



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 7C36 / pdb_00007c36
BMRB ID : 36354
Title : c-Myc DNA binding protein structure
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Deposited on : 2020-05-11

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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

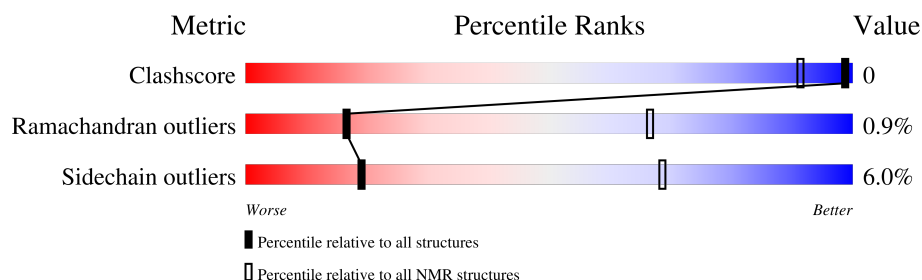
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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	167	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:3-A:10, A:17-A:78 (70)	0.58	4
2	A:84-A:116, A:122-A:167 (79)	0.64	2

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2542 atoms, of which 1279 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA-binding motif, single-stranded-interacting protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2542	794	1279	216	244	9	

There are 5 discrepancies between the modelled and reference sequences:

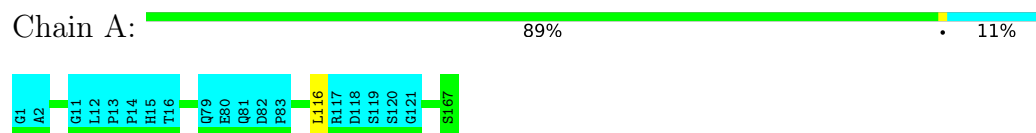
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P29558
A	2	ALA	-	expression tag	UNP P29558
A	3	MET	-	expression tag	UNP P29558
A	4	GLY	-	expression tag	UNP P29558
A	167	SER	-	expression tag	UNP P29558

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: RNA-binding motif, single-stranded-interacting protein 1

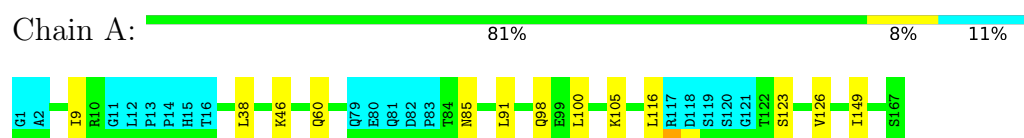


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

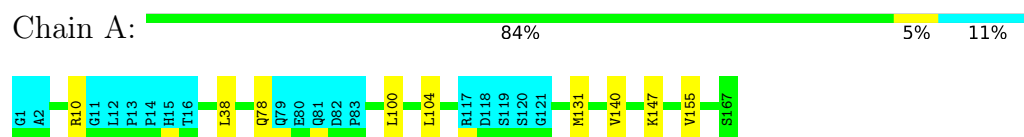
4.2.1 Score per residue for model 1

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



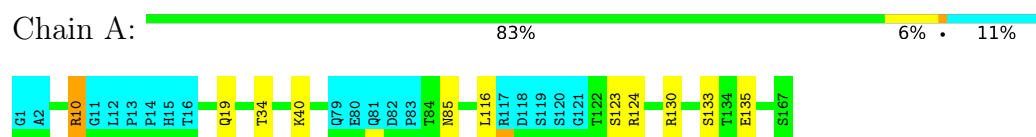
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



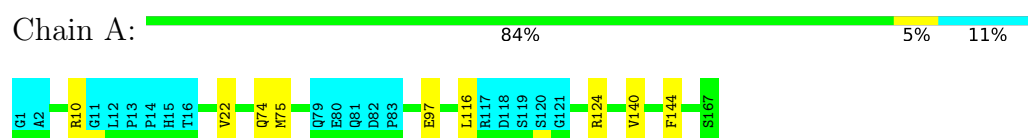
4.2.3 Score per residue for model 3

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



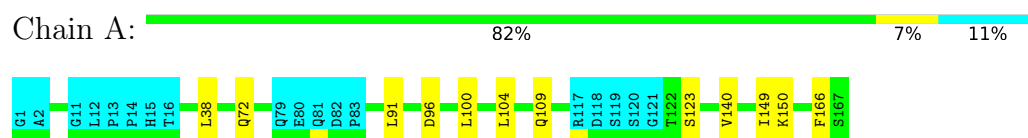
4.2.4 Score per residue for model 4

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



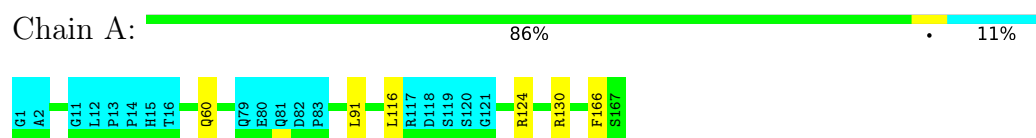
4.2.5 Score per residue for model 5

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



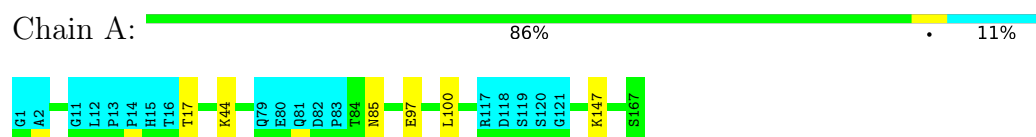
4.2.6 Score per residue for model 6

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



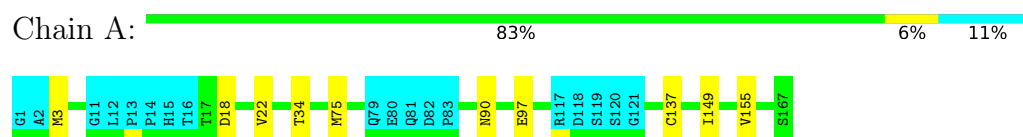
4.2.7 Score per residue for model 7

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



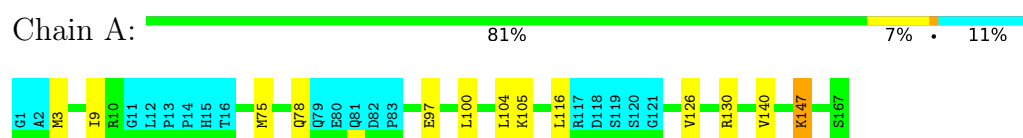
4.2.8 Score per residue for model 8

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



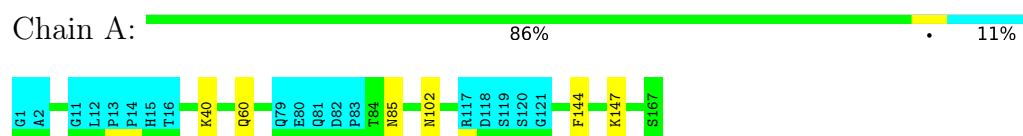
4.2.9 Score per residue for model 9

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



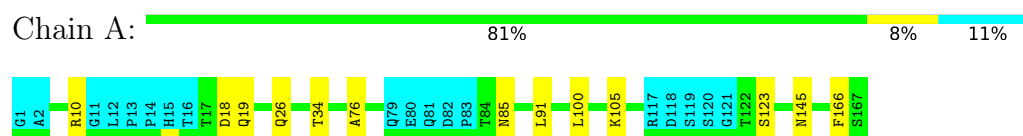
4.2.10 Score per residue for model 10

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



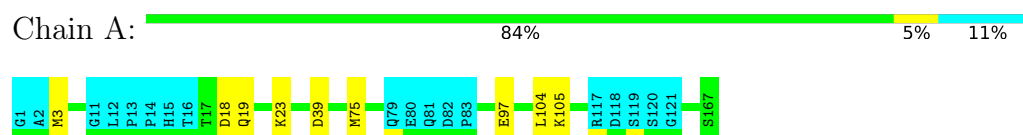
4.2.11 Score per residue for model 11

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



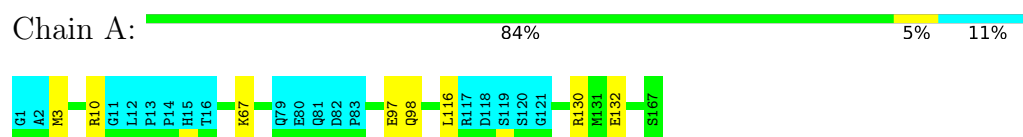
4.2.12 Score per residue for model 12

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



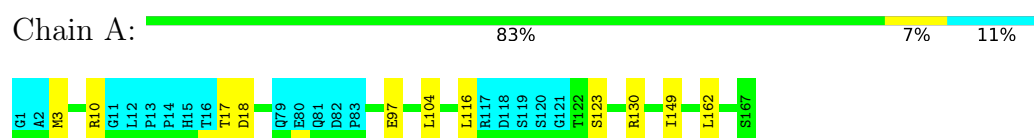
4.2.13 Score per residue for model 13

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



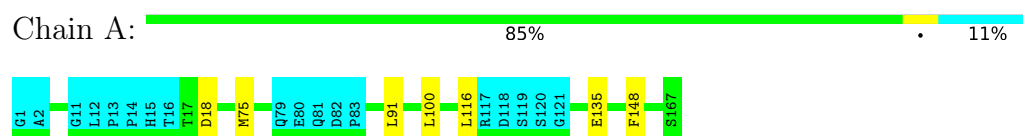
4.2.14 Score per residue for model 14

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



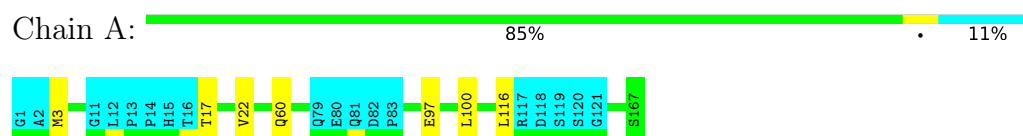
4.2.15 Score per residue for model 15

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



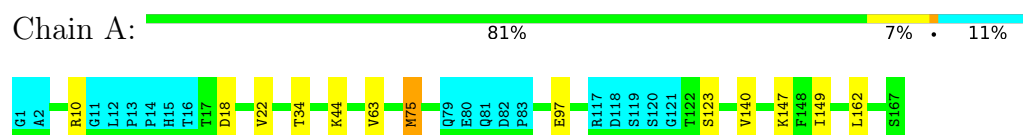
4.2.16 Score per residue for model 16

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



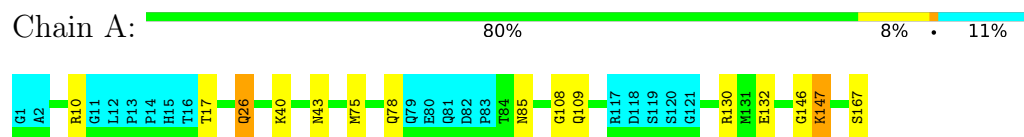
4.2.17 Score per residue for model 17

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



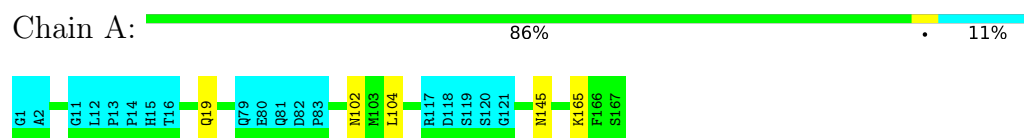
4.2.18 Score per residue for model 18

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



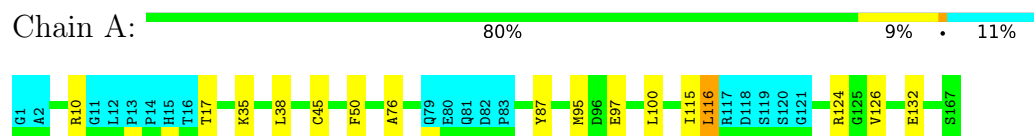
4.2.19 Score per residue for model 19

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



4.2.20 Score per residue for model 20

- Molecule 1: RNA-binding motif, single-stranded-interacting protein 1



5 Refinement protocol and experimental data overview

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

Of the 10000 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
CYANA	structure calculation	3.98.13
Amber	refinement	18

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	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.74±0.01	0±0/1153 (0.0± 0.0%)	1.29±0.03	0±1/1554 (0.0± 0.0%)
All	All	0.74	0/23060 (0.0%)	1.29	9/31080 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.4±0.8
All	All	0	8

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	GLN	OE1-CD-NE2	-5.91	116.69	122.60	4	1
1	A	85	ASN	CA-CB-CG	5.51	118.11	112.60	18	3
1	A	72	GLN	OE1-CD-NE2	-5.46	117.14	122.60	5	1
1	A	144	PHE	CA-CB-CG	5.19	118.99	113.80	10	1
1	A	26	GLN	OE1-CD-NE2	-5.11	117.49	122.60	18	1
1	A	126	VAL	CA-C-N	5.03	127.56	120.57	20	1
1	A	126	VAL	C-N-CA	5.03	127.56	120.57	20	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	147	LYS	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	10	ARG	Sidechain	1
1	A	116	LEU	Peptide	1
1	A	124	ARG	Sidechain	1
1	A	144	PHE	Sidechain	1
1	A	87	TYR	Sidechain	1
1	A	115	ILE	Peptide	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1134	1164	1164	0±1
All	All	22680	23280	23280	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:VAL:HG21	1:A:75:MET:SD	0.47	2.49	17	1
1:A:104:LEU:HD21	1:A:140:VAL:HG21	0.45	1.88	5	2
1:A:35:LYS:HE2	1:A:50:PHE:CE2	0.43	2.48	20	1
1:A:104:LEU:HD21	1:A:140:VAL:CG2	0.41	2.45	5	1
1:A:104:LEU:HD22	1:A:131:MET:SD	0.41	2.55	2	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/167 (89%)	138±3 (93±2%)	9±2 (6±1%)	1±1 (1±1%)	16	66
All	All	2960/3340 (89%)	2750 (93%)	182 (6%)	28 (1%)	16	66

All 15 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	3	MET	4
1	A	149	ILE	3
1	A	18	ASP	3
1	A	147	LYS	2
1	A	22	VAL	2
1	A	109	GLN	2
1	A	116	LEU	2
1	A	76	ALA	2
1	A	162	LEU	2
1	A	40	LYS	1
1	A	90	ASN	1
1	A	98	GLN	1
1	A	108	GLY	1
1	A	146	GLY	1
1	A	124	ARG	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	126/140 (90%)	118±2 (94±2%)	8±2 (6±2%)	19	68
All	All	2520/2800 (90%)	2368 (94%)	152 (6%)	19	68

All 50 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	97	GLU	10
1	A	100	LEU	9
1	A	10	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	116	LEU	8
1	A	75	MET	7
1	A	123	SER	6
1	A	130	ARG	6
1	A	91	LEU	5
1	A	17	THR	5
1	A	38	LEU	4
1	A	60	GLN	4
1	A	105	LYS	4
1	A	19	GLN	4
1	A	34	THR	4
1	A	147	LYS	4
1	A	104	LEU	4
1	A	85	ASN	3
1	A	78	GLN	3
1	A	140	VAL	3
1	A	166	PHE	3
1	A	18	ASP	3
1	A	132	GLU	3
1	A	9	ILE	2
1	A	126	VAL	2
1	A	155	VAL	2
1	A	135	GLU	2
1	A	124	ARG	2
1	A	44	LYS	2
1	A	22	VAL	2
1	A	149	ILE	2
1	A	3	MET	2
1	A	40	LYS	2
1	A	102	ASN	2
1	A	26	GLN	2
1	A	145	ASN	2
1	A	46	LYS	1
1	A	98	GLN	1
1	A	133	SER	1
1	A	96	ASP	1
1	A	150	LYS	1
1	A	137	CYS	1
1	A	23	LYS	1
1	A	39	ASP	1
1	A	67	LYS	1
1	A	148	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	43	ASN	1
1	A	167	SER	1
1	A	165	LYS	1
1	A	45	CYS	1
1	A	95	MET	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	154	1.03 ± 0.09	Should be applied
$^{13}\text{C}_\beta$	141	1.23 ± 0.14	Should be applied
$^{13}\text{C}'$	153	-0.01 ± 0.15	None needed (< 0.5 ppm)
^{15}N	133	0.44 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1554 atoms were assigned a chemical shift out of a possible 1982. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	683/740 (92%)	277/301 (92%)	281/298 (94%)	125/141 (89%)
Sidechain	827/1129 (73%)	558/737 (76%)	269/352 (76%)	0/40 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	44/113 (39%)	22/55 (40%)	22/57 (39%)	0/1 (0%)
Overall	1554/1982 (78%)	857/1093 (78%)	572/707 (81%)	125/182 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1661 atoms were assigned a chemical shift out of a possible 2188. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	740/827 (89%)	300/337 (89%)	307/334 (92%)	133/156 (85%)
Sidechain	877/1241 (71%)	591/808 (73%)	286/388 (74%)	0/45 (0%)
Aromatic	44/120 (37%)	22/59 (37%)	22/59 (37%)	0/2 (0%)
Overall	1661/2188 (76%)	913/1204 (76%)	615/781 (79%)	133/203 (66%)

7.1.4 Statistically unusual chemical shifts ⓘ

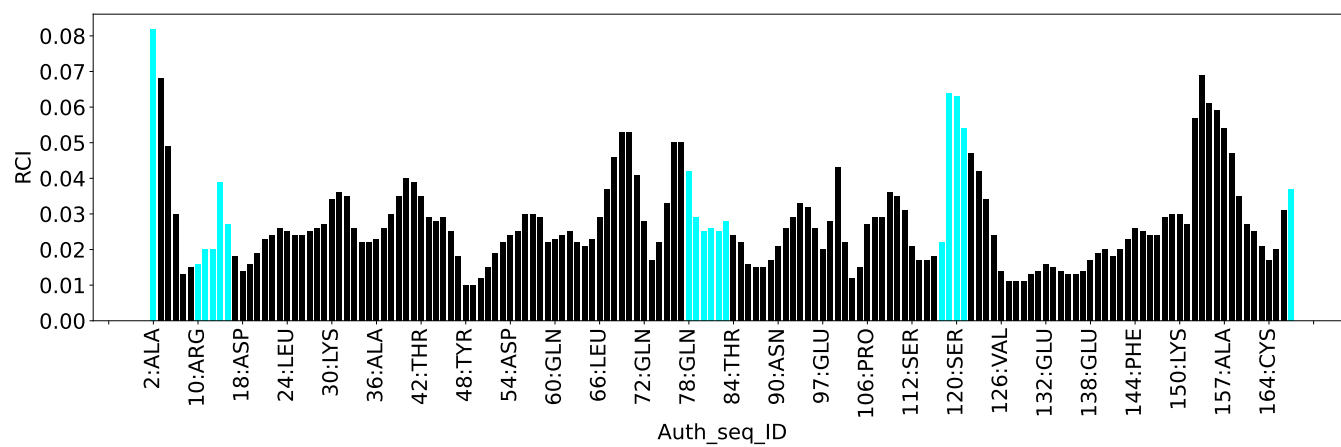
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	103	MET	CG	39.74	25.46 – 38.60	5.9
1	A	66	LEU	CG	32.34	21.37 – 32.19	5.1
1	A	89	SER	HB2	5.17	2.61 – 5.13	5.1
1	A	82	ASP	HB2	1.41	1.41 – 4.01	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2184
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	878
Medium range ($ i-j >1$ and $ i-j <5$)	459
Long range ($ i-j \geq 5$)	847
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	13.1
Number of long range restraints per residue ¹	5.1

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)	45.2	0.2
0.2-0.5 (Medium)	80.5	0.5
>0.5 (Large)	32.2	1.95

