19	0.11
(1,539)	1:31:A:CYS:HB3	1:32:A:THR:HG23	19	0.11
(1,515)	1:67:A:LYS:HG2	1:67:A:LYS:HE2	16	0.11
(1,515)	1:67:A:LYS:HG2	1:67:A:LYS:HE3	16	0.11
(1,464)	1:16:A:SER:HA	1:20:A:GLN:HG3	7	0.11
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	1	0.11
(1,458)	1:11:A:THR:HA	1:26:A:GLN:HB3	15	0.11
(1,439)	1:63:A:SER:HA	1:64:A:CYS:HB2	20	0.11
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	12	0.11
(1,421)	1:25:A:CYS:HA	1:26:A:GLN:HB3	14	0.11
(1,390)	1:10:A:CYS:HB3	1:15:A:ARG:HG2	14	0.11
(1,390)	1:10:A:CYS:HB3	1:15:A:ARG:HG3	14	0.11
(1,310)	1:64:A:CYS:H	1:64:A:CYS:HB2	1	0.11
(1,282)	1:55:A:PRO:HA	1:58:A:CYS:H	3	0.11
(1,282)	1:55:A:PRO:HA	1:58:A:CYS:H	6	0.11
(1,260)	1:9:A:LYS:H	1:10:A:CYS:HB2	12	0.11
(1,205)	1:9:A:LYS:HG3	1:10:A:CYS:H	10	0.11
(1,161)	1:31:A:CYS:H	1:32:A:THR:HB	9	0.11
(1,140)	1:41:A:CYS:H	1:66:A:CYS:HA	2	0.11
(1,134)	1:41:A:CYS:H	1:54:A:GLY:HA2	5	0.11
(1,117)	1:11:A:THR:H	1:28:A:GLY:H	15	0.11
(1,114)	1:11:A:THR:H	1:15:A:ARG:HG2	6	0.11
(1,110)	1:11:A:THR:H	1:12:A:SER:HA	7	0.11
(1,64)	1:55:A:PRO:HA	1:57:A:SER:H	5	0.11
(1,24)	1:21:A:CYS:HA	1:25:A:CYS:H	19	0.11
(4,1173)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	17	0.1
(4,1172)	1:38:A:THR:HG21	1:67:A:LYS:HA	13	0.1
(4,1172)	1:38:A:THR:HG22	1:67:A:LYS:HA	13	0.1
(4,1172)	1:38:A:THR:HG23	1:67:A:LYS:HA	13	0.1
(4,1160)	1:14:A:CYS:HA	1:21:A:CYS:HA	19	0.1
(4,955)	1:7:A:GLY:HA3	1:10:A:CYS:HB2	19	0.1
(4,903)	1:38:A:THR:HB	1:55:A:PRO:HG3	7	0.1
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG21	6	0.1
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG22	6	0.1
(4,860)	1:9:A:LYS:HB3	1:11:A:THR:HG23	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	3	0.1
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	3	0.1
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	3	0.1
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	4	0.1
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	4	0.1
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	4	0.1
(4,854)	1:11:A:THR:HG21	1:12:A:SER:HA	13	0.1
(4,854)	1:11:A:THR:HG22	1:12:A:SER:HA	13	0.1
(4,854)	1:11:A:THR:HG23	1:12:A:SER:HA	13	0.1
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	19	0.1
(4,812)	1:46:A:CYS:HB2	1:51:A:GLU:HB3	19	0.1
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	5	0.1
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	6	0.1
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	11	0.1
(4,779)	1:24:A:LYS:HA	1:24:A:LYS:HB3	16	0.1
(4,632)	1:55:A:PRO:HG2	1:56:A:ASP:HA	15	0.1
(4,624)	1:28:A:GLY:HA3	1:31:A:CYS:HB2	8	0.1
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG21	5	0.1
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG22	5	0.1
(4,621)	1:31:A:CYS:HB2	1:32:A:THR:HG23	5	0.1
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG21	5	0.1
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG22	5	0.1
(4,621)	1:31:A:CYS:HB3	1:32:A:THR:HG23	5	0.1
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	7	0.1
(4,581)	1:16:A:SER:HB2	1:20:A:GLN:HE22	7	0.1
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE22	7	0.1
(4,581)	1:16:A:SER:HB3	1:20:A:GLN:HE21	7	0.1
(4,578)	1:16:A:SER:HB3	1:20:A:GLN:HB2	7	0.1
(4,578)	1:16:A:SER:HB2	1:20:A:GLN:HB2	7	0.1
(4,528)	1:16:A:SER:HA	1:20:A:GLN:HG3	13	0.1
(4,417)	1:8:A:GLU:HA	1:9:A:LYS:HB2	2	0.1
(4,150)	1:41:A:CYS:H	1:66:A:CYS:HA	6	0.1
(4,128)	1:11:A:THR:H	1:28:A:GLY:H	6	0.1
(4,56)	1:61:A:GLY:H	1:64:A:CYS:HB3	16	0.1
(1,964)	1:48:A:CYS:HB2	1:66:A:CYS:HB2	17	0.1
(1,963)	1:38:A:THR:HG21	1:67:A:LYS:HA	13	0.1
(1,963)	1:38:A:THR:HG22	1:67:A:LYS:HA	13	0.1
(1,963)	1:38:A:THR:HG23	1:67:A:LYS:HA	13	0.1
(1,952)	1:14:A:CYS:HA	1:21:A:CYS:HA	19	0.1
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG21	6	0.1
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG22	6	0.1
(1,740)	1:9:A:LYS:HB3	1:11:A:THR:HG23	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,703)	1:46:A:CYS:HB2	1:51:A:GLU:HB2	19	0.1
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG21	5	0.1
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG22	5	0.1
(1,539)	1:31:A:CYS:HB2	1:32:A:THR:HG23	5	0.1
(1,464)	1:16:A:SER:HA	1:20:A:GLN:HG3	13	0.1
(1,374)	1:8:A:GLU:HA	1:9:A:LYS:HB2	2	0.1
(1,140)	1:41:A:CYS:H	1:66:A:CYS:HA	6	0.1
(1,117)	1:11:A:THR:H	1:28:A:GLY:H	6	0.1
(1,50)	1:61:A:GLY:H	1:64:A:CYS:HB3	16	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found