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

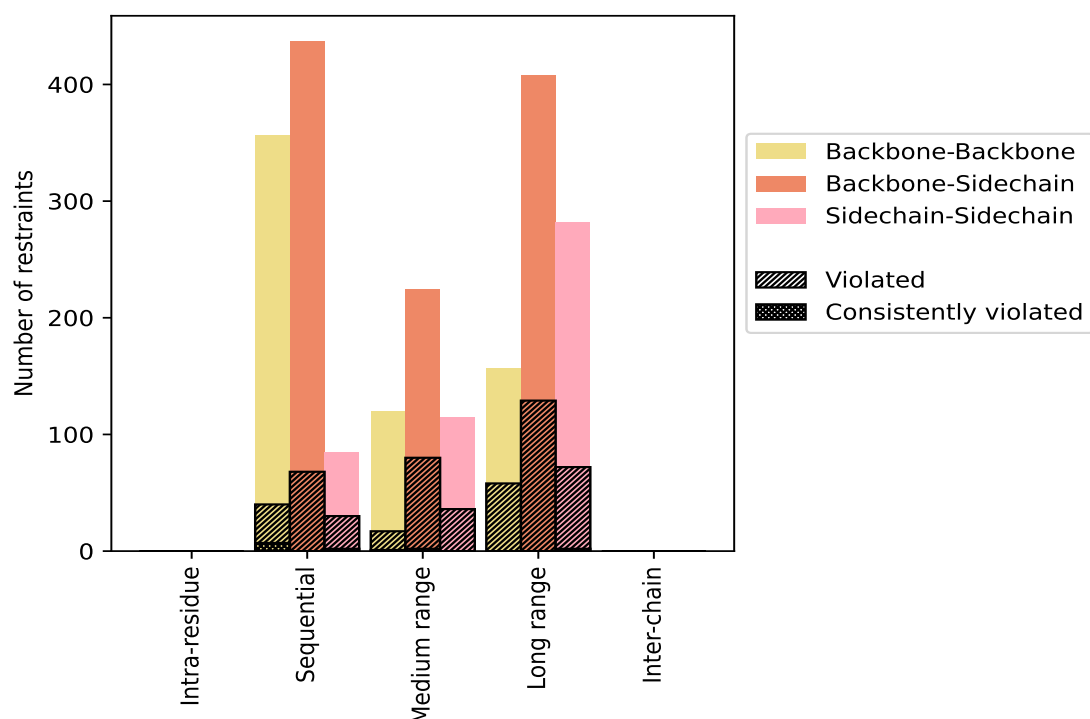
9.1 Summary of distance violations

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$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	878	40.2	138	15.7	6.3	9	1.0	0.4
Backbone-Backbone	356	16.3	40	11.2	1.8	7	2.0	0.3
Backbone-Sidechain	437	20.0	68	15.6	3.1	0	0.0	0.0
Sidechain-Sidechain	85	3.9	30	35.3	1.4	2	2.4	0.1
Medium range ($ i-j >1$ & $ i-j <5$)	459	21.0	133	29.0	6.1	3	0.7	0.1
Backbone-Backbone	120	5.5	17	14.2	0.8	1	0.8	0.0
Backbone-Sidechain	224	10.3	80	35.7	3.7	2	0.9	0.1
Sidechain-Sidechain	115	5.3	36	31.3	1.6	0	0.0	0.0
Long range ($ i-j \geq 5$)	847	38.8	259	30.6	11.9	2	0.2	0.1
Backbone-Backbone	157	7.2	58	36.9	2.7	0	0.0	0.0
Backbone-Sidechain	408	18.7	129	31.6	5.9	0	0.0	0.0
Sidechain-Sidechain	282	12.9	72	25.5	3.3	2	0.7	0.1
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	2184	100.0	530	24.3	24.3	14	0.6	0.6
Backbone-Backbone	633	29.0	115	18.2	5.3	8	1.3	0.4
Backbone-Sidechain	1069	48.9	277	25.9	12.7	2	0.2	0.1
Sidechain-Sidechain	482	22.1	138	28.6	6.3	4	0.8	0.2

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	0	47	39	72	0	158	0.36	1.23	0.23	0.3
2	0	60	37	66	0	163	0.34	1.13	0.22	0.28
3	0	49	45	62	0	156	0.38	1.54	0.28	0.3
4	0	46	39	55	0	140	0.35	1.36	0.24	0.29
5	0	55	34	72	0	161	0.36	1.16	0.22	0.3
6	0	51	36	81	0	168	0.37	1.74	0.27	0.31
7	0	51	29	64	0	144	0.33	1.29	0.2	0.26
8	0	45	42	65	0	152	0.37	1.34	0.23	0.31
9	0	46	43	69	0	158	0.37	1.95	0.28	0.28
10	0	48	39	49	0	136	0.37	1.34	0.24	0.31

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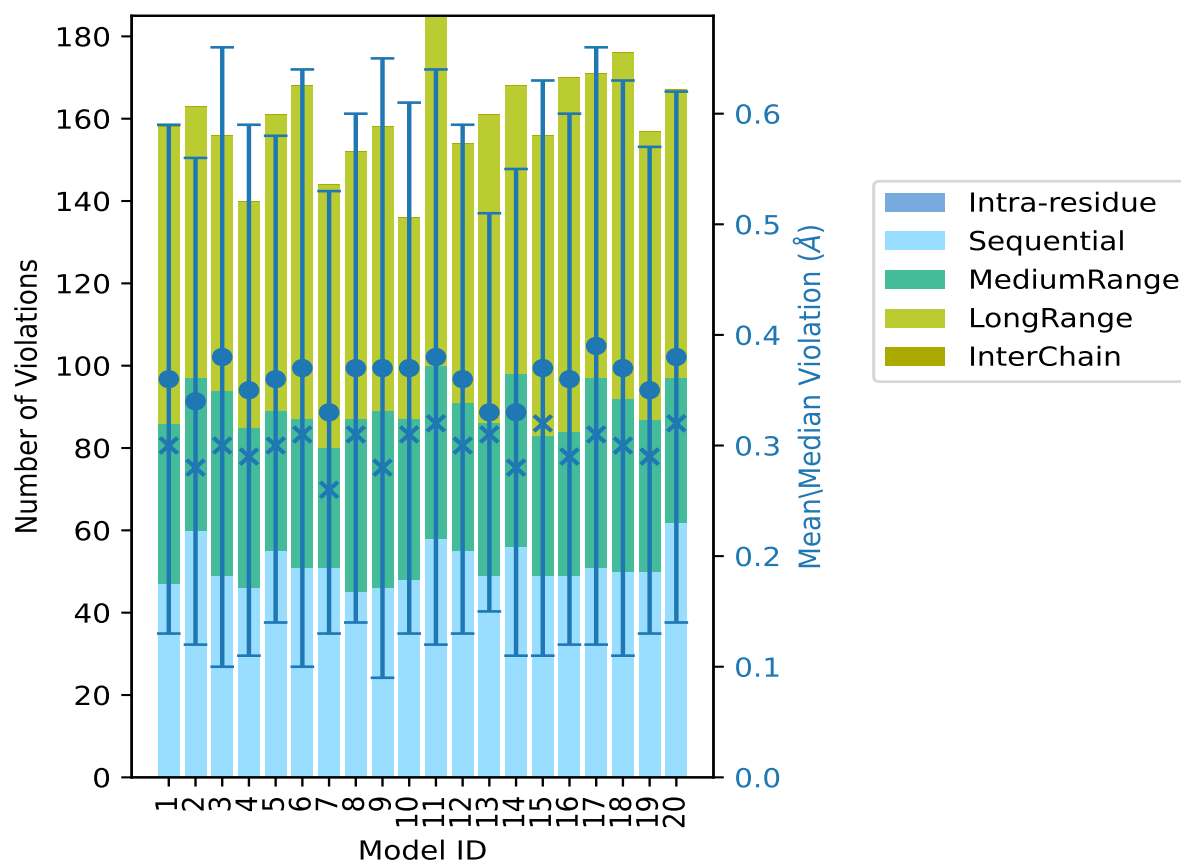
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	58	42	85	0	185	0.38	1.55	0.26	0.32
12	0	55	36	63	0	154	0.36	1.77	0.23	0.3
13	0	49	37	75	0	161	0.33	1.05	0.18	0.31
14	0	56	42	70	0	168	0.33	1.51	0.22	0.28
15	0	49	34	73	0	156	0.37	1.61	0.26	0.32
16	0	49	35	86	0	170	0.36	1.71	0.24	0.29
17	0	51	46	74	0	171	0.39	1.55	0.27	0.31
18	0	50	42	84	0	176	0.37	1.41	0.26	0.3
19	0	50	37	70	0	157	0.35	1.17	0.22	0.29
20	0	62	35	70	0	167	0.38	1.28	0.24	0.32

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

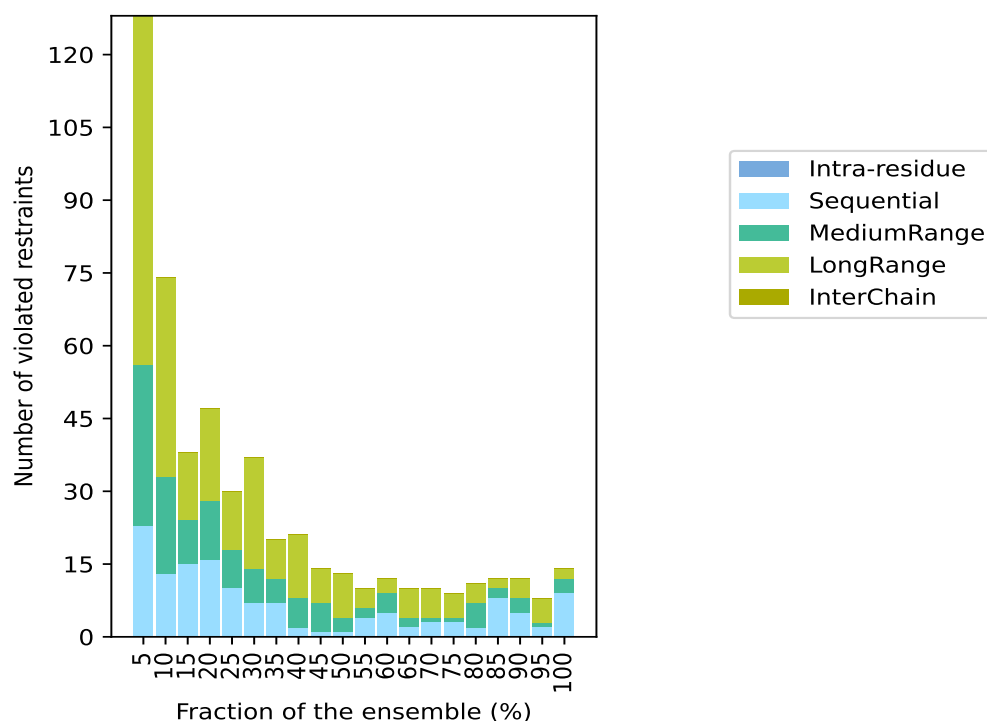
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1654(IR:0, SQ:740, MR:326, LR:588, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	23	33	72	0	128	1	5.0
0	13	20	41	0	74	2	10.0
0	15	9	14	0	38	3	15.0
0	16	12	19	0	47	4	20.0
0	10	8	12	0	30	5	25.0
0	7	7	23	0	37	6	30.0
0	7	5	8	0	20	7	35.0
0	2	6	13	0	21	8	40.0
0	1	6	7	0	14	9	45.0
0	1	3	9	0	13	10	50.0
0	4	2	4	0	10	11	55.0
0	5	4	3	0	12	12	60.0
0	2	2	6	0	10	13	65.0
0	3	1	6	0	10	14	70.0
0	3	1	5	0	9	15	75.0
0	2	5	4	0	11	16	80.0
0	8	2	2	0	12	17	85.0
0	5	3	4	0	12	18	90.0
0	2	1	5	0	8	19	95.0
0	9	3	2	0	14	20	100.0

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

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

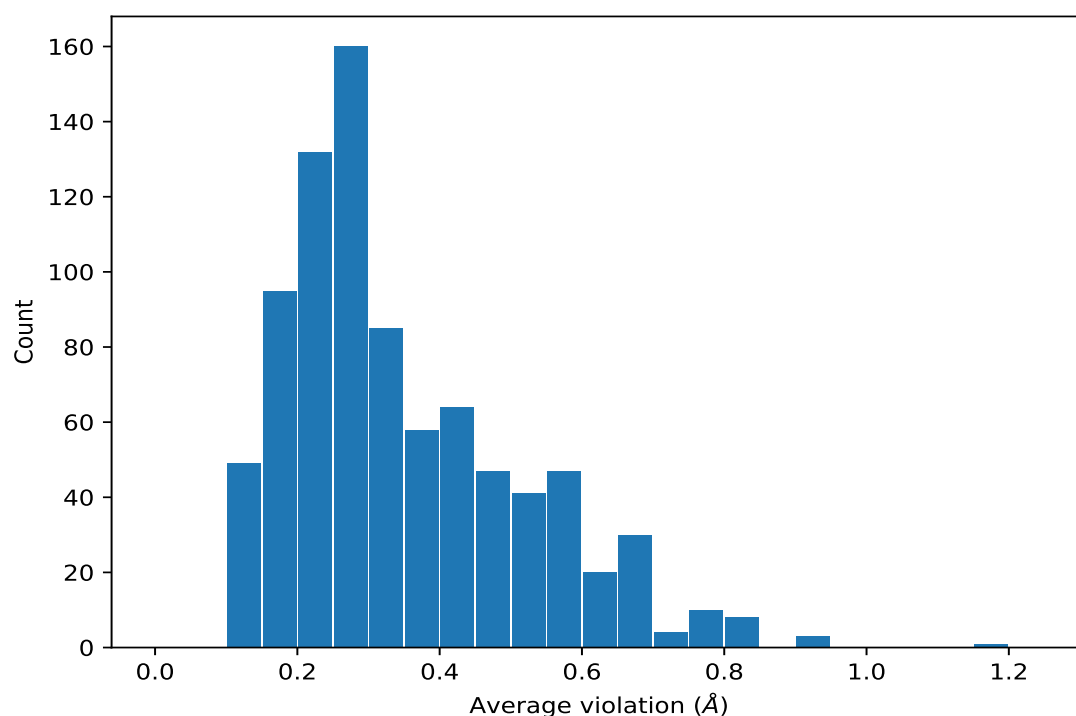
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	20	0.62	0.17	0.62
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	20	0.57	0.25	0.54
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	20	0.53	0.14	0.54
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	20	0.53	0.14	0.54
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	20	0.5	0.15	0.52
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	20	0.46	0.04	0.48
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	20	0.46	0.04	0.46
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	20	0.46	0.06	0.46
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	20	0.44	0.15	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	20	0.44	0.15	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	20	0.44	0.15	0.44
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	20	0.38	0.04	0.38
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	20	0.33	0.1	0.34
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	20	0.3	0.08	0.32
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	20	0.28	0.08	0.28
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	20	0.28	0.08	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	20	0.25	0.09	0.23
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	20	0.25	0.09	0.23
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	20	0.14	0.02	0.14
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	19	0.51	0.33	0.35
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	19	0.45	0.12	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	19	0.45	0.12	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	19	0.45	0.12	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	19	0.45	0.12	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	19	0.45	0.12	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	19	0.45	0.12	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	19	0.4	0.22	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	19	0.4	0.22	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	19	0.4	0.22	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	19	0.4	0.22	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	19	0.4	0.22	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	19	0.4	0.22	0.33
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	19	0.37	0.06	0.39
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	19	0.36	0.26	0.29
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	19	0.32	0.12	0.33
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	19	0.24	0.09	0.23
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	19	0.22	0.07	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	19	0.22	0.07	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	19	0.22	0.07	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	19	0.22	0.07	0.21
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	18	0.81	0.38	0.77
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	18	0.73	0.27	0.76
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	18	0.73	0.27	0.76
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	18	0.49	0.18	0.48
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	18	0.46	0.3	0.36
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	18	0.38	0.17	0.36
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	18	0.35	0.18	0.34
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	18	0.35	0.18	0.34
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	18	0.34	0.15	0.35
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	18	0.34	0.15	0.35
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	18	0.34	0.15	0.33
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	18	0.34	0.15	0.33
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	18	0.33	0.09	0.32
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	18	0.28	0.16	0.24
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	18	0.28	0.16	0.24
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	18	0.27	0.08	0.28
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	18	0.22	0.06	0.22
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	17	0.6	0.13	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	17	0.54	0.27	0.57
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	17	0.54	0.27	0.57
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	17	0.5	0.23	0.43
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	17	0.5	0.23	0.43
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	17	0.39	0.15	0.36
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	17	0.39	0.14	0.4
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	17	0.38	0.14	0.36
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	17	0.31	0.15	0.27
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	17	0.31	0.15	0.27
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	17	0.31	0.15	0.27
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	17	0.31	0.1	0.29
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	17	0.31	0.1	0.29
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	17	0.29	0.11	0.27
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	17	0.27	0.1	0.27
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	17	0.27	0.1	0.27
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	17	0.26	0.09	0.23
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	17	0.26	0.12	0.23
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	17	0.26	0.12	0.23
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	16	0.83	0.46	0.68
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	16	0.83	0.46	0.68
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	16	0.68	0.14	0.72
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	16	0.63	0.37	0.53
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	16	0.39	0.2	0.33
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	16	0.35	0.15	0.34
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	16	0.34	0.15	0.3
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	16	0.32	0.12	0.3
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	16	0.32	0.12	0.33
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	16	0.3	0.07	0.32
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	16	0.3	0.07	0.32
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	16	0.21	0.08	0.2
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	16	0.2	0.07	0.19
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	16	0.2	0.07	0.19
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	15	0.54	0.32	0.47
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	15	0.54	0.32	0.47
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	15	0.42	0.18	0.41
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	15	0.41	0.15	0.44
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	15	0.36	0.16	0.31
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	15	0.34	0.15	0.32
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	15	0.33	0.14	0.3
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	15	0.33	0.08	0.35
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	15	0.31	0.14	0.3
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	15	0.22	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	14	0.6	0.12	0.57
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	14	0.6	0.12	0.57
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	14	0.57	0.3	0.57
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	14	0.52	0.2	0.44
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	14	0.46	0.3	0.28
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	14	0.46	0.3	0.28
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	14	0.41	0.35	0.34
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	14	0.34	0.12	0.33
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	14	0.28	0.13	0.26
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	14	0.24	0.06	0.23
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	14	0.23	0.07	0.21
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	14	0.21	0.08	0.2
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	14	0.21	0.08	0.2
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	13	0.82	0.33	0.78
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	13	0.82	0.33	0.78
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	13	0.82	0.33	0.78
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	13	0.43	0.2	0.37
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	13	0.41	0.26	0.36
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	13	0.41	0.19	0.32
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	13	0.39	0.14	0.42
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	13	0.3	0.1	0.27
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	13	0.3	0.13	0.3
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	13	0.3	0.13	0.3
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	13	0.23	0.07	0.26
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	13	0.2	0.08	0.16
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	13	0.2	0.08	0.16
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	13	0.19	0.06	0.21
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	12	0.95	0.32	0.95
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	12	0.4	0.14	0.39
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	12	0.4	0.14	0.39
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	12	0.39	0.18	0.38
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	12	0.38	0.2	0.32
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	12	0.38	0.2	0.32
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	12	0.38	0.2	0.32
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	12	0.38	0.2	0.32
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	12	0.38	0.2	0.32
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	12	0.38	0.2	0.32
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	12	0.35	0.15	0.3
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	12	0.29	0.13	0.3
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	12	0.27	0.06	0.26
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	12	0.24	0.09	0.22
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	12	0.23	0.14	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	12	0.23	0.14	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	12	0.23	0.08	0.24
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	12	0.23	0.08	0.24
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	12	0.23	0.08	0.24
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	12	0.23	0.08	0.24
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	12	0.23	0.08	0.24
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	12	0.23	0.08	0.24
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	12	0.19	0.13	0.12
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	12	0.17	0.04	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	12	0.17	0.04	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	12	0.17	0.04	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	12	0.17	0.04	0.16
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	11	0.52	0.24	0.45
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	11	0.52	0.24	0.45
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	11	0.44	0.14	0.47
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	11	0.44	0.14	0.47
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	11	0.44	0.14	0.47
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	11	0.44	0.14	0.47
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	11	0.43	0.26	0.38
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	11	0.43	0.26	0.38
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	11	0.38	0.13	0.42
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	11	0.37	0.2	0.28
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	11	0.36	0.13	0.36
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	11	0.36	0.13	0.36
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	11	0.36	0.13	0.36
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	11	0.36	0.13	0.36
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	11	0.36	0.16	0.31
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	11	0.33	0.19	0.33
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	11	0.33	0.19	0.33
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	11	0.33	0.19	0.33
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	11	0.33	0.19	0.33
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	11	0.33	0.18	0.25
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	11	0.32	0.11	0.32
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	11	0.32	0.11	0.32
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	10	1.18	0.49	1.25
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	10	0.54	0.25	0.48
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	10	0.54	0.25	0.48
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	10	0.54	0.25	0.48
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	10	0.51	0.32	0.4
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	10	0.51	0.32	0.4
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	10	0.47	0.32	0.4
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	10	0.47	0.32	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	10	0.41	0.33	0.34
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	10	0.41	0.33	0.34
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	10	0.38	0.18	0.37
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	10	0.35	0.22	0.3
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	10	0.35	0.22	0.3
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	10	0.29	0.11	0.28
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	10	0.22	0.1	0.2
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	10	0.22	0.05	0.23
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	10	0.22	0.05	0.23
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	10	0.2	0.06	0.2
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	10	0.2	0.06	0.2
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	10	0.2	0.07	0.16
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	10	0.2	0.07	0.16
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	10	0.18	0.09	0.15
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	9	0.76	0.48	1.0
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	9	0.57	0.34	0.48
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	9	0.57	0.34	0.48
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	9	0.55	0.26	0.6
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	9	0.54	0.41	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	9	0.54	0.41	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	9	0.54	0.41	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	9	0.54	0.41	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	9	0.54	0.41	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	9	0.54	0.41	0.29
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	9	0.4	0.36	0.23
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	9	0.38	0.25	0.28
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	9	0.38	0.25	0.28
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	9	0.38	0.12	0.34
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	9	0.38	0.12	0.34
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	9	0.36	0.15	0.41
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	9	0.36	0.15	0.41
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	9	0.36	0.15	0.41
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	9	0.36	0.15	0.41
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	9	0.31	0.13	0.31
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	9	0.31	0.13	0.31
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	9	0.27	0.1	0.22
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	9	0.27	0.1	0.22
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	9	0.24	0.1	0.2
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	9	0.24	0.1	0.2
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	9	0.23	0.12	0.2
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	9	0.23	0.12	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	9	0.23	0.06	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	9	0.23	0.06	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	9	0.23	0.06	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	9	0.23	0.06	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	9	0.23	0.06	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	9	0.23	0.06	0.23
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	9	0.23	0.05	0.23
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	9	0.23	0.05	0.23
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	9	0.23	0.05	0.23
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	8	0.57	0.41	0.34
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	8	0.56	0.28	0.52
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	8	0.56	0.28	0.52
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	8	0.52	0.43	0.42
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	8	0.46	0.2	0.44
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	8	0.46	0.2	0.44
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	8	0.46	0.2	0.44
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	8	0.46	0.2	0.44
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	8	0.41	0.17	0.42
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	8	0.38	0.33	0.24
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	8	0.38	0.33	0.24
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	8	0.37	0.13	0.34
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	8	0.37	0.13	0.34
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	8	0.31	0.18	0.24
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	8	0.31	0.18	0.24
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	8	0.3	0.14	0.31
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	8	0.29	0.12	0.25
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	8	0.29	0.12	0.29
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	8	0.29	0.13	0.28
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	8	0.29	0.13	0.28
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	8	0.25	0.1	0.22
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	8	0.25	0.1	0.22
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	8	0.23	0.07	0.24
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	8	0.23	0.07	0.24
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	8	0.23	0.07	0.24
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	8	0.23	0.1	0.24
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	8	0.22	0.05	0.21
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	8	0.21	0.06	0.22
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	8	0.21	0.06	0.22
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	8	0.2	0.07	0.16
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	8	0.2	0.07	0.16
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	8	0.18	0.06	0.18
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	8	0.18	0.04	0.16
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	8	0.16	0.07	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	7	0.79	0.22	0.76
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	7	0.79	0.22	0.76
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	7	0.79	0.22	0.76
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	7	0.66	0.17	0.56
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	7	0.66	0.17	0.56
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	7	0.66	0.17	0.56
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	7	0.59	0.27	0.57
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	7	0.56	0.45	0.34
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	7	0.42	0.2	0.33
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	7	0.42	0.2	0.33
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	7	0.4	0.23	0.28
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	7	0.4	0.23	0.28
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	7	0.36	0.14	0.32
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	7	0.36	0.14	0.32
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	7	0.36	0.14	0.32
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	7	0.36	0.14	0.32
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	7	0.35	0.19	0.3
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	7	0.35	0.19	0.3
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	7	0.35	0.19	0.3
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	7	0.35	0.19	0.3
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	7	0.33	0.1	0.37
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	7	0.33	0.1	0.37
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	7	0.29	0.12	0.32
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	7	0.28	0.14	0.24
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	7	0.28	0.14	0.24
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	7	0.27	0.15	0.22
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	7	0.25	0.08	0.23
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	7	0.24	0.07	0.23
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	7	0.24	0.07	0.23
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	7	0.18	0.04	0.16
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	7	0.18	0.04	0.16
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	7	0.17	0.04	0.17
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	7	0.16	0.06	0.15
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	7	0.16	0.06	0.15
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	7	0.16	0.06	0.15
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	7	0.16	0.06	0.15
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	7	0.15	0.04	0.15
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	7	0.13	0.02	0.13
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	6	0.63	0.37	0.55
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	6	0.63	0.37	0.55
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	6	0.6	0.44	0.39
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	6	0.6	0.44	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	6	0.58	0.2	0.63
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	6	0.56	0.42	0.36
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	6	0.56	0.42	0.36
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	6	0.56	0.42	0.36
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	6	0.56	0.42	0.36
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	6	0.56	0.37	0.48
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	6	0.54	0.22	0.54
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	6	0.54	0.22	0.54
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	6	0.51	0.39	0.42
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	6	0.51	0.39	0.42
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	6	0.5	0.4	0.38
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	6	0.5	0.4	0.38
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	6	0.5	0.4	0.38
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	6	0.5	0.4	0.38
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	6	0.49	0.26	0.56
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	6	0.47	0.25	0.46
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	6	0.47	0.25	0.46
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	6	0.46	0.25	0.43
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	6	0.46	0.25	0.43
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	6	0.46	0.25	0.43
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	6	0.45	0.23	0.46
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	6	0.45	0.23	0.46
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	6	0.45	0.23	0.46
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	6	0.45	0.23	0.46
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	6	0.45	0.23	0.46
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	6	0.45	0.23	0.46
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	6	0.4	0.24	0.32
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	6	0.38	0.16	0.38
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	6	0.36	0.12	0.4
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	6	0.36	0.12	0.4
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	6	0.36	0.13	0.36
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	6	0.32	0.22	0.23
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	6	0.32	0.22	0.23
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	6	0.31	0.12	0.28
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	6	0.29	0.12	0.26
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	6	0.29	0.12	0.26
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	6	0.28	0.06	0.28
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	6	0.28	0.06	0.28
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	6	0.28	0.06	0.28
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	6	0.28	0.06	0.28
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	6	0.27	0.13	0.28
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	6	0.27	0.13	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	6	0.27	0.13	0.28
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	6	0.27	0.13	0.28
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	6	0.27	0.13	0.28
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	6	0.27	0.13	0.28
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	6	0.27	0.11	0.24
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	6	0.26	0.1	0.24
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	6	0.26	0.14	0.22
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	6	0.26	0.14	0.22
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	6	0.26	0.14	0.22
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	6	0.26	0.14	0.22
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	6	0.25	0.11	0.22
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	6	0.25	0.11	0.22
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	6	0.25	0.11	0.22
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	6	0.25	0.11	0.22
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	6	0.25	0.08	0.23
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	6	0.23	0.09	0.23
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	6	0.23	0.09	0.23
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	6	0.22	0.1	0.16
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	6	0.22	0.1	0.16
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	6	0.19	0.05	0.18
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	6	0.19	0.07	0.17
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	6	0.19	0.07	0.17
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	6	0.19	0.07	0.17
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	6	0.19	0.07	0.17
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	6	0.18	0.05	0.18
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	6	0.17	0.07	0.15
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	6	0.17	0.07	0.15
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	6	0.17	0.06	0.16
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	6	0.17	0.06	0.16
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	6	0.17	0.05	0.15
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	6	0.16	0.03	0.18
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	6	0.15	0.05	0.13
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	6	0.15	0.05	0.13
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	6	0.15	0.05	0.13
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	6	0.12	0.01	0.12
(1,33)	1:60:A:GLN:HG2	1:61:A:LYS:HA	5	0.62	0.33	0.46
(1,33)	1:60:A:GLN:HG3	1:61:A:LYS:HA	5	0.62	0.33	0.46
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG2	5	0.61	0.24	0.6
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG3	5	0.61	0.24	0.6
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG21	5	0.53	0.25	0.51
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG22	5	0.53	0.25	0.51
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG23	5	0.53	0.25	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG2	5	0.46	0.24	0.41
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG3	5	0.46	0.24	0.41
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD11	5	0.45	0.07	0.43
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD12	5	0.45	0.07	0.43
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD13	5	0.45	0.07	0.43
(1,1669)	1:165:A:LYS:HD2	1:166:A:PHE:H	5	0.4	0.07	0.41
(1,1669)	1:165:A:LYS:HD3	1:166:A:PHE:H	5	0.4	0.07	0.41
(1,1540)	1:30:A:LYS:HE2	1:31:A:ILE:H	5	0.38	0.21	0.34
(1,1540)	1:30:A:LYS:HE3	1:31:A:ILE:H	5	0.38	0.21	0.34
(1,676)	1:151:A:THR:HA	1:155:A:VAL:HB	5	0.37	0.15	0.28
(1,2114)	1:112:A:SER:HG	1:113:A:THR:HA	5	0.37	0.21	0.3
(1,313)	1:106:A:PRO:HD2	1:108:A:GLY:H	5	0.36	0.06	0.34
(1,313)	1:106:A:PRO:HD3	1:108:A:GLY:H	5	0.36	0.06	0.34
(1,614)	1:162:A:LEU:HG	1:90:A:ASN:HB2	5	0.35	0.17	0.42
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB2	5	0.35	0.05	0.35
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB3	5	0.35	0.05	0.35
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB2	5	0.35	0.05	0.35
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB3	5	0.35	0.05	0.35
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD1	5	0.34	0.19	0.35
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD2	5	0.34	0.19	0.35
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD1	5	0.34	0.19	0.35
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD2	5	0.34	0.19	0.35
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG12	5	0.34	0.14	0.32
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG13	5	0.34	0.14	0.32
(1,522)	1:139:A:ALA:HA	1:143:A:HIS:H	5	0.33	0.18	0.23
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB2	5	0.33	0.25	0.29
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB3	5	0.33	0.25	0.29
(1,611)	1:156:A:SER:HA	1:155:A:VAL:H	5	0.32	0.19	0.23
(1,937)	1:113:A:THR:H	1:112:A:SER:HB2	5	0.3	0.04	0.31
(1,937)	1:113:A:THR:H	1:112:A:SER:HB3	5	0.3	0.04	0.31
(1,60)	1:157:A:ALA:HB1	1:90:A:ASN:HA	5	0.29	0.1	0.27
(1,60)	1:157:A:ALA:HB2	1:90:A:ASN:HA	5	0.29	0.1	0.27
(1,60)	1:157:A:ALA:HB3	1:90:A:ASN:HA	5	0.29	0.1	0.27
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE1	5	0.25	0.15	0.18
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE2	5	0.25	0.15	0.18
(1,520)	1:111:A:ILE:HB	1:132:A:GLU:H	5	0.24	0.1	0.25
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG11	5	0.22	0.1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG12	5	0.22	0.1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG13	5	0.22	0.1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG21	5	0.22	0.1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG22	5	0.22	0.1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG23	5	0.22	0.1	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG2	5	0.21	0.05	0.18
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG3	5	0.21	0.05	0.18
(1,1465)	1:47:A:GLY:H	1:48:A:TYR:H	5	0.21	0.07	0.2
(1,1816)	1:53:A:PHE:HB2	1:30:A:LYS:H	5	0.21	0.08	0.17
(1,1816)	1:53:A:PHE:HB3	1:30:A:LYS:H	5	0.21	0.08	0.17
(1,102)	1:115:A:ILE:HB	1:124:A:ARG:H	5	0.2	0.04	0.21
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD11	5	0.19	0.07	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD12	5	0.19	0.07	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD13	5	0.19	0.07	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD21	5	0.19	0.07	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD22	5	0.19	0.07	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD23	5	0.19	0.07	0.15
(1,2009)	1:48:A:TYR:HD2	1:9:A:ILE:H	5	0.19	0.08	0.15
(1,722)	1:61:A:LYS:HB2	1:64:A:SER:H	5	0.17	0.02	0.17
(1,722)	1:61:A:LYS:HB3	1:64:A:SER:H	5	0.17	0.02	0.17
(1,2178)	1:31:A:ILE:HA	1:53:A:PHE:HA	5	0.16	0.04	0.13
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG2	4	0.94	0.35	1.09
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG3	4	0.94	0.35	1.09
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB2	4	0.7	0.13	0.7
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB3	4	0.7	0.13	0.7
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB2	4	0.7	0.13	0.7
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB3	4	0.7	0.13	0.7
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB2	4	0.7	0.44	0.62
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB3	4	0.7	0.44	0.62
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG11	4	0.61	0.42	0.63
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG12	4	0.61	0.42	0.63
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG13	4	0.61	0.42	0.63
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG11	4	0.61	0.42	0.63
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG12	4	0.61	0.42	0.63
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG13	4	0.61	0.42	0.63
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD11	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD12	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD13	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD11	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD12	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD13	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD11	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD12	4	0.59	0.5	0.38
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD13	4	0.59	0.5	0.38
(1,1961)	1:19:A:GLN:HG2	1:22:A:VAL:HB	4	0.59	0.31	0.56
(1,1961)	1:19:A:GLN:HG3	1:22:A:VAL:HB	4	0.59	0.31	0.56
(1,2144)	1:134:A:THR:HB	1:166:A:PHE:HZ	4	0.54	0.27	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB2	4	0.47	0.32	0.38
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB3	4	0.47	0.32	0.38
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB2	4	0.47	0.32	0.38
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB3	4	0.47	0.32	0.38
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD11	4	0.44	0.19	0.4
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD12	4	0.44	0.19	0.4
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD13	4	0.44	0.19	0.4
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD21	4	0.44	0.19	0.4
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD22	4	0.44	0.19	0.4
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD23	4	0.44	0.19	0.4
(1,308)	1:103:A:MET:HB2	1:104:A:LEU:HB2	4	0.44	0.19	0.39
(1,308)	1:103:A:MET:HB3	1:104:A:LEU:HB2	4	0.44	0.19	0.39
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG2	4	0.43	0.07	0.42
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG3	4	0.43	0.07	0.42
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB2	4	0.4	0.26	0.32
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB3	4	0.4	0.26	0.32
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB2	4	0.4	0.38	0.21
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB3	4	0.4	0.38	0.21
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB2	4	0.4	0.38	0.21
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB3	4	0.4	0.38	0.21
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB2	4	0.37	0.15	0.42
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB3	4	0.37	0.15	0.42
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG21	4	0.34	0.14	0.3
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG22	4	0.34	0.14	0.3
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG23	4	0.34	0.14	0.3
(1,1581)	1:93:A:LEU:HA	1:122:A:THR:HA	4	0.3	0.06	0.28
(1,352)	1:86:A:LEU:HG	1:85:A:ASN:H	4	0.3	0.17	0.3
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG2	4	0.28	0.14	0.22
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG3	4	0.28	0.14	0.22
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE1	4	0.27	0.08	0.24
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE2	4	0.27	0.08	0.24
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB2	4	0.27	0.15	0.22
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB3	4	0.27	0.15	0.22
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB2	4	0.27	0.15	0.22
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB3	4	0.27	0.15	0.22
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG2	4	0.26	0.23	0.15
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG3	4	0.26	0.23	0.15
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD2	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD3	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD2	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD3	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD2	4	0.26	0.08	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD3	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD2	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD3	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD2	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD3	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD2	4	0.26	0.08	0.26
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD3	4	0.26	0.08	0.26
(1,28)	1:45:A:CYS:HB2	1:15:A:HIS:HA	4	0.26	0.08	0.24
(1,28)	1:45:A:CYS:HB3	1:15:A:HIS:HA	4	0.26	0.08	0.24
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG2	4	0.26	0.16	0.18
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG3	4	0.26	0.16	0.18
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD11	4	0.26	0.12	0.25
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD12	4	0.26	0.12	0.25
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD13	4	0.26	0.12	0.25
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD21	4	0.26	0.12	0.25
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD22	4	0.26	0.12	0.25
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD23	4	0.26	0.12	0.25
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB2	4	0.25	0.09	0.26
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB3	4	0.25	0.09	0.26
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB2	4	0.25	0.09	0.26
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB3	4	0.25	0.09	0.26
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG12	4	0.25	0.1	0.28
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG13	4	0.25	0.1	0.28
(1,398)	1:123:A:SER:HA	1:126:A:VAL:H	4	0.24	0.1	0.2
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB2	4	0.24	0.07	0.24
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB3	4	0.24	0.07	0.24
(1,716)	1:165:A:LYS:HB2	1:86:A:LEU:HA	4	0.2	0.04	0.22
(1,716)	1:165:A:LYS:HB3	1:86:A:LEU:HA	4	0.2	0.04	0.22
(1,1128)	1:30:A:LYS:HE2	1:54:A:ASP:H	4	0.2	0.06	0.21
(1,1128)	1:30:A:LYS:HE3	1:54:A:ASP:H	4	0.2	0.06	0.21
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG2	4	0.2	0.07	0.22
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG3	4	0.2	0.07	0.22
(1,244)	1:67:A:LYS:HE2	1:64:A:SER:HA	4	0.19	0.04	0.2
(1,244)	1:67:A:LYS:HE3	1:64:A:SER:HA	4	0.19	0.04	0.2
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB2	4	0.19	0.08	0.19
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB3	4	0.19	0.08	0.19
(1,1150)	1:130:A:ARG:HA	1:112:A:SER:H	4	0.18	0.05	0.15
(1,1012)	1:43:A:ASN:HB3	1:44:A:LYS:HA	4	0.18	0.04	0.16
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB2	4	0.16	0.05	0.15
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB3	4	0.16	0.05	0.15
(1,1052)	1:15:A:HIS:HB3	1:16:A:THR:HA	4	0.16	0.04	0.18
(1,99)	1:41:A:THR:HB	1:40:A:LYS:H	4	0.16	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD11	4	0.16	0.05	0.14
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD12	4	0.16	0.05	0.14
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD13	4	0.16	0.05	0.14
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD21	4	0.16	0.05	0.14
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD22	4	0.16	0.05	0.14
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD23	4	0.16	0.05	0.14
(1,900)	1:32:A:VAL:HB	1:33:A:SER:HA	4	0.15	0.05	0.12
(1,405)	1:129:A:ALA:HB1	1:112:A:SER:H	4	0.14	0.02	0.15
(1,405)	1:129:A:ALA:HB2	1:112:A:SER:H	4	0.14	0.02	0.15
(1,405)	1:129:A:ALA:HB3	1:112:A:SER:H	4	0.14	0.02	0.15
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB2	4	0.14	0.02	0.14
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB3	4	0.14	0.02	0.14
(1,1891)	1:43:A:ASN:HA	1:38:A:LEU:HA	4	0.13	0.03	0.12
(1,425)	1:110:A:VAL:HA	1:111:A:ILE:HA	4	0.13	0.01	0.12
(1,1408)	1:9:A:ILE:HA	1:10:A:ARG:H	4	0.12	0.0	0.12
(1,1980)	1:7:A:LEU:HA	1:8:A:TYR:H	4	0.11	0.01	0.11
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB2	3	0.78	0.04	0.77
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB3	3	0.78	0.04	0.77
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB2	3	0.78	0.04	0.77
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB3	3	0.78	0.04	0.77
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB2	3	0.67	0.37	0.53
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB3	3	0.67	0.37	0.53
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB2	3	0.67	0.37	0.53
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB3	3	0.67	0.37	0.53
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB2	3	0.63	0.35	0.58
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB3	3	0.63	0.35	0.58
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB2	3	0.63	0.35	0.58
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB3	3	0.63	0.35	0.58
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB2	3	0.6	0.21	0.54
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB3	3	0.6	0.21	0.54
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB2	3	0.57	0.34	0.7
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB3	3	0.57	0.34	0.7
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB2	3	0.57	0.34	0.7
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB3	3	0.57	0.34	0.7
(1,1655)	1:162:A:LEU:HG	1:164:A:CYS:H	3	0.46	0.11	0.5
(1,2139)	1:163:A:LEU:HG	1:164:A:CYS:HA	3	0.42	0.24	0.43
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG2	3	0.34	0.05	0.38
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG3	3	0.34	0.05	0.38
(1,1500)	1:40:A:LYS:HG2	1:39:A:ASP:HA	3	0.31	0.19	0.23
(1,1500)	1:40:A:LYS:HG3	1:39:A:ASP:HA	3	0.31	0.19	0.23
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG2	3	0.29	0.19	0.18
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG3	3	0.29	0.19	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1072)	1:77:A:LYS:HB2	1:4:A:GLY:H	3	0.29	0.22	0.14
(1,1072)	1:77:A:LYS:HB3	1:4:A:GLY:H	3	0.29	0.22	0.14
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB2	3	0.28	0.17	0.2
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB3	3	0.28	0.17	0.2
(1,2130)	1:48:A:TYR:HD1	1:46:A:LYS:H	3	0.28	0.09	0.23
(1,2084)	1:90:A:ASN:H	1:89:A:SER:HG	3	0.27	0.1	0.28
(1,1255)	1:41:A:THR:HG21	1:42:A:THR:HB	3	0.26	0.05	0.24
(1,1255)	1:41:A:THR:HG22	1:42:A:THR:HB	3	0.26	0.05	0.24
(1,1255)	1:41:A:THR:HG23	1:42:A:THR:HB	3	0.26	0.05	0.24
(1,1291)	1:48:A:TYR:HD1	1:10:A:ARG:HA	3	0.26	0.04	0.26
(1,1291)	1:48:A:TYR:HD2	1:10:A:ARG:HA	3	0.26	0.04	0.26
(1,1661)	1:162:A:LEU:HG	1:164:A:CYS:HA	3	0.25	0.05	0.27
(1,1801)	1:44:A:LYS:HD2	1:42:A:THR:HB	3	0.25	0.06	0.29
(1,1801)	1:44:A:LYS:HD3	1:42:A:THR:HB	3	0.25	0.06	0.29
(1,1425)	1:87:A:TYR:HA	1:86:A:LEU:H	3	0.25	0.09	0.29
(1,1041)	1:23:A:LYS:H	1:19:A:GLN:HA	3	0.25	0.08	0.26
(1,1939)	1:43:A:ASN:HB3	1:42:A:THR:HA	3	0.24	0.11	0.2
(1,432)	1:86:A:LEU:HA	1:167:A:SER:HA	3	0.23	0.06	0.23
(1,969)	1:30:A:LYS:HD2	1:31:A:ILE:H	3	0.22	0.1	0.2
(1,969)	1:30:A:LYS:HD3	1:31:A:ILE:H	3	0.22	0.1	0.2
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD2	3	0.22	0.12	0.13
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD3	3	0.22	0.12	0.13
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG21	3	0.21	0.04	0.21
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG22	3	0.21	0.04	0.21
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG23	3	0.21	0.04	0.21
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG2	3	0.2	0.08	0.17
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG3	3	0.2	0.08	0.17
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG2	3	0.2	0.08	0.17
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG3	3	0.2	0.08	0.17
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG2	3	0.2	0.08	0.17
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG3	3	0.2	0.08	0.17
(1,1156)	1:130:A:ARG:HB2	1:86:A:LEU:H	3	0.19	0.07	0.19
(1,1156)	1:130:A:ARG:HB3	1:86:A:LEU:H	3	0.19	0.07	0.19
(1,2086)	1:126:A:VAL:HG11	1:89:A:SER:HG	3	0.18	0.04	0.17
(1,2086)	1:126:A:VAL:HG12	1:89:A:SER:HG	3	0.18	0.04	0.17
(1,2086)	1:126:A:VAL:HG13	1:89:A:SER:HG	3	0.18	0.04	0.17
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG21	3	0.17	0.08	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG22	3	0.17	0.08	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG23	3	0.17	0.08	0.11
(1,1539)	1:33:A:SER:HA	1:34:A:THR:H	3	0.16	0.05	0.15
(1,991)	1:44:A:LYS:HB2	1:15:A:HIS:HA	3	0.16	0.05	0.15
(1,991)	1:44:A:LYS:HB3	1:15:A:HIS:HA	3	0.16	0.05	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG21	3	0.15	0.03	0.14
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG22	3	0.15	0.03	0.14
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG23	3	0.15	0.03	0.14
(1,1169)	1:129:A:ALA:HA	1:112:A:SER:H	3	0.13	0.04	0.11
(1,684)	1:158:A:PRO:HA	1:159:A:THR:HB	3	0.13	0.02	0.12
(1,1569)	1:89:A:SER:HA	1:90:A:ASN:HB2	3	0.12	0.01	0.12
(1,2001)	1:33:A:SER:H	1:34:A:THR:H	3	0.11	0.01	0.11
(1,1686)	1:164:A:CYS:HA	1:88:A:ILE:H	3	0.11	0.01	0.11
(1,1978)	1:6:A:ASN:HA	1:7:A:LEU:H	3	0.11	0.01	0.12
(1,1956)	1:77:A:LYS:HB2	1:3:A:MET:HA	2	0.83	0.13	0.83
(1,1956)	1:77:A:LYS:HB3	1:3:A:MET:HA	2	0.83	0.13	0.83
(1,1958)	1:77:A:LYS:HA	1:3:A:MET:HG2	2	0.78	0.5	0.78
(1,1958)	1:77:A:LYS:HA	1:3:A:MET:HG3	2	0.78	0.5	0.78
(1,1935)	1:42:A:THR:HB	1:44:A:LYS:HE2	2	0.72	0.05	0.72
(1,1935)	1:42:A:THR:HB	1:44:A:LYS:HE3	2	0.72	0.05	0.72
(1,2094)	1:163:A:LEU:HB2	1:90:A:ASN:HD21	2	0.7	0.1	0.7
(1,2094)	1:163:A:LEU:HB2	1:90:A:ASN:HD22	2	0.7	0.1	0.7
(1,2094)	1:163:A:LEU:HB3	1:90:A:ASN:HD21	2	0.7	0.1	0.7
(1,2094)	1:163:A:LEU:HB3	1:90:A:ASN:HD22	2	0.7	0.1	0.7
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG21	2	0.67	0.23	0.67
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG22	2	0.67	0.23	0.67
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG23	2	0.67	0.23	0.67
(1,1955)	1:77:A:LYS:HD2	1:79:A:GLN:HB2	2	0.66	0.45	0.66
(1,1955)	1:77:A:LYS:HD2	1:79:A:GLN:HB3	2	0.66	0.45	0.66
(1,1955)	1:77:A:LYS:HD3	1:79:A:GLN:HB2	2	0.66	0.45	0.66
(1,1955)	1:77:A:LYS:HD3	1:79:A:GLN:HB3	2	0.66	0.45	0.66
(1,1909)	1:77:A:LYS:HA	1:3:A:MET:HB2	2	0.66	0.12	0.66
(1,1909)	1:77:A:LYS:HA	1:3:A:MET:HB3	2	0.66	0.12	0.66
(1,202)	1:111:A:ILE:HG21	1:80:A:GLU:HA	2	0.66	0.1	0.66
(1,202)	1:111:A:ILE:HG22	1:80:A:GLU:HA	2	0.66	0.1	0.66
(1,202)	1:111:A:ILE:HG23	1:80:A:GLU:HA	2	0.66	0.1	0.66
(1,949)	1:23:A:LYS:HE2	1:19:A:GLN:HA	2	0.63	0.29	0.63
(1,949)	1:23:A:LYS:HE3	1:19:A:GLN:HA	2	0.63	0.29	0.63
(1,2071)	1:128:A:PHE:H	1:88:A:ILE:HG12	2	0.6	0.28	0.6
(1,2071)	1:128:A:PHE:H	1:88:A:ILE:HG13	2	0.6	0.28	0.6
(1,2134)	1:163:A:LEU:HB2	1:90:A:ASN:HD21	2	0.6	0.1	0.6
(1,2134)	1:163:A:LEU:HB2	1:90:A:ASN:HD22	2	0.6	0.1	0.6
(1,2134)	1:163:A:LEU:HB3	1:90:A:ASN:HD21	2	0.6	0.1	0.6
(1,2134)	1:163:A:LEU:HB3	1:90:A:ASN:HD22	2	0.6	0.1	0.6
(1,1450)	1:80:A:GLU:HG2	1:77:A:LYS:H	2	0.6	0.24	0.6
(1,1450)	1:80:A:GLU:HG3	1:77:A:LYS:H	2	0.6	0.24	0.6
(1,55)	1:37:A:ILE:HA	1:38:A:LEU:HG	2	0.58	0.01	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2117)	1:101:A:GLU:HG2	1:113:A:THR:H	2	0.5	0.15	0.5
(1,2117)	1:101:A:GLU:HG3	1:113:A:THR:H	2	0.5	0.15	0.5
(1,2117)	1:101:A:GLU:HG2	1:113:A:THR:H	2	0.5	0.15	0.5
(1,2117)	1:101:A:GLU:HG3	1:113:A:THR:H	2	0.5	0.15	0.5
(1,289)	1:93:A:LEU:HB2	1:95:A:MET:H	2	0.49	0.23	0.49
(1,289)	1:93:A:LEU:HB3	1:95:A:MET:H	2	0.49	0.23	0.49
(1,665)	1:149:A:ILE:HG12	1:160:A:GLU:H	2	0.46	0.11	0.46
(1,665)	1:149:A:ILE:HG13	1:160:A:GLU:H	2	0.46	0.11	0.46
(1,387)	1:116:A:LEU:HA	1:124:A:ARG:HD2	2	0.45	0.27	0.45
(1,387)	1:116:A:LEU:HA	1:124:A:ARG:HD3	2	0.45	0.27	0.45
(1,973)	1:60:A:GLN:HG2	1:64:A:SER:H	2	0.44	0.01	0.44
(1,973)	1:60:A:GLN:HG3	1:64:A:SER:H	2	0.44	0.01	0.44
(1,194)	1:97:A:GLU:HB2	1:115:A:ILE:HG12	2	0.42	0.01	0.42
(1,194)	1:97:A:GLU:HB2	1:115:A:ILE:HG13	2	0.42	0.01	0.42
(1,194)	1:97:A:GLU:HB3	1:115:A:ILE:HG12	2	0.42	0.01	0.42
(1,194)	1:97:A:GLU:HB3	1:115:A:ILE:HG13	2	0.42	0.01	0.42
(1,484)	1:109:A:GLN:HB2	1:136:A:LYS:HE2	2	0.42	0.08	0.42
(1,484)	1:109:A:GLN:HB2	1:136:A:LYS:HE3	2	0.42	0.08	0.42
(1,484)	1:109:A:GLN:HB3	1:136:A:LYS:HE2	2	0.42	0.08	0.42
(1,484)	1:109:A:GLN:HB3	1:136:A:LYS:HE3	2	0.42	0.08	0.42
(1,1853)	1:31:A:ILE:HB	1:22:A:VAL:HA	2	0.42	0.13	0.42
(1,1015)	1:23:A:LYS:HG2	1:22:A:VAL:HB	2	0.4	0.05	0.4
(1,1015)	1:23:A:LYS:HG3	1:22:A:VAL:HB	2	0.4	0.05	0.4
(1,1682)	1:166:A:PHE:HA	1:137:A:CYS:HB2	2	0.39	0.05	0.39
(1,1682)	1:166:A:PHE:HA	1:137:A:CYS:HB3	2	0.39	0.05	0.39
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD11	2	0.38	0.26	0.38
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD12	2	0.38	0.26	0.38
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD13	2	0.38	0.26	0.38
(1,415)	1:116:A:LEU:HA	1:128:A:PHE:HE1	2	0.34	0.24	0.34
(1,415)	1:116:A:LEU:HA	1:128:A:PHE:HE2	2	0.34	0.24	0.34
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG21	2	0.34	0.13	0.34
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG22	2	0.34	0.13	0.34
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG23	2	0.34	0.13	0.34
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB1	2	0.34	0.2	0.34
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB2	2	0.34	0.2	0.34
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB3	2	0.34	0.2	0.34
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB1	2	0.34	0.2	0.34
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB2	2	0.34	0.2	0.34
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB3	2	0.34	0.2	0.34
(1,703)	1:163:A:LEU:HD11	1:164:A:CYS:H	2	0.33	0.07	0.33
(1,703)	1:163:A:LEU:HD12	1:164:A:CYS:H	2	0.33	0.07	0.33
(1,703)	1:163:A:LEU:HD13	1:164:A:CYS:H	2	0.33	0.07	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,703)	1:163:A:LEU:HD21	1:164:A:CYS:H	2	0.33	0.07	0.33
(1,703)	1:163:A:LEU:HD22	1:164:A:CYS:H	2	0.33	0.07	0.33
(1,703)	1:163:A:LEU:HD23	1:164:A:CYS:H	2	0.33	0.07	0.33
(1,1839)	1:50:A:PHE:HE1	1:34:A:THR:HA	2	0.3	0.1	0.3
(1,1839)	1:50:A:PHE:HE2	1:34:A:THR:HA	2	0.3	0.1	0.3
(1,1782)	1:37:A:ILE:HB	1:49:A:GLY:H	2	0.29	0.03	0.29
(1,187)	1:95:A:MET:HB2	1:115:A:ILE:HB	2	0.29	0.01	0.29
(1,187)	1:95:A:MET:HB3	1:115:A:ILE:HB	2	0.29	0.01	0.29
(1,678)	1:150:A:LYS:HG2	1:151:A:THR:HB	2	0.28	0.09	0.28
(1,678)	1:150:A:LYS:HG3	1:151:A:THR:HB	2	0.28	0.09	0.28
(1,705)	1:160:A:GLU:HA	1:149:A:ILE:H	2	0.28	0.11	0.28
(1,1304)	1:37:A:ILE:HG12	1:46:A:LYS:HB2	2	0.26	0.1	0.26
(1,1304)	1:37:A:ILE:HG12	1:46:A:LYS:HB3	2	0.26	0.1	0.26
(1,1304)	1:37:A:ILE:HG13	1:46:A:LYS:HB2	2	0.26	0.1	0.26
(1,1304)	1:37:A:ILE:HG13	1:46:A:LYS:HB3	2	0.26	0.1	0.26
(1,1348)	1:17:A:THR:H	1:21:A:LEU:H	2	0.26	0.06	0.26
(1,475)	1:138:A:GLU:HG2	1:166:A:PHE:HB2	2	0.26	0.07	0.26
(1,475)	1:138:A:GLU:HG2	1:166:A:PHE:HB3	2	0.26	0.07	0.26
(1,475)	1:138:A:GLU:HG3	1:166:A:PHE:HB2	2	0.26	0.07	0.26
(1,475)	1:138:A:GLU:HG3	1:166:A:PHE:HB3	2	0.26	0.07	0.26
(1,1707)	1:44:A:LYS:HA	1:38:A:LEU:HB2	2	0.26	0.12	0.26
(1,1707)	1:44:A:LYS:HA	1:38:A:LEU:HB3	2	0.26	0.12	0.26
(1,2109)	1:114:A:ARG:HH21	1:112:A:SER:HB2	2	0.26	0.06	0.26
(1,2109)	1:114:A:ARG:HH21	1:112:A:SER:HB3	2	0.26	0.06	0.26
(1,2109)	1:114:A:ARG:HH22	1:112:A:SER:HB2	2	0.26	0.06	0.26
(1,2109)	1:114:A:ARG:HH22	1:112:A:SER:HB3	2	0.26	0.06	0.26
(1,781)	1:71:A:VAL:HG11	1:10:A:ARG:HG2	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG11	1:10:A:ARG:HG3	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG12	1:10:A:ARG:HG2	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG12	1:10:A:ARG:HG3	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG13	1:10:A:ARG:HG2	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG13	1:10:A:ARG:HG3	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG21	1:10:A:ARG:HG2	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG21	1:10:A:ARG:HG3	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG22	1:10:A:ARG:HG2	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG22	1:10:A:ARG:HG3	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG23	1:10:A:ARG:HG2	2	0.25	0.1	0.25
(1,781)	1:71:A:VAL:HG23	1:10:A:ARG:HG3	2	0.25	0.1	0.25
(1,2108)	1:112:A:SER:HG	1:113:A:THR:H	2	0.24	0.02	0.24
(1,693)	1:155:A:VAL:HB	1:94:A:SER:HB2	2	0.24	0.05	0.24
(1,693)	1:155:A:VAL:HB	1:94:A:SER:HB3	2	0.24	0.05	0.24
(1,1352)	1:61:A:LYS:HD2	1:28:A:TYR:HA	2	0.23	0.12	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1352)	1:61:A:LYS:HD3	1:28:A:TYR:HA	2	0.23	0.12	0.23
(1,719)	1:164:A:CYS:HB2	1:88:A:ILE:HG12	2	0.22	0.01	0.22
(1,719)	1:164:A:CYS:HB2	1:88:A:ILE:HG13	2	0.22	0.01	0.22
(1,719)	1:164:A:CYS:HB3	1:88:A:ILE:HG12	2	0.22	0.01	0.22
(1,719)	1:164:A:CYS:HB3	1:88:A:ILE:HG13	2	0.22	0.01	0.22
(1,1953)	1:72:A:GLN:HG2	1:10:A:ARG:HG2	2	0.22	0.11	0.22
(1,1953)	1:72:A:GLN:HG2	1:10:A:ARG:HG3	2	0.22	0.11	0.22
(1,1953)	1:72:A:GLN:HG3	1:10:A:ARG:HG2	2	0.22	0.11	0.22
(1,1953)	1:72:A:GLN:HG3	1:10:A:ARG:HG3	2	0.22	0.11	0.22
(1,2054)	1:75:A:MET:HE1	1:3:A:MET:HG2	2	0.22	0.12	0.22
(1,2054)	1:75:A:MET:HE1	1:3:A:MET:HG3	2	0.22	0.12	0.22
(1,2054)	1:75:A:MET:HE2	1:3:A:MET:HG2	2	0.22	0.12	0.22
(1,2054)	1:75:A:MET:HE2	1:3:A:MET:HG3	2	0.22	0.12	0.22
(1,2054)	1:75:A:MET:HE3	1:3:A:MET:HG2	2	0.22	0.12	0.22
(1,2054)	1:75:A:MET:HE3	1:3:A:MET:HG3	2	0.22	0.12	0.22
(1,21)	1:24:A:LEU:HA	1:26:A:GLN:H	2	0.22	0.12	0.22
(1,1901)	1:77:A:LYS:HB2	1:79:A:GLN:HG2	2	0.21	0.02	0.21
(1,1901)	1:77:A:LYS:HB2	1:79:A:GLN:HG3	2	0.21	0.02	0.21
(1,1901)	1:77:A:LYS:HB3	1:79:A:GLN:HG2	2	0.21	0.02	0.21
(1,1901)	1:77:A:LYS:HB3	1:79:A:GLN:HG3	2	0.21	0.02	0.21
(1,68)	1:114:A:ARG:HA	1:97:A:GLU:H	2	0.21	0.1	0.21
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD11	2	0.2	0.06	0.2
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD12	2	0.2	0.06	0.2
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD13	2	0.2	0.06	0.2
(1,556)	1:136:A:LYS:HD2	1:108:A:GLY:H	2	0.2	0.06	0.2
(1,556)	1:136:A:LYS:HD3	1:108:A:GLY:H	2	0.2	0.06	0.2
(1,1534)	1:64:A:SER:HB2	1:67:A:LYS:HD2	2	0.2	0.08	0.2
(1,1534)	1:64:A:SER:HB2	1:67:A:LYS:HD3	2	0.2	0.08	0.2
(1,1534)	1:64:A:SER:HB3	1:67:A:LYS:HD2	2	0.2	0.08	0.2
(1,1534)	1:64:A:SER:HB3	1:67:A:LYS:HD3	2	0.2	0.08	0.2
(1,27)	1:50:A:PHE:HE1	1:52:A:ASP:HB3	2	0.19	0.08	0.19
(1,27)	1:50:A:PHE:HE2	1:52:A:ASP:HB3	2	0.19	0.08	0.19
(1,1495)	1:58:A:ALA:HA	1:61:A:LYS:HE2	2	0.19	0.06	0.19
(1,1495)	1:58:A:ALA:HA	1:61:A:LYS:HE3	2	0.19	0.06	0.19
(1,968)	1:27:A:PRO:HG2	1:25:A:CYS:HA	2	0.18	0.08	0.18
(1,968)	1:27:A:PRO:HG3	1:25:A:CYS:HA	2	0.18	0.08	0.18
(1,1114)	1:133:A:SER:HA	1:132:A:GLU:HG2	2	0.18	0.05	0.18
(1,1114)	1:133:A:SER:HA	1:132:A:GLU:HG3	2	0.18	0.05	0.18
(1,2046)	1:7:A:LEU:HD11	1:75:A:MET:HA	2	0.18	0.02	0.18
(1,2046)	1:7:A:LEU:HD12	1:75:A:MET:HA	2	0.18	0.02	0.18
(1,2046)	1:7:A:LEU:HD13	1:75:A:MET:HA	2	0.18	0.02	0.18
(1,347)	1:95:A:MET:HA	1:94:A:SER:H	2	0.18	0.01	0.18

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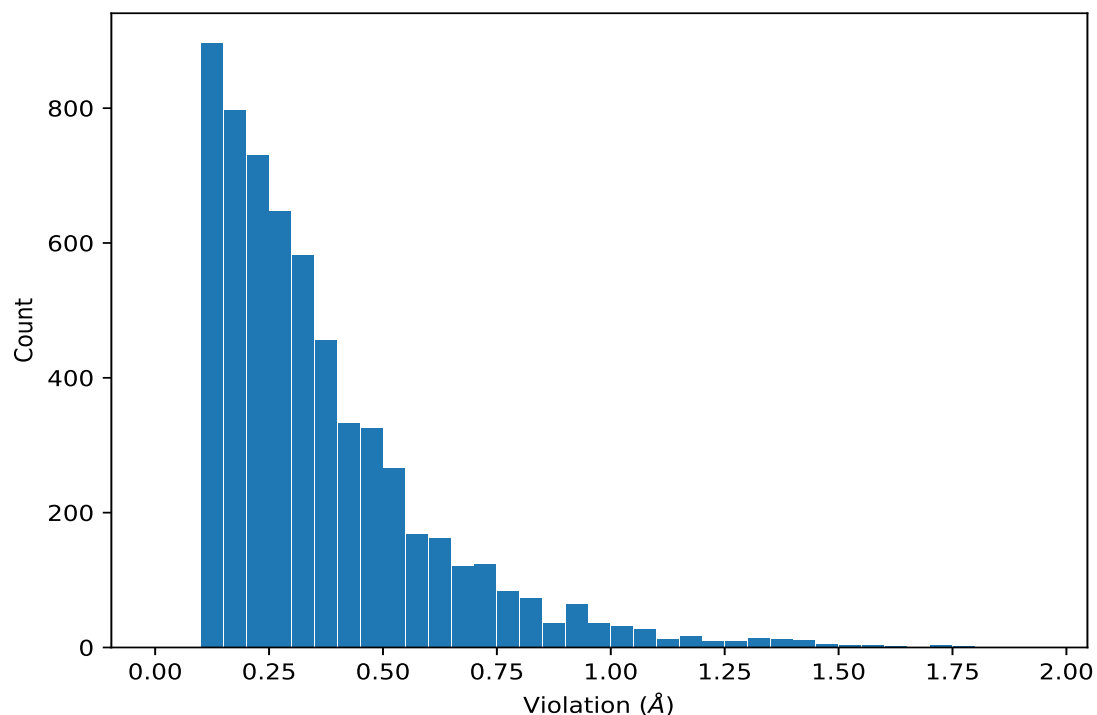
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,340)	1:84:A:THR:HB	1:85:A:ASN:HA	2	0.18	0.03	0.18
(1,2167)	1:6:A:ASN:H	1:4:A:GLY:HA2	2	0.18	0.06	0.18
(1,2167)	1:6:A:ASN:H	1:4:A:GLY:HA3	2	0.18	0.06	0.18
(1,1085)	1:4:A:GLY:HA2	1:77:A:LYS:HA	2	0.17	0.06	0.17
(1,1085)	1:4:A:GLY:HA3	1:77:A:LYS:HA	2	0.17	0.06	0.17
(1,1590)	1:92:A:PRO:HD2	1:160:A:GLU:H	2	0.17	0.04	0.17
(1,1590)	1:92:A:PRO:HD3	1:160:A:GLU:H	2	0.17	0.04	0.17
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG21	2	0.16	0.04	0.16
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG22	2	0.16	0.04	0.16
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG23	2	0.16	0.04	0.16
(1,958)	1:27:A:PRO:HG2	1:23:A:LYS:HB2	2	0.16	0.05	0.16
(1,958)	1:27:A:PRO:HG2	1:23:A:LYS:HB3	2	0.16	0.05	0.16
(1,958)	1:27:A:PRO:HG3	1:23:A:LYS:HB2	2	0.16	0.05	0.16
(1,958)	1:27:A:PRO:HG3	1:23:A:LYS:HB3	2	0.16	0.05	0.16
(1,1905)	1:16:A:THR:HG21	1:21:A:LEU:HA	2	0.16	0.03	0.16
(1,1905)	1:16:A:THR:HG22	1:21:A:LEU:HA	2	0.16	0.03	0.16
(1,1905)	1:16:A:THR:HG23	1:21:A:LEU:HA	2	0.16	0.03	0.16
(1,50)	1:51:A:VAL:HA	1:35:A:LYS:H	2	0.15	0.0	0.15
(1,1137)	1:83:A:PRO:HD2	1:84:A:THR:HB	2	0.15	0.02	0.15
(1,1137)	1:83:A:PRO:HD3	1:84:A:THR:HB	2	0.15	0.02	0.15
(1,460)	1:114:A:ARG:HB2	1:115:A:ILE:H	2	0.14	0.02	0.14
(1,460)	1:114:A:ARG:HB3	1:115:A:ILE:H	2	0.14	0.02	0.14
(1,521)	1:111:A:ILE:HB	1:130:A:ARG:HA	2	0.14	0.01	0.14
(1,585)	1:141:A:ILE:HD11	1:164:A:CYS:HB2	2	0.12	0.01	0.12
(1,585)	1:141:A:ILE:HD11	1:164:A:CYS:HB3	2	0.12	0.01	0.12
(1,585)	1:141:A:ILE:HD12	1:164:A:CYS:HB2	2	0.12	0.01	0.12
(1,585)	1:141:A:ILE:HD12	1:164:A:CYS:HB3	2	0.12	0.01	0.12
(1,585)	1:141:A:ILE:HD13	1:164:A:CYS:HB2	2	0.12	0.01	0.12
(1,585)	1:141:A:ILE:HD13	1:164:A:CYS:HB3	2	0.12	0.01	0.12
(1,1384)	1:32:A:VAL:HA	1:30:A:LYS:HE2	2	0.12	0.01	0.12
(1,1384)	1:32:A:VAL:HA	1:30:A:LYS:HE3	2	0.12	0.01	0.12
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG21	2	0.12	0.02	0.12
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG22	2	0.12	0.02	0.12
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG23	2	0.12	0.02	0.12
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG21	2	0.12	0.02	0.12
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG22	2	0.12	0.02	0.12
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG23	2	0.12	0.02	0.12
(1,1378)	1:26:A:GLN:HB2	1:29:A:GLY:H	2	0.12	0.01	0.12
(1,1378)	1:26:A:GLN:HB3	1:29:A:GLY:H	2	0.12	0.01	0.12
(1,1899)	1:75:A:MET:HA	1:74:A:GLN:H	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	9	1.95
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	12	1.77
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	12	1.77
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	6	1.74
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	6	1.74
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	16	1.71
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	15	1.61
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	15	1.6
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	17	1.55
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	17	1.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	11	1.55
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	3	1.54
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	14	1.51
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	14	1.51
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	9	1.48
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	17	1.47
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	17	1.47
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	17	1.47
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	17	1.47
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD11	11	1.44
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD12	11	1.44
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD13	11	1.44
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD11	11	1.44
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD12	11	1.44
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD13	11	1.44
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD11	11	1.44
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD12	11	1.44
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD13	11	1.44
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	11	1.43
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	18	1.41
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	17	1.38
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	17	1.38
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	17	1.38
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	17	1.38
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	17	1.38
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	17	1.38
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	9	1.37
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	9	1.37
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	16	1.36
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB2	4	1.36
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB3	4	1.36
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	6	1.36
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	6	1.34
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	9	1.34
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	9	1.34
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	8	1.34
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	8	1.34
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	10	1.34
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	18	1.34
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	18	1.34
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	18	1.34
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	18	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	4	1.32
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	4	1.32
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	4	1.32
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	3	1.32
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	7	1.29
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	18	1.29
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	18	1.29
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	18	1.29
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	18	1.29
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	18	1.29
(1,1958)	1:77:A:LYS:HA	1:3:A:MET:HG2	20	1.28
(1,1958)	1:77:A:LYS:HA	1:3:A:MET:HG3	20	1.28
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	11	1.27
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	14	1.26
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	20	1.24
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	10	1.24
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	1	1.23
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	1	1.23
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	20	1.22
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG2	17	1.22
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG3	17	1.22
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG2	6	1.21
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG3	6	1.21
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	18	1.2
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	3	1.19
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	18	1.19
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	18	1.19
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	3	1.18
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB2	4	1.18
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB3	4	1.18
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB2	4	1.18
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB3	4	1.18
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	11	1.18
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	19	1.17
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	3	1.17
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	3	1.17
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	3	1.17
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	11	1.16
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	1	1.16
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	5	1.16
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	5	1.16
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	2	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	2	1.13
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	2	1.13
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	8	1.13
(1,1955)	1:77:A:LYS:HD2	1:79:A:GLN:HB2	20	1.11
(1,1955)	1:77:A:LYS:HD2	1:79:A:GLN:HB3	20	1.11
(1,1955)	1:77:A:LYS:HD3	1:79:A:GLN:HB2	20	1.11
(1,1955)	1:77:A:LYS:HD3	1:79:A:GLN:HB3	20	1.11
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	19	1.11
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	14	1.1
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	14	1.1
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	14	1.1
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	6	1.1
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	19	1.09
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	19	1.09
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB2	18	1.08
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB3	18	1.08
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB2	18	1.08
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB3	18	1.08
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	17	1.08
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	17	1.08
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	6	1.07
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	6	1.07
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	8	1.07
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	8	1.06
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB2	1	1.06
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB3	1	1.06
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB2	1	1.06
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB3	1	1.06
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	15	1.06
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG11	13	1.05
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG12	13	1.05
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG13	13	1.05
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG11	13	1.05
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG12	13	1.05
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG13	13	1.05
(1,1961)	1:19:A:GLN:HG2	1:22:A:VAL:HB	3	1.05
(1,1961)	1:19:A:GLN:HG3	1:22:A:VAL:HB	3	1.05
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	16	1.05
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	16	1.05
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	4	1.04
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	17	1.04
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	17	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	17	1.04
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	15	1.03
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	3	1.03
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	3	1.03
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	14	1.03
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	3	1.02
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	4	1.02
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	9	1.02
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	9	1.02
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	4	1.01
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	4	1.01
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	2	1.01
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	2	1.01
(1,33)	1:60:A:GLN:HG2	1:61:A:LYS:HA	9	1.01
(1,33)	1:60:A:GLN:HG3	1:61:A:LYS:HA	9	1.01
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG11	5	1.0
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG12	5	1.0
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG13	5	1.0
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG11	5	1.0
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG12	5	1.0
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG13	5	1.0
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	9	1.0
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	9	1.0
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	2	1.0
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	6	1.0
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	6	1.0
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	6	1.0
(1,33)	1:60:A:GLN:HG2	1:61:A:LYS:HA	17	1.0
(1,33)	1:60:A:GLN:HG3	1:61:A:LYS:HA	17	1.0
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	2	0.99
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	15	0.99
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	15	0.99
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	15	0.98
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	5	0.98
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB2	3	0.98
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB3	3	0.98
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB2	3	0.98
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB3	3	0.98
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	7	0.98
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	7	0.98
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	7	0.98
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	7	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG2	1	0.97
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG3	1	0.97
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	20	0.97
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	20	0.97
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	3	0.97
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	3	0.97
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG2	16	0.97
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG3	16	0.97
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	2	0.96
(1,1956)	1:77:A:LYS:HB2	1:3:A:MET:HA	20	0.96
(1,1956)	1:77:A:LYS:HB3	1:3:A:MET:HA	20	0.96
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	3	0.96
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	5	0.96
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	5	0.96
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	5	0.96
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	16	0.95
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	3	0.95
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	3	0.95
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	3	0.95
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	3	0.95
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	3	0.95
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	3	0.95
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	2	0.95
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	2	0.95
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	1	0.94
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	16	0.94
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	16	0.94
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	16	0.94
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	16	0.94
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	16	0.94
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	16	0.94
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	15	0.94
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	15	0.94
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	6	0.94
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	6	0.94
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	6	0.94
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	18	0.93
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	10	0.93
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	10	0.93
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	10	0.93
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	13	0.93
(1,188)	1:95:A:MET:HB2	1:115:A:ILE:HG12	15	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:95:A:MET:HB2	1:115:A:ILE:HG13	15	0.93
(1,188)	1:95:A:MET:HB3	1:115:A:ILE:HG12	15	0.93
(1,188)	1:95:A:MET:HB3	1:115:A:ILE:HG13	15	0.93
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	12	0.92
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	10	0.92
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	10	0.92
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	15	0.92
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	15	0.92
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	15	0.92
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	17	0.92
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	8	0.92
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	8	0.92
(1,949)	1:23:A:LYS:HE2	1:19:A:GLN:HA	15	0.92
(1,949)	1:23:A:LYS:HE3	1:19:A:GLN:HA	15	0.92
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	5	0.92
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	12	0.92
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	12	0.92
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	1	0.92
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	1	0.92
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	17	0.91
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	17	0.91
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	17	0.91
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	2	0.91
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	1	0.91
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	1	0.91
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	1	0.91
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	6	0.91
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	6	0.91
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	15	0.91
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	15	0.91
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	18	0.91
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	18	0.91
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB2	9	0.9
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB3	9	0.9
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB2	9	0.9
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB3	9	0.9
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	6	0.9
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	1	0.9
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	1	0.9
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	4	0.9
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG21	17	0.9
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG22	17	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG23	17	0.9
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	18	0.9
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	5	0.9
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	5	0.9
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	9	0.89
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	3	0.89
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	14	0.89
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	19	0.89
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	12	0.89
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	12	0.89
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	17	0.89
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	10	0.89
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	10	0.89
(1,2071)	1:128:A:PHE:H	1:88:A:ILE:HG12	11	0.88
(1,2071)	1:128:A:PHE:H	1:88:A:ILE:HG13	11	0.88
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	11	0.88
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	11	0.88
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	11	0.88
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	11	0.88
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	11	0.88
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	11	0.88
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB2	4	0.88
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB3	4	0.88
(1,2144)	1:134:A:THR:HB	1:166:A:PHE:HZ	12	0.87
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	5	0.87
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	4	0.86
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	11	0.86
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	11	0.86
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	2	0.86
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	11	0.86
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	11	0.86
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	14	0.86
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	14	0.86
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	7	0.86
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	13	0.85
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	13	0.85
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	17	0.85
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	17	0.85
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	8	0.85
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	8	0.85
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	14	0.84
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	10	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	10	0.84
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	10	0.84
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB2	10	0.84
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB3	10	0.84
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB2	10	0.84
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB3	10	0.84
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	1	0.84
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	16	0.84
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	19	0.84
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	19	0.83
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	20	0.83
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	2	0.83
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB2	4	0.83
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB3	4	0.83
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB2	19	0.83
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB3	19	0.83
(1,1450)	1:80:A:GLU:HG2	1:77:A:LYS:H	4	0.83
(1,1450)	1:80:A:GLU:HG3	1:77:A:LYS:H	4	0.83
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	19	0.83
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB2	3	0.83
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB3	3	0.83
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB2	3	0.83
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB3	3	0.83
(1,307)	1:107:A:PHE:HB2	1:140:A:VAL:HA	18	0.83
(1,307)	1:107:A:PHE:HB3	1:140:A:VAL:HA	18	0.83
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	3	0.83
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	3	0.83
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	17	0.82
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	10	0.82
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	10	0.82
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	10	0.82
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	10	0.82
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB2	2	0.82
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB3	2	0.82
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB2	2	0.82
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB3	2	0.82
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	8	0.82
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	8	0.82
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	19	0.81
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG2	19	0.81
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG3	19	0.81
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	18	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	18	0.81
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	18	0.81
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	18	0.81
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	18	0.81
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	18	0.81
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG21	12	0.81
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG22	12	0.81
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG23	12	0.81
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG21	19	0.81
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG22	19	0.81
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG23	19	0.81
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	1	0.81
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	11	0.81
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	11	0.81
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	11	0.81
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	14	0.81
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	14	0.81
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	20	0.81
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	20	0.81
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	20	0.81
(1,2094)	1:163:A:LEU:HB2	1:90:A:ASN:HD21	9	0.8
(1,2094)	1:163:A:LEU:HB2	1:90:A:ASN:HD22	9	0.8
(1,2094)	1:163:A:LEU:HB3	1:90:A:ASN:HD21	9	0.8
(1,2094)	1:163:A:LEU:HB3	1:90:A:ASN:HD22	9	0.8
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	8	0.8
(1,853)	1:20:A:ASP:HB3	1:17:A:THR:H	11	0.8
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	12	0.8
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	11	0.8
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	11	0.8
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	12	0.79
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG2	16	0.79
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG3	16	0.79
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	8	0.79
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	17	0.79
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	17	0.79
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	17	0.79
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	18	0.79
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB2	18	0.79
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB3	18	0.79
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	5	0.79
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	20	0.79
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	13	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	13	0.79
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	5	0.78
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	16	0.78
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	10	0.78
(1,1909)	1:77:A:LYS:HA	1:3:A:MET:HB2	20	0.78
(1,1909)	1:77:A:LYS:HA	1:3:A:MET:HB3	20	0.78
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	8	0.78
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	8	0.78
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	8	0.78
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	20	0.78
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	20	0.78
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	2	0.78
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	7	0.78
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	12	0.78
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	7	0.78
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	7	0.78
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	18	0.78
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	18	0.78
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	6	0.77
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	18	0.77
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	18	0.77
(1,1935)	1:42:A:THR:HB	1:44:A:LYS:HE2	10	0.77
(1,1935)	1:42:A:THR:HB	1:44:A:LYS:HE3	10	0.77
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB2	17	0.77
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB3	17	0.77
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB2	17	0.77
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB3	17	0.77
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	6	0.77
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	6	0.77
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	20	0.77
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	2	0.77
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	16	0.77
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	16	0.77
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	17	0.76
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	1	0.76
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	8	0.76
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	15	0.76
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	16	0.76
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	16	0.76
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	10	0.76
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	10	0.76
(1,202)	1:111:A:ILE:HG21	1:80:A:GLU:HA	18	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:111:A:ILE:HG22	1:80:A:GLU:HA	18	0.76
(1,202)	1:111:A:ILE:HG23	1:80:A:GLU:HA	18	0.76
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	20	0.76
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	20	0.76
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	20	0.76
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	19	0.76
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	19	0.76
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	15	0.75
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	15	0.75
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	15	0.75
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	13	0.75
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	13	0.75
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	17	0.75
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	10	0.75
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	10	0.75
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	10	0.75
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	10	0.75
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	10	0.75
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	6	0.75
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	6	0.75
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	14	0.75
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	14	0.75
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	14	0.75
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	17	0.75
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	17	0.75
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	17	0.75
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	9	0.75
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	9	0.75
(1,1)	1:20:A:ASP:HB2	1:21:A:LEU:HA	10	0.75
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	13	0.74
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	7	0.74
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	7	0.74
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB2	9	0.74
(1,1456)	1:60:A:GLN:HG2	1:64:A:SER:HB3	9	0.74
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB2	9	0.74
(1,1456)	1:60:A:GLN:HG3	1:64:A:SER:HB3	9	0.74
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	15	0.74
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	8	0.74
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	10	0.74
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	9	0.74
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	9	0.74
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:103:A:MET:HB2	1:104:A:LEU:HB2	18	0.74
(1,308)	1:103:A:MET:HB3	1:104:A:LEU:HB2	18	0.74
(1,2114)	1:112:A:SER:HG	1:113:A:THR:HA	20	0.73
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	20	0.73
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	20	0.73
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	20	0.73
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	10	0.73
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	9	0.73
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	9	0.73
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	9	0.73
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	20	0.73
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	20	0.73
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	20	0.73
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD11	8	0.73
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD12	8	0.73
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD13	8	0.73
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD21	8	0.73
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD22	8	0.73
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD23	8	0.73
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	9	0.73
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	9	0.73
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	12	0.72
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	7	0.72
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	10	0.72
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	8	0.72
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	8	0.72
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	8	0.72
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	9	0.72
(1,387)	1:116:A:LEU:HA	1:124:A:ARG:HD2	16	0.72
(1,387)	1:116:A:LEU:HA	1:124:A:ARG:HD3	16	0.72
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	1	0.72
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	1	0.72
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	1	0.72
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	1	0.72
(1,289)	1:93:A:LEU:HB2	1:95:A:MET:H	17	0.72
(1,289)	1:93:A:LEU:HB3	1:95:A:MET:H	17	0.72
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	10	0.72
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	10	0.72
(1,2139)	1:163:A:LEU:HG	1:164:A:CYS:HA	1	0.71
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	1	0.71
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	1	0.71
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	6	0.71
(1,2053)	1:63:A:VAL:HG21	1:75:A:MET:HE1	5	0.71
(1,2053)	1:63:A:VAL:HG21	1:75:A:MET:HE2	5	0.71
(1,2053)	1:63:A:VAL:HG21	1:75:A:MET:HE3	5	0.71
(1,2053)	1:63:A:VAL:HG22	1:75:A:MET:HE1	5	0.71
(1,2053)	1:63:A:VAL:HG22	1:75:A:MET:HE2	5	0.71
(1,2053)	1:63:A:VAL:HG22	1:75:A:MET:HE3	5	0.71
(1,2053)	1:63:A:VAL:HG23	1:75:A:MET:HE1	5	0.71
(1,2053)	1:63:A:VAL:HG23	1:75:A:MET:HE2	5	0.71
(1,2053)	1:63:A:VAL:HG23	1:75:A:MET:HE3	5	0.71
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	15	0.71
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	15	0.71
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	8	0.71
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	20	0.71
(1,1124)	1:79:A:GLN:HA	1:111:A:ILE:HG21	3	0.71
(1,1124)	1:79:A:GLN:HA	1:111:A:ILE:HG22	3	0.71
(1,1124)	1:79:A:GLN:HA	1:111:A:ILE:HG23	3	0.71
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	8	0.71
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	14	0.71
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	16	0.71
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	16	0.71
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	9	0.71
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	9	0.71
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	17	0.71
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	17	0.71
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	5	0.7
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	5	0.7
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	5	0.7
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	5	0.7
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	5	0.7
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	5	0.7
(1,2134)	1:163:A:LEU:HB2	1:90:A:ASN:HD21	9	0.7
(1,2134)	1:163:A:LEU:HB2	1:90:A:ASN:HD22	9	0.7
(1,2134)	1:163:A:LEU:HB3	1:90:A:ASN:HD21	9	0.7
(1,2134)	1:163:A:LEU:HB3	1:90:A:ASN:HD22	9	0.7
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB2	13	0.7
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB3	13	0.7
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB2	13	0.7
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB3	13	0.7
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	4	0.7
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	5	0.7
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	2	0.7
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	2	0.7
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	2	0.7
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	2	0.7
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	2	0.7
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	2	0.7
(1,1985)	1:8:A:TYR:HD1	1:74:A:GLN:HG2	20	0.7
(1,1985)	1:8:A:TYR:HD1	1:74:A:GLN:HG3	20	0.7
(1,1985)	1:8:A:TYR:HD2	1:74:A:GLN:HG2	20	0.7
(1,1985)	1:8:A:TYR:HD2	1:74:A:GLN:HG3	20	0.7
(1,1956)	1:77:A:LYS:HB2	1:3:A:MET:HA	11	0.7
(1,1956)	1:77:A:LYS:HB3	1:3:A:MET:HA	11	0.7
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	19	0.7
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	5	0.7
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	6	0.7
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	7	0.7
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	11	0.7
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	8	0.7
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	13	0.7
(1,391)	1:116:A:LEU:HB2	1:126:A:VAL:H	20	0.7
(1,391)	1:116:A:LEU:HB3	1:126:A:VAL:H	20	0.7
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	18	0.7
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	18	0.7
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	7	0.7
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	7	0.7
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	7	0.7
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	7	0.7
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	10	0.69
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	10	0.69
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	10	0.69
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	10	0.69
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	18	0.69
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	18	0.69
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	18	0.69
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	18	0.69
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	18	0.69
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	18	0.69
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	17	0.69
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	17	0.69
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	19	0.69
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	11	0.69
(1,1540)	1:30:A:LYS:HE2	1:31:A:ILE:H	20	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1540)	1:30:A:LYS:HE3	1:31:A:ILE:H	20	0.69
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	3	0.69
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	3	0.69
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	20	0.69
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	13	0.69
(1,493)	1:111:A:ILE:HB	1:79:A:GLN:HB2	3	0.69
(1,493)	1:111:A:ILE:HB	1:79:A:GLN:HB3	3	0.69
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	2	0.69
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	11	0.69
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	14	0.69
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	8	0.68
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	8	0.68
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	8	0.68
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	8	0.68
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	8	0.68
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	8	0.68
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	1	0.68
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	1	0.68
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	10	0.68
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	12	0.68
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	12	0.68
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	12	0.68
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	12	0.68
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	12	0.68
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	12	0.68
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	17	0.68
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	3	0.68
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	15	0.68
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	13	0.68
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	13	0.68
(1,151)	1:95:A:MET:HG2	1:115:A:ILE:HG12	15	0.68
(1,151)	1:95:A:MET:HG2	1:115:A:ILE:HG13	15	0.68
(1,151)	1:95:A:MET:HG3	1:115:A:ILE:HG12	15	0.68
(1,151)	1:95:A:MET:HG3	1:115:A:ILE:HG13	15	0.68
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	5	0.68
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	20	0.68
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	11	0.68
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	11	0.68
(1,2144)	1:134:A:THR:HB	1:166:A:PHE:HZ	16	0.67
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	9	0.67
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	9	0.67
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	9	0.67
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	9	0.67
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	9	0.67
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	16	0.67
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	16	0.67
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	1	0.67
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	1	0.67
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	11	0.67
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	11	0.67
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	11	0.67
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	13	0.67
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	13	0.67
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	13	0.67
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	13	0.67
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	13	0.67
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	13	0.67
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	16	0.67
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	16	0.67
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	16	0.67
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	16	0.67
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	16	0.67
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	16	0.67
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	1	0.67
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	12	0.67
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	9	0.67
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	5	0.67
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	5	0.67
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	6	0.67
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	6	0.67
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	20	0.67
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	20	0.67
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	11	0.66
(1,1935)	1:42:A:THR:HB	1:44:A:LYS:HE2	12	0.66
(1,1935)	1:42:A:THR:HB	1:44:A:LYS:HE3	12	0.66
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	19	0.66
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD1	11	0.66
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD2	11	0.66
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD1	11	0.66
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD2	11	0.66
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG2	18	0.66
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG3	18	0.66
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2117)	1:101:A:GLU:HG2	1:113:A:THR:H	1	0.65
(1,2117)	1:101:A:GLU:HG3	1:113:A:THR:H	1	0.65
(1,2117)	1:101:A:GLU:HG2	1:113:A:THR:H	1	0.65
(1,2117)	1:101:A:GLU:HG3	1:113:A:THR:H	1	0.65
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	2	0.65
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	1	0.65
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	18	0.65
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	18	0.65
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	12	0.65
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	16	0.65
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	1	0.65
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	1	0.65
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	1	0.65
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	1	0.65
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	1	0.65
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	1	0.65
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	8	0.65
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	16	0.65
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	11	0.65
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	11	0.65
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	3	0.65
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	15	0.65
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	14	0.64
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	17	0.64
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD11	12	0.64
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD12	12	0.64
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD13	12	0.64
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	16	0.64
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	16	0.64
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	16	0.64
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	16	0.64
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	16	0.64
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	16	0.64
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	16	0.64
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	16	0.64
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	17	0.64
(1,1330)	1:34:A:THR:HG21	1:9:A:ILE:HD11	11	0.64
(1,1330)	1:34:A:THR:HG21	1:9:A:ILE:HD12	11	0.64
(1,1330)	1:34:A:THR:HG21	1:9:A:ILE:HD13	11	0.64
(1,1330)	1:34:A:THR:HG22	1:9:A:ILE:HD11	11	0.64
(1,1330)	1:34:A:THR:HG22	1:9:A:ILE:HD12	11	0.64
(1,1330)	1:34:A:THR:HG22	1:9:A:ILE:HD13	11	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:34:A:THR:HG23	1:9:A:ILE:HD11	11	0.64
(1,1330)	1:34:A:THR:HG23	1:9:A:ILE:HD12	11	0.64
(1,1330)	1:34:A:THR:HG23	1:9:A:ILE:HD13	11	0.64
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	15	0.64
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	20	0.64
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	1	0.64
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	1	0.64
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	3	0.64
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	3	0.64
(1,2115)	1:130:A:ARG:H	1:104:A:LEU:HD21	18	0.63
(1,2115)	1:130:A:ARG:H	1:104:A:LEU:HD22	18	0.63
(1,2115)	1:130:A:ARG:H	1:104:A:LEU:HD23	18	0.63
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	16	0.63
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	2	0.63
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	19	0.63
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	17	0.63
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	17	0.63
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	17	0.63
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	18	0.63
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	18	0.63
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	11	0.63
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	14	0.63
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	1	0.63
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	1	0.63
(1,522)	1:139:A:ALA:HA	1:143:A:HIS:H	12	0.63
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	16	0.63
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	16	0.63
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	13	0.63
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	13	0.63
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	16	0.63
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	3	0.63
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	8	0.62
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG2	14	0.62
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG3	14	0.62
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	6	0.62
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	6	0.62
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	6	0.62
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	6	0.62
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	20	0.62
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	11	0.62
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	17	0.62
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	6	0.62
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	6	0.62
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	1	0.62
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	1	0.62
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	7	0.62
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	5	0.62
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	3	0.62
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	3	0.62
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	9	0.62
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	9	0.62
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	12	0.62
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	13	0.62
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	19	0.61
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	19	0.61
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	13	0.61
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	7	0.61
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	7	0.61
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	19	0.61
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	19	0.61
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	2	0.61
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	2	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	9	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	9	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	9	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	9	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	9	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	9	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	17	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	17	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	17	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	17	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	17	0.61
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	17	0.61
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	2	0.61
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	9	0.61
(1,1072)	1:77:A:LYS:HB2	1:4:A:GLY:H	11	0.61
(1,1072)	1:77:A:LYS:HB3	1:4:A:GLY:H	11	0.61
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	13	0.61
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	13	0.61
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	13	0.61
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	13	0.61
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	5	0.61
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	5	0.61
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	19	0.61
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	14	0.61
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	19	0.61
(1,136)	1:78:A:GLN:HB2	1:2:A:ALA:HB1	16	0.61
(1,136)	1:78:A:GLN:HB2	1:2:A:ALA:HB2	16	0.61
(1,136)	1:78:A:GLN:HB2	1:2:A:ALA:HB3	16	0.61
(1,136)	1:78:A:GLN:HB3	1:2:A:ALA:HB1	16	0.61
(1,136)	1:78:A:GLN:HB3	1:2:A:ALA:HB2	16	0.61
(1,136)	1:78:A:GLN:HB3	1:2:A:ALA:HB3	16	0.61
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	16	0.61
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	16	0.61
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	8	0.61
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	19	0.61
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	15	0.6
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	13	0.6
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG2	15	0.6
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG3	15	0.6
(1,2094)	1:163:A:LEU:HB2	1:90:A:ASN:HD21	13	0.6
(1,2094)	1:163:A:LEU:HB2	1:90:A:ASN:HD22	13	0.6
(1,2094)	1:163:A:LEU:HB3	1:90:A:ASN:HD21	13	0.6
(1,2094)	1:163:A:LEU:HB3	1:90:A:ASN:HD22	13	0.6
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	19	0.6
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	20	0.6
(1,1962)	1:8:A:TYR:HB3	1:10:A:ARG:HD2	12	0.6
(1,1962)	1:8:A:TYR:HB3	1:10:A:ARG:HD3	12	0.6
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	15	0.6
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	2	0.6
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	2	0.6
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	12	0.6
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	12	0.6
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	5	0.6
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	5	0.6
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	5	0.6
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	14	0.6
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	14	0.6
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	14	0.6
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	2	0.6
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	5	0.6
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	1	0.6
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	1	0.6
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	1	0.6
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	3	0.6
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	14	0.6
(1,611)	1:156:A:SER:HA	1:155:A:VAL:H	18	0.6
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	19	0.6
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	19	0.6
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	3	0.6
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	3	0.6
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	20	0.6
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	20	0.6
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	6	0.6
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	6	0.6
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	6	0.6
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	5	0.6
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	5	0.6
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	1	0.6
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	20	0.59
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	20	0.59
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	14	0.59
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	16	0.59
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	4	0.59
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	4	0.59
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB2	6	0.59
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB3	6	0.59
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB2	6	0.59
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB3	6	0.59
(1,415)	1:116:A:LEU:HA	1:128:A:PHE:HE1	20	0.59
(1,415)	1:116:A:LEU:HA	1:128:A:PHE:HE2	20	0.59
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	20	0.59
(1,55)	1:37:A:ILE:HA	1:38:A:LEU:HG	6	0.59
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	11	0.58
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB2	20	0.58
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB3	20	0.58
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB2	20	0.58
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB3	20	0.58
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	9	0.58
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	9	0.58
(1,1961)	1:19:A:GLN:HG2	1:22:A:VAL:HB	20	0.58
(1,1961)	1:19:A:GLN:HG3	1:22:A:VAL:HB	20	0.58
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	15	0.58
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	3	0.58
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	3	0.58
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	17	0.58
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	17	0.58
(1,1655)	1:162:A:LEU:HG	1:164:A:CYS:H	13	0.58
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	16	0.58
(1,772)	1:72:A:GLN:HB2	1:10:A:ARG:HG2	18	0.58
(1,772)	1:72:A:GLN:HB2	1:10:A:ARG:HG3	18	0.58
(1,772)	1:72:A:GLN:HB3	1:10:A:ARG:HG2	18	0.58
(1,772)	1:72:A:GLN:HB3	1:10:A:ARG:HG3	18	0.58
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	16	0.58
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	7	0.58
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	7	0.58
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	5	0.58
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	4	0.58
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	4	0.58
(1,55)	1:37:A:ILE:HA	1:38:A:LEU:HG	11	0.58
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD11	5	0.57
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD12	5	0.57
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD13	5	0.57
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	20	0.57
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	12	0.57
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	7	0.57
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	7	0.57
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	20	0.57
(1,1500)	1:40:A:LYS:HG2	1:39:A:ASP:HA	4	0.57
(1,1500)	1:40:A:LYS:HG3	1:39:A:ASP:HA	4	0.57
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	13	0.57
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	13	0.57
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	13	0.57
(1,1175)	1:23:A:LYS:HG2	1:19:A:GLN:HA	5	0.57
(1,1175)	1:23:A:LYS:HG3	1:19:A:GLN:HA	5	0.57
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	4	0.57
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	4	0.57
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	4	0.57
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	4	0.57
(1,1039)	1:19:A:GLN:HG2	1:20:A:ASP:HA	6	0.57
(1,1039)	1:19:A:GLN:HG3	1:20:A:ASP:HA	6	0.57
(1,676)	1:151:A:THR:HA	1:155:A:VAL:HB	3	0.57
(1,665)	1:149:A:ILE:HG12	1:160:A:GLU:H	14	0.57
(1,665)	1:149:A:ILE:HG13	1:160:A:GLU:H	14	0.57
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	20	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	14	0.57
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	14	0.57
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	5	0.57
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	6	0.57
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	6	0.57
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	6	0.57
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	6	0.57
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	3	0.57
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	11	0.57
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	7	0.57
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	7	0.57
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	14	0.57
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	14	0.57
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	19	0.56
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	2	0.56
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	18	0.56
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	2	0.56
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	2	0.56
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	7	0.56
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	7	0.56
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	7	0.56
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	16	0.56
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	16	0.56
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	16	0.56
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	11	0.56
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	11	0.56
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	5	0.56
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	5	0.56
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	9	0.56
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	9	0.56
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	16	0.56
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	16	0.56
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	16	0.56
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	16	0.56
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	16	0.56
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	16	0.56
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	17	0.56
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	17	0.56
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	17	0.56
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	19	0.56
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	19	0.56
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	19	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	19	0.56
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	2	0.56
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	2	0.56
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	2	0.56
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	2	0.56
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	1	0.56
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	8	0.56
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	8	0.56
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	12	0.56
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG2	8	0.56
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG3	8	0.56
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB2	16	0.56
(1,887)	1:78:A:GLN:HB2	1:81:A:GLN:HB3	16	0.56
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB2	16	0.56
(1,887)	1:78:A:GLN:HB3	1:81:A:GLN:HB3	16	0.56
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	1	0.56
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	2	0.56
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	6	0.56
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	10	0.56
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	10	0.56
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	2	0.55
(1,2044)	1:74:A:GLN:HG2	1:76:A:ALA:H	18	0.55
(1,2044)	1:74:A:GLN:HG3	1:76:A:ALA:H	18	0.55
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	9	0.55
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	9	0.55
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	9	0.55
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	3	0.55
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	3	0.55
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	7	0.55
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	7	0.55
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	13	0.55
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	13	0.55
(1,1853)	1:31:A:ILE:HB	1:22:A:VAL:HA	6	0.55
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	20	0.55
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	20	0.55
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	7	0.55
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG12	11	0.55
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG13	11	0.55
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	16	0.55
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	16	0.55
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	17	0.55
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	16	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	18	0.55
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	2	0.55
(1,676)	1:151:A:THR:HA	1:155:A:VAL:HB	10	0.55
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	9	0.55
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	12	0.55
(1,614)	1:162:A:LEU:HG	1:90:A:ASN:HB2	12	0.55
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	14	0.55
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	14	0.55
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	12	0.55
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	12	0.55
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	12	0.55
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	12	0.55
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	5	0.55
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	5	0.55
(1,202)	1:111:A:ILE:HG21	1:80:A:GLU:HA	12	0.55
(1,202)	1:111:A:ILE:HG22	1:80:A:GLU:HA	12	0.55
(1,202)	1:111:A:ILE:HG23	1:80:A:GLU:HA	12	0.55
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	8	0.55
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	19	0.54
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	20	0.54
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	20	0.54
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	20	0.54
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	13	0.54
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	13	0.54
(1,1961)	1:19:A:GLN:HG2	1:22:A:VAL:HB	11	0.54
(1,1961)	1:19:A:GLN:HG3	1:22:A:VAL:HB	11	0.54
(1,1909)	1:77:A:LYS:HA	1:3:A:MET:HB2	11	0.54
(1,1909)	1:77:A:LYS:HA	1:3:A:MET:HB3	11	0.54
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	10	0.54
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	10	0.54
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	12	0.54
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	9	0.54
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	11	0.54
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	17	0.54
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	2	0.54
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	2	0.54
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG21	19	0.54
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG22	19	0.54
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG23	19	0.54
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	20	0.54
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	20	0.54
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	20	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	20	0.54
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	20	0.54
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	20	0.54
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	10	0.54
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	8	0.54
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	7	0.54
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	12	0.54
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	1	0.54
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	1	0.54
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	17	0.54
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG2	17	0.54
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG3	17	0.54
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	2	0.54
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	2	0.54
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	16	0.54
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB2	19	0.54
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB3	19	0.54
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	6	0.54
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	17	0.54
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	17	0.54
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	17	0.54
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	17	0.54
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	2	0.54
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	2	0.54
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	4	0.54
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	4	0.54
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	13	0.54
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	16	0.54
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	16	0.54
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	10	0.54
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	11	0.53
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	11	0.53
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	5	0.53
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	5	0.53
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	5	0.53
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB2	8	0.53
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB3	8	0.53
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB2	8	0.53
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB3	8	0.53
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	7	0.53
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	17	0.53
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	6	0.53
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	6	0.53
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	6	0.53
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	6	0.53
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	6	0.53
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB1	18	0.53
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB2	18	0.53
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB3	18	0.53
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB1	18	0.53
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB2	18	0.53
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB3	18	0.53
(1,1540)	1:30:A:LYS:HE2	1:31:A:ILE:H	2	0.53
(1,1540)	1:30:A:LYS:HE3	1:31:A:ILE:H	2	0.53
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	14	0.53
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	1	0.53
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	9	0.53
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	17	0.53
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	8	0.53
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	3	0.53
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	8	0.53
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	8	0.53
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	2	0.53
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	7	0.53
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE1	11	0.53
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE2	11	0.53
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	5	0.52
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	5	0.52
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	4	0.52
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	4	0.52
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	4	0.52
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	16	0.52
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	16	0.52
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	20	0.52
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	20	0.52
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	20	0.52
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	20	0.52
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	20	0.52
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	20	0.52
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	5	0.52
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	5	0.52
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	16	0.52
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	16	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	15	0.52
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	7	0.52
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	7	0.52
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	7	0.52
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	7	0.52
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	7	0.52
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG2	13	0.52
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG3	13	0.52
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	5	0.52
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	6	0.52
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	15	0.52
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	8	0.52
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	20	0.52
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD11	17	0.52
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD12	17	0.52
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD13	17	0.52
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD21	17	0.52
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD22	17	0.52
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD23	17	0.52
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	5	0.52
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	5	0.52
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	5	0.52
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	5	0.52
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	16	0.52
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	16	0.52
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	16	0.52
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	16	0.52
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	18	0.52
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG2	6	0.52
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG3	6	0.52
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	14	0.52
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	15	0.52
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	15	0.52
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	20	0.52
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	20	0.52
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	8	0.52
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	12	0.52
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	14	0.52
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB2	5	0.52
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB3	5	0.52
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	7	0.52
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	18	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	14	0.51
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	8	0.51
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	4	0.51
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	4	0.51
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	4	0.51
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	19	0.51
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	9	0.51
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	9	0.51
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	9	0.51
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	9	0.51
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB2	6	0.51
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB3	6	0.51
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	16	0.51
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	19	0.51
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	3	0.51
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	4	0.51
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	4	0.51
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	4	0.51
(1,1369)	1:74:A:GLN:HB2	1:10:A:ARG:HG2	17	0.51
(1,1369)	1:74:A:GLN:HB2	1:10:A:ARG:HG3	17	0.51
(1,1369)	1:74:A:GLN:HB3	1:10:A:ARG:HG2	17	0.51
(1,1369)	1:74:A:GLN:HB3	1:10:A:ARG:HG3	17	0.51
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	10	0.51
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	17	0.51
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	20	0.51
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG21	6	0.51
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG22	6	0.51
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG23	6	0.51
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	15	0.51
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	15	0.51
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	2	0.51
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	2	0.51
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB2	5	0.51
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB3	5	0.51
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB2	5	0.51
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB3	5	0.51
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	1	0.51
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	11	0.51
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	12	0.51
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	11	0.51
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	18	0.51
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	11	0.51
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	11	0.51
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	13	0.51
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	12	0.51
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	2	0.51
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	2	0.51
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	2	0.51
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	2	0.51
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	5	0.51
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	20	0.51
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	20	0.51
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	20	0.51
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	20	0.51
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	3	0.51
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	11	0.51
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	11	0.51
(1,2134)	1:163:A:LEU:HB2	1:90:A:ASN:HD21	13	0.5
(1,2134)	1:163:A:LEU:HB2	1:90:A:ASN:HD22	13	0.5
(1,2134)	1:163:A:LEU:HB3	1:90:A:ASN:HD21	13	0.5
(1,2134)	1:163:A:LEU:HB3	1:90:A:ASN:HD22	13	0.5
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	16	0.5
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	16	0.5
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	5	0.5
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	5	0.5
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	1	0.5
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	18	0.5
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	18	0.5
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	9	0.5
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	9	0.5
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	19	0.5
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	19	0.5
(1,1669)	1:165:A:LYS:HD2	1:166:A:PHE:H	8	0.5
(1,1669)	1:165:A:LYS:HD3	1:166:A:PHE:H	8	0.5
(1,1655)	1:162:A:LEU:HG	1:164:A:CYS:H	3	0.5
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	11	0.5
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	11	0.5
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	11	0.5
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	6	0.5
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	10	0.5
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	10	0.5
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	10	0.5
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	16	0.5
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	16	0.5
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	16	0.5
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	16	0.5
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	5	0.5
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	9	0.5
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	10	0.5
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	4	0.5
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	4	0.5
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	14	0.5
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	18	0.5
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	9	0.5
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB2	14	0.5
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB3	14	0.5
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB2	14	0.5
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB3	14	0.5
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	8	0.5
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	8	0.5
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	15	0.5
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	20	0.5
(1,614)	1:162:A:LEU:HG	1:90:A:ASN:HB2	7	0.5
(1,484)	1:109:A:GLN:HB2	1:136:A:LYS:HE2	19	0.5
(1,484)	1:109:A:GLN:HB2	1:136:A:LYS:HE3	19	0.5
(1,484)	1:109:A:GLN:HB3	1:136:A:LYS:HE2	19	0.5
(1,484)	1:109:A:GLN:HB3	1:136:A:LYS:HE3	19	0.5
(1,396)	1:120:A:SER:HA	1:122:A:THR:H	9	0.5
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	1	0.5
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	1	0.5
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	3	0.5
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	8	0.5
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	13	0.5
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	13	0.5
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	17	0.49
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	17	0.49
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	15	0.49
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	11	0.49
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	11	0.49
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	11	0.49
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	15	0.49
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	15	0.49
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	15	0.49
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	11	0.49
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	9	0.49
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	9	0.49
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	11	0.49
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	11	0.49
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	12	0.49
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	4	0.49
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	4	0.49
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	4	0.49
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	4	0.49
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	4	0.49
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	4	0.49
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	10	0.49
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	6	0.49
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	7	0.49
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	6	0.49
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	6	0.49
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	6	0.49
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	6	0.49
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	5	0.49
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	6	0.49
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	6	0.49
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	6	0.49
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	6	0.49
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	8	0.49
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	11	0.49
(1,779)	1:77:A:LYS:HA	1:3:A:MET:H	20	0.49
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	10	0.49
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	10	0.49
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	8	0.49
(1,611)	1:156:A:SER:HA	1:155:A:VAL:H	6	0.49
(1,533)	1:136:A:LYS:HE2	1:109:A:GLN:H	18	0.49
(1,533)	1:136:A:LYS:HE3	1:109:A:GLN:H	18	0.49
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	17	0.49
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	1	0.49
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	6	0.49
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	5	0.49
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	5	0.49
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	17	0.49
(1,2144)	1:134:A:THR:HB	1:166:A:PHE:HZ	8	0.48
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	13	0.48
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	14	0.48
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	14	0.48
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	19	0.48
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	2	0.48
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	6	0.48
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	17	0.48
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	13	0.48
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	2	0.48
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	2	0.48
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	2	0.48
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	2	0.48
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	2	0.48
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	2	0.48
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	2	0.48
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB2	4	0.48
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB3	4	0.48
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	7	0.48
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG21	15	0.48
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG22	15	0.48
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG23	15	0.48
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	11	0.48
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	11	0.48
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	11	0.48
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	11	0.48
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	11	0.48
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	11	0.48
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	18	0.48
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	18	0.48
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	18	0.48
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	18	0.48
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	10	0.48
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	10	0.48
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	10	0.48
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	15	0.48
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	15	0.48
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	12	0.48
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	18	0.48
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	20	0.48
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	2	0.48
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	12	0.48
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	19	0.48
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	4	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	4	0.48
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	15	0.48
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	5	0.48
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	5	0.48
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	13	0.48
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	13	0.48
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	20	0.48
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	20	0.48
(1,313)	1:106:A:PRO:HD2	1:108:A:GLY:H	10	0.48
(1,313)	1:106:A:PRO:HD3	1:108:A:GLY:H	10	0.48
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	12	0.48
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	20	0.48
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	4	0.48
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	4	0.48
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	8	0.47
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	8	0.47
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	20	0.47
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	1	0.47
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	17	0.47
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	19	0.47
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	19	0.47
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	19	0.47
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	9	0.47
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	9	0.47
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	9	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	3	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	3	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	3	0.47
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	3	0.47
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	3	0.47
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	3	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	5	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	5	0.47
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	5	0.47
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	5	0.47
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	5	0.47
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	5	0.47
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	12	0.47
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	6	0.47
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	12	0.47
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	12	0.47
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	20	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	20	0.47
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	3	0.47
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	3	0.47
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	3	0.47
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	3	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	1	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	1	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	1	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	1	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	1	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	1	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	5	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	5	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	5	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	5	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	5	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	5	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	19	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	19	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	19	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	19	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	19	0.47
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	19	0.47
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	15	0.47
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	11	0.47
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	2	0.47
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	4	0.47
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	4	0.47
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	17	0.47
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	8	0.47
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	8	0.47
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	8	0.47
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	8	0.47
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	5	0.47
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	5	0.47
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	5	0.47
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	5	0.47
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	7	0.47
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD11	19	0.47
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD12	19	0.47
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD13	19	0.47
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD11	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD12	19	0.47
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD13	19	0.47
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD11	19	0.47
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD12	19	0.47
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD13	19	0.47
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	18	0.47
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	18	0.47
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	9	0.47
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	9	0.47
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	2	0.47
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	9	0.47
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	1	0.47
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	2	0.47
(1,352)	1:86:A:LEU:HG	1:85:A:ASN:H	4	0.47
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	3	0.47
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	3	0.47
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	20	0.47
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	20	0.47
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	19	0.47
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	5	0.47
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	5	0.47
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	18	0.46
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	18	0.46
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD11	6	0.46
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD12	6	0.46
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD13	6	0.46
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	13	0.46
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	2	0.46
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	10	0.46
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	10	0.46
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	15	0.46
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	15	0.46
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	12	0.46
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	12	0.46
(1,1669)	1:165:A:LYS:HD2	1:166:A:PHE:H	7	0.46
(1,1669)	1:165:A:LYS:HD3	1:166:A:PHE:H	7	0.46
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	12	0.46
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	1	0.46
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	1	0.46
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	19	0.46
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	19	0.46
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG2	10	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG3	10	0.46
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	3	0.46
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	3	0.46
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	3	0.46
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	3	0.46
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	12	0.46
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	15	0.46
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	15	0.46
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	15	0.46
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	15	0.46
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	3	0.46
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	8	0.46
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	7	0.46
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	11	0.46
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	15	0.46
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	11	0.46
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	11	0.46
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	11	0.46
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	11	0.46
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	17	0.46
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	8	0.46
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	17	0.46
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	17	0.46
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	12	0.46
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	12	0.46
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	20	0.46
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	7	0.46
(1,522)	1:139:A:ALA:HA	1:143:A:HIS:H	13	0.46
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	6	0.46
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	17	0.46
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	3	0.46
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	3	0.46
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	6	0.46
(1,352)	1:86:A:LEU:HG	1:85:A:ASN:H	18	0.46
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	14	0.46
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	16	0.46
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	1	0.46
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	1	0.46
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	1	0.46
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	1	0.46
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	16	0.46
(1,33)	1:60:A:GLN:HG2	1:61:A:LYS:HA	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:60:A:GLN:HG3	1:61:A:LYS:HA	1	0.46
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	15	0.46
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	20	0.46
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	13	0.46
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	13	0.46
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	13	0.46
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	13	0.46
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	13	0.46
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	13	0.46
(1,2114)	1:112:A:SER:HG	1:113:A:THR:HA	11	0.45
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	18	0.45
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	9	0.45
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	12	0.45
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	12	0.45
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	4	0.45
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	2	0.45
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	17	0.45
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	17	0.45
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	17	0.45
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	5	0.45
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	11	0.45
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	11	0.45
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	11	0.45
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	11	0.45
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	11	0.45
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	11	0.45
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	11	0.45
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	14	0.45
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	20	0.45
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	3	0.45
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	3	0.45
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	3	0.45
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	3	0.45
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	6	0.45
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	16	0.45
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	16	0.45
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	5	0.45
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	6	0.45
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	19	0.45
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	19	0.45
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	13	0.45
(1,1015)	1:23:A:LYS:HG2	1:22:A:VAL:HB	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:23:A:LYS:HG3	1:22:A:VAL:HB	13	0.45
(1,984)	1:128:A:PHE:HB2	1:88:A:ILE:HG12	11	0.45
(1,984)	1:128:A:PHE:HB2	1:88:A:ILE:HG13	11	0.45
(1,984)	1:128:A:PHE:HB3	1:88:A:ILE:HG12	11	0.45
(1,984)	1:128:A:PHE:HB3	1:88:A:ILE:HG13	11	0.45
(1,973)	1:60:A:GLN:HG2	1:64:A:SER:H	9	0.45
(1,973)	1:60:A:GLN:HG3	1:64:A:SER:H	9	0.45
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	7	0.45
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	6	0.45
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	15	0.45
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	19	0.45
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	3	0.45
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	9	0.45
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	9	0.45
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	14	0.45
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	15	0.45
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	15	0.45
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	18	0.45
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	18	0.45
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	18	0.45
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	2	0.45
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	15	0.44
(1,2028)	1:59:A:ALA:HB1	1:53:A:PHE:HE1	1	0.44
(1,2028)	1:59:A:ALA:HB2	1:53:A:PHE:HE1	1	0.44
(1,2028)	1:59:A:ALA:HB3	1:53:A:PHE:HE1	1	0.44
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	9	0.44
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	9	0.44
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	16	0.44
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	19	0.44
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	19	0.44
(1,1682)	1:166:A:PHE:HA	1:137:A:CYS:HB2	16	0.44
(1,1682)	1:166:A:PHE:HA	1:137:A:CYS:HB3	16	0.44
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	15	0.44
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	15	0.44
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	18	0.44
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	18	0.44
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	6	0.44
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	11	0.44
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	8	0.44
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	9	0.44
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	20	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	3	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	3	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	3	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	11	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	11	0.44
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	11	0.44
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	19	0.44
(1,1170)	1:20:A:ASP:HA	1:24:A:LEU:HG	14	0.44
(1,973)	1:60:A:GLN:HG2	1:64:A:SER:H	17	0.44
(1,973)	1:60:A:GLN:HG3	1:64:A:SER:H	17	0.44
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	14	0.44
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	6	0.44
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG21	1	0.44
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG22	1	0.44
(1,673)	1:151:A:THR:HA	1:149:A:ILE:HG23	1	0.44
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	11	0.44
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	14	0.44
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	14	0.44
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	14	0.44
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	14	0.44
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	17	0.44
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	2	0.44
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	11	0.44
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	18	0.44
(1,117)	1:60:A:GLN:HA	1:75:A:MET:HG2	1	0.44
(1,117)	1:60:A:GLN:HA	1:75:A:MET:HG3	1	0.44
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	13	0.44
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	13	0.44
(1,33)	1:60:A:GLN:HG2	1:61:A:LYS:HA	16	0.44
(1,33)	1:60:A:GLN:HG3	1:61:A:LYS:HA	16	0.44
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	9	0.44
(1,2139)	1:163:A:LEU:HG	1:164:A:CYS:HA	7	0.43
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD11	11	0.43
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD12	11	0.43
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD13	11	0.43
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	5	0.43
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	5	0.43
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	5	0.43
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	17	0.43
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	17	0.43
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	11	0.43
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	15	0.43
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	10	0.43
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	10	0.43
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	6	0.43
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	2	0.43
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	5	0.43
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	5	0.43
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	6	0.43
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	6	0.43
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	15	0.43
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB2	6	0.43
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB3	6	0.43
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB2	6	0.43
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB3	6	0.43
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	3	0.43
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	14	0.43
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	16	0.43
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	16	0.43
(1,785)	1:74:A:GLN:HG2	1:75:A:MET:H	18	0.43
(1,785)	1:74:A:GLN:HG3	1:75:A:MET:H	18	0.43
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	3	0.43
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	3	0.43
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	10	0.43
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	12	0.43
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	11	0.43
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	14	0.43
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	20	0.43
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	20	0.43
(1,513)	1:110:A:VAL:HB	1:132:A:GLU:H	10	0.43
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	18	0.43
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	18	0.43
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	16	0.43
(1,416)	1:122:A:THR:HB	1:120:A:SER:HB2	9	0.43
(1,416)	1:122:A:THR:HB	1:120:A:SER:HB3	9	0.43
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	8	0.43
(1,308)	1:103:A:MET:HB2	1:104:A:LEU:HB2	9	0.43
(1,308)	1:103:A:MET:HB3	1:104:A:LEU:HB2	9	0.43
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	3	0.43
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	3	0.43
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	2	0.43
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	4	0.43
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	9	0.43
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	5	0.43
(1,194)	1:97:A:GLU:HB2	1:115:A:ILE:HG12	4	0.43
(1,194)	1:97:A:GLU:HB2	1:115:A:ILE:HG13	4	0.43
(1,194)	1:97:A:GLU:HB3	1:115:A:ILE:HG12	4	0.43
(1,194)	1:97:A:GLU:HB3	1:115:A:ILE:HG13	4	0.43
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	12	0.43
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	13	0.42
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	2	0.42
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	2	0.42
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	2	0.42
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	6	0.42
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	4	0.42
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	17	0.42
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	18	0.42
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	1	0.42
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	1	0.42
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB2	8	0.42
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB3	8	0.42
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	4	0.42
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	14	0.42
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	14	0.42
(1,1750)	1:37:A:ILE:HB	1:46:A:LYS:HG2	1	0.42
(1,1750)	1:37:A:ILE:HB	1:46:A:LYS:HG3	1	0.42
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	9	0.42
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	12	0.42
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	12	0.42
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	12	0.42
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	13	0.42
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	14	0.42
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	2	0.42
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	2	0.42
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD11	1	0.42
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD12	1	0.42
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD13	1	0.42
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD21	1	0.42
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD22	1	0.42
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD23	1	0.42
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	13	0.42
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	5	0.42
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	12	0.42
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	18	0.42
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	3	0.42
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	16	0.42
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	16	0.42
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	15	0.42
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	15	0.42
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	14	0.42
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	20	0.42
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	1	0.42
(1,614)	1:162:A:LEU:HG	1:90:A:ASN:HB2	14	0.42
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	16	0.42
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	16	0.42
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	3	0.42
(1,398)	1:123:A:SER:HA	1:126:A:VAL:H	12	0.42
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	3	0.42
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	18	0.42
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	12	0.42
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	12	0.42
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	7	0.42
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	10	0.42
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	12	0.42
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	12	0.42
(1,194)	1:97:A:GLU:HB2	1:115:A:ILE:HG12	10	0.42
(1,194)	1:97:A:GLU:HB2	1:115:A:ILE:HG13	10	0.42
(1,194)	1:97:A:GLU:HB3	1:115:A:ILE:HG12	10	0.42
(1,194)	1:97:A:GLU:HB3	1:115:A:ILE:HG13	10	0.42
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	7	0.42
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	19	0.42
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	19	0.42
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	12	0.42
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	12	0.42
(1,60)	1:157:A:ALA:HB1	1:90:A:ASN:HA	20	0.42
(1,60)	1:157:A:ALA:HB2	1:90:A:ASN:HA	20	0.42
(1,60)	1:157:A:ALA:HB3	1:90:A:ASN:HA	20	0.42
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	11	0.42
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	15	0.41
(1,2130)	1:48:A:TYR:HD1	1:46:A:LYS:H	17	0.41
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	5	0.41
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	7	0.41
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	12	0.41
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD11	1	0.41
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD12	1	0.41
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD13	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	1	0.41
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	18	0.41
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	12	0.41
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	12	0.41
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG2	12	0.41
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG3	12	0.41
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	17	0.41
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	17	0.41
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	10	0.41
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	4	0.41
(1,1919)	1:67:A:LYS:HE2	1:72:A:GLN:HA	3	0.41
(1,1919)	1:67:A:LYS:HE3	1:72:A:GLN:HA	3	0.41
(1,1839)	1:50:A:PHE:HE1	1:34:A:THR:HA	19	0.41
(1,1839)	1:50:A:PHE:HE2	1:34:A:THR:HA	19	0.41
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	3	0.41
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	15	0.41
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	1	0.41
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	9	0.41
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	9	0.41
(1,1669)	1:165:A:LYS:HD2	1:166:A:PHE:H	3	0.41
(1,1669)	1:165:A:LYS:HD3	1:166:A:PHE:H	3	0.41
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	11	0.41
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	11	0.41
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	11	0.41
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	11	0.41
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	18	0.41
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	18	0.41
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	18	0.41
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	18	0.41
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	18	0.41
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	18	0.41
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	19	0.41
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	19	0.41
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	6	0.41
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	6	0.41
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	6	0.41
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	6	0.41
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	5	0.41
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	12	0.41
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	12	0.41
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	10	0.41
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	17	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	19	0.41
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	19	0.41
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	3	0.41
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	2	0.41
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	15	0.41
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	15	0.41
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	11	0.41
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	17	0.41
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	17	0.41
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	18	0.41
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	18	0.41
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	18	0.41
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	18	0.41
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	1	0.41
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	3	0.41
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	16	0.41
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	4	0.41
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	8	0.41
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	16	0.41
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	16	0.41
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	5	0.41
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	5	0.41
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	11	0.4
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	18	0.4
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	18	0.4
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	8	0.4
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	11	0.4
(1,1939)	1:43:A:ASN:HB3	1:42:A:THR:HA	18	0.4
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	14	0.4
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	11	0.4
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	5	0.4
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	17	0.4
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	17	0.4
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG12	13	0.4
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG13	13	0.4
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	17	0.4
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	17	0.4
(1,1694)	1:33:A:SER:HB2	1:32:A:VAL:HA	2	0.4
(1,1694)	1:33:A:SER:HB3	1:32:A:VAL:HA	2	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	14	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	14	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	14	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	14	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	14	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	15	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	15	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	15	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	15	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	15	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	15	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	20	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	20	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	20	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	20	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	20	0.4
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	20	0.4
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG21	12	0.4
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG22	12	0.4
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG23	12	0.4
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	1	0.4
(1,1581)	1:93:A:LEU:HA	1:122:A:THR:HA	10	0.4
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	10	0.4
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	14	0.4
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	11	0.4
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	12	0.4
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	20	0.4
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	20	0.4
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	15	0.4
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	4	0.4
(1,703)	1:163:A:LEU:HD11	1:164:A:CYS:H	1	0.4
(1,703)	1:163:A:LEU:HD12	1:164:A:CYS:H	1	0.4
(1,703)	1:163:A:LEU:HD13	1:164:A:CYS:H	1	0.4
(1,703)	1:163:A:LEU:HD21	1:164:A:CYS:H	1	0.4
(1,703)	1:163:A:LEU:HD22	1:164:A:CYS:H	1	0.4
(1,703)	1:163:A:LEU:HD23	1:164:A:CYS:H	1	0.4
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	6	0.4
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	6	0.4
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	6	0.4
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	6	0.4
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	11	0.4
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	11	0.4
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	15	0.4
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	15	0.4
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	15	0.4
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	15	0.4
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	15	0.4
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	16	0.4
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	4	0.4
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	17	0.4
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	20	0.4
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	11	0.4
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	11	0.4
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	11	0.4
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	11	0.4
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	1	0.4
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	10	0.4
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	12	0.4
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	12	0.4
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	19	0.4
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	4	0.4
(1,2084)	1:90:A:ASN:H	1:89:A:SER:HG	17	0.39
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	9	0.39
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	11	0.39
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	6	0.39
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	15	0.39
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	15	0.39
(1,1794)	1:48:A:TYR:HB2	1:10:A:ARG:HB2	18	0.39
(1,1794)	1:48:A:TYR:HB2	1:10:A:ARG:HB3	18	0.39
(1,1794)	1:48:A:TYR:HB3	1:10:A:ARG:HB2	18	0.39
(1,1794)	1:48:A:TYR:HB3	1:10:A:ARG:HB3	18	0.39
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	4	0.39
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	4	0.39
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	11	0.39
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	11	0.39
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	8	0.39
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	13	0.39
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	13	0.39
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	17	0.39
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	11	0.39
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	1	0.39
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	12	0.39
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	7	0.39
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	7	0.39
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	7	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	18	0.39
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	18	0.39
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	18	0.39
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD2	9	0.39
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD3	9	0.39
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD2	9	0.39
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD3	9	0.39
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD2	9	0.39
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD3	9	0.39
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD2	9	0.39
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD3	9	0.39
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD2	9	0.39
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD3	9	0.39
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD2	9	0.39
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD3	9	0.39
(1,1341)	1:66:A:LEU:HA	1:65:A:ALA:H	3	0.39
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	18	0.39
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	4	0.39
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	1	0.39
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	15	0.39
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	2	0.39
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	2	0.39
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	10	0.39
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD2	3	0.39
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD3	3	0.39
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	5	0.39
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	19	0.39
(1,705)	1:160:A:GLU:HA	1:149:A:ILE:H	8	0.39
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	1	0.39
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	1	0.39
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	1	0.39
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	1	0.39
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	17	0.39
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	4	0.39
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	6	0.39
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	13	0.39
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	20	0.39
(1,520)	1:111:A:ILE:HB	1:132:A:GLU:H	6	0.39
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE1	5	0.39
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE2	5	0.39
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	5	0.39
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	10	0.39
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	10	0.39
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	10	0.39
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	4	0.39
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	6	0.39
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	15	0.39
(1,60)	1:157:A:ALA:HB1	1:90:A:ASN:HA	4	0.39
(1,60)	1:157:A:ALA:HB2	1:90:A:ASN:HA	4	0.39
(1,60)	1:157:A:ALA:HB3	1:90:A:ASN:HA	4	0.39
(1,28)	1:45:A:CYS:HB2	1:15:A:HIS:HA	5	0.39
(1,28)	1:45:A:CYS:HB3	1:15:A:HIS:HA	5	0.39
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	20	0.38
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	20	0.38
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	5	0.38
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	18	0.38
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	6	0.38
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	19	0.38
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD11	7	0.38
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD12	7	0.38
(1,2088)	1:89:A:SER:HA	1:91:A:LEU:HD13	7	0.38
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	4	0.38
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	3	0.38
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	12	0.38
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	6	0.38
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	6	0.38
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	6	0.38
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	20	0.38
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	20	0.38
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	11	0.38
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	20	0.38
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	20	0.38
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	6	0.38
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	8	0.38
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	8	0.38
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	17	0.38
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	17	0.38
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	10	0.38
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	2	0.38
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	2	0.38
(1,1741)	1:129:A:ALA:H	1:86:A:LEU:H	15	0.38
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	12	0.38
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	12	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	12	0.38
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	12	0.38
(1,1707)	1:44:A:LYS:HA	1:38:A:LEU:HB2	11	0.38
(1,1707)	1:44:A:LYS:HA	1:38:A:LEU:HB3	11	0.38
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG2	7	0.38
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG3	7	0.38
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG2	16	0.38
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG3	16	0.38
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG2	17	0.38
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG3	17	0.38
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	3	0.38
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	8	0.38
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	17	0.38
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	17	0.38
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	17	0.38
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	17	0.38
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	6	0.38
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	6	0.38
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG21	14	0.38
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG22	14	0.38
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG23	14	0.38
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	18	0.38
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	9	0.38
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	9	0.38
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	10	0.38
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	10	0.38
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	3	0.38
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	9	0.38
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	10	0.38
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	7	0.38
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	7	0.38
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	9	0.38
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	9	0.38
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	17	0.38
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	1	0.38
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	7	0.38
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	15	0.38
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	11	0.38
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB2	8	0.38
(1,361)	1:80:A:GLU:HA	1:77:A:LYS:HB3	8	0.38
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	14	0.38
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	14	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	16	0.38
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	16	0.38
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	15	0.38
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	13	0.38
(1,181)	1:95:A:MET:HG2	1:115:A:ILE:HB	15	0.38
(1,181)	1:95:A:MET:HG3	1:115:A:ILE:HB	15	0.38
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	1	0.38
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	1	0.38
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG2	7	0.37
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG3	7	0.37
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	10	0.37
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	20	0.37
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	15	0.37
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	15	0.37
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	2	0.37
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	2	0.37
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	2	0.37
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	5	0.37
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB2	20	0.37
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB3	20	0.37
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	11	0.37
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	19	0.37
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	19	0.37
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	1	0.37
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	1	0.37
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	6	0.37
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	6	0.37
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	18	0.37
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	18	0.37
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	18	0.37
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	18	0.37
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	14	0.37
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	14	0.37
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	14	0.37
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	14	0.37
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	14	0.37
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	14	0.37
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG11	5	0.37
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG12	5	0.37
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG13	5	0.37
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG21	5	0.37
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG22	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG23	5	0.37
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	1	0.37
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	20	0.37
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	20	0.37
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	20	0.37
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	20	0.37
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	15	0.37
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	15	0.37
(1,1304)	1:37:A:ILE:HG12	1:46:A:LYS:HB2	15	0.37
(1,1304)	1:37:A:ILE:HG12	1:46:A:LYS:HB3	15	0.37
(1,1304)	1:37:A:ILE:HG13	1:46:A:LYS:HB2	15	0.37
(1,1304)	1:37:A:ILE:HG13	1:46:A:LYS:HB3	15	0.37
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	16	0.37
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD1	18	0.37
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD2	18	0.37
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD1	18	0.37
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD2	18	0.37
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB2	20	0.37
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB3	20	0.37
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB2	20	0.37
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB3	20	0.37
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	2	0.37
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	11	0.37
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	8	0.37
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	19	0.37
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	19	0.37
(1,1000)	1:78:A:GLN:HA	1:3:A:MET:HA	16	0.37
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	4	0.37
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	14	0.37
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	10	0.37
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	17	0.37
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	15	0.37
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	15	0.37
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	20	0.37
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	20	0.37
(1,678)	1:150:A:LYS:HG2	1:151:A:THR:HB	9	0.37
(1,678)	1:150:A:LYS:HG3	1:151:A:THR:HB	9	0.37
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	10	0.37
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	5	0.37
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	3	0.37
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	3	0.37
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	13	0.37
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	3	0.37
(1,313)	1:106:A:PRO:HD2	1:108:A:GLY:H	12	0.37
(1,313)	1:106:A:PRO:HD3	1:108:A:GLY:H	12	0.37
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	3	0.37
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	3	0.37
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	6	0.37
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	6	0.37
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	14	0.37
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	14	0.37
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	4	0.37
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	4	0.37
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	19	0.37
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	19	0.37
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	19	0.37
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	19	0.37
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	19	0.37
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	19	0.37
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	16	0.36
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	18	0.36
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	8	0.36
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	4	0.36
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	4	0.36
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	10	0.36
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	10	0.36
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	10	0.36
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG2	16	0.36
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG3	16	0.36
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	5	0.36
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	6	0.36
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	14	0.36
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	5	0.36
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	5	0.36
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	7	0.36
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	7	0.36
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	11	0.36
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	11	0.36
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	14	0.36
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	14	0.36
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	19	0.36
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	19	0.36
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	20	0.36
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	2	0.36
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	11	0.36
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	11	0.36
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	8	0.36
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	18	0.36
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	18	0.36
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	4	0.36
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	4	0.36
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	14	0.36
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB2	12	0.36
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB3	12	0.36
(1,1450)	1:80:A:GLU:HG2	1:77:A:LYS:H	20	0.36
(1,1450)	1:80:A:GLU:HG3	1:77:A:LYS:H	20	0.36
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	4	0.36
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	4	0.36
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	4	0.36
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	4	0.36
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	13	0.36
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	13	0.36
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	16	0.36
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	4	0.36
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	8	0.36
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	6	0.36
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	6	0.36
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	11	0.36
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	12	0.36
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	12	0.36
(1,969)	1:30:A:LYS:HD2	1:31:A:ILE:H	20	0.36
(1,969)	1:30:A:LYS:HD3	1:31:A:ILE:H	20	0.36
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	13	0.36
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	20	0.36
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	17	0.36
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	4	0.36
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	4	0.36
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG2	13	0.36
(1,778)	1:73:A:ALA:HA	1:10:A:ARG:HG3	13	0.36
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	6	0.36
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	19	0.36
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	6	0.36
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	1	0.36
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	7	0.36
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	13	0.36
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	7	0.36
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	20	0.36
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	9	0.36
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	13	0.36
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	13	0.36
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	17	0.36
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	18	0.36
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	20	0.36
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	20	0.36
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	5	0.36
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	9	0.36
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB2	20	0.36
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB3	20	0.36
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB2	20	0.36
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB3	20	0.36
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	2	0.36
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	2	0.36
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	19	0.36
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	19	0.36
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	17	0.36
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	17	0.36
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	17	0.36
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	17	0.36
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	17	0.36
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	17	0.36
(1,2117)	1:101:A:GLU:HG2	1:113:A:THR:H	4	0.35
(1,2117)	1:101:A:GLU:HG3	1:113:A:THR:H	4	0.35
(1,2117)	1:101:A:GLU:HG2	1:113:A:THR:H	4	0.35
(1,2117)	1:101:A:GLU:HG3	1:113:A:THR:H	4	0.35
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	1	0.35
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	2	0.35
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	16	0.35
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	13	0.35
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	2	0.35
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	14	0.35
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	14	0.35
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	5	0.35
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	13	0.35
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	13	0.35
(1,1816)	1:53:A:PHE:HB2	1:30:A:LYS:H	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1816)	1:53:A:PHE:HB3	1:30:A:LYS:H	6	0.35
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	10	0.35
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	10	0.35
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	14	0.35
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	16	0.35
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	14	0.35
(1,1692)	1:19:A:GLN:HB2	1:17:A:THR:HB	13	0.35
(1,1692)	1:19:A:GLN:HB3	1:17:A:THR:HB	13	0.35
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	4	0.35
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	7	0.35
(1,1669)	1:165:A:LYS:HD2	1:166:A:PHE:H	13	0.35
(1,1669)	1:165:A:LYS:HD3	1:166:A:PHE:H	13	0.35
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	8	0.35
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	18	0.35
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	4	0.35
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	8	0.35
(1,1352)	1:61:A:LYS:HD2	1:28:A:TYR:HA	1	0.35
(1,1352)	1:61:A:LYS:HD3	1:28:A:TYR:HA	1	0.35
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	13	0.35
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	13	0.35
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	4	0.35
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD1	7	0.35
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD2	7	0.35
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD1	7	0.35
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD2	7	0.35
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB2	4	0.35
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB3	4	0.35
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB2	4	0.35
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB3	4	0.35
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	1	0.35
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	9	0.35
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	13	0.35
(1,1015)	1:23:A:LYS:HG2	1:22:A:VAL:HB	5	0.35
(1,1015)	1:23:A:LYS:HG3	1:22:A:VAL:HB	5	0.35
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	3	0.35
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	18	0.35
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	2	0.35
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	2	0.35
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	6	0.35
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	6	0.35
(1,781)	1:71:A:VAL:HG11	1:10:A:ARG:HG2	18	0.35
(1,781)	1:71:A:VAL:HG11	1:10:A:ARG:HG3	18	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:71:A:VAL:HG12	1:10:A:ARG:HG2	18	0.35
(1,781)	1:71:A:VAL:HG12	1:10:A:ARG:HG3	18	0.35
(1,781)	1:71:A:VAL:HG13	1:10:A:ARG:HG2	18	0.35
(1,781)	1:71:A:VAL:HG13	1:10:A:ARG:HG3	18	0.35
(1,781)	1:71:A:VAL:HG21	1:10:A:ARG:HG2	18	0.35
(1,781)	1:71:A:VAL:HG21	1:10:A:ARG:HG3	18	0.35
(1,781)	1:71:A:VAL:HG22	1:10:A:ARG:HG2	18	0.35
(1,781)	1:71:A:VAL:HG22	1:10:A:ARG:HG3	18	0.35
(1,781)	1:71:A:VAL:HG23	1:10:A:ARG:HG2	18	0.35
(1,781)	1:71:A:VAL:HG23	1:10:A:ARG:HG3	18	0.35
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	14	0.35
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	14	0.35
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	14	0.35
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	18	0.35
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	18	0.35
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	19	0.35
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	19	0.35
(1,665)	1:149:A:ILE:HG12	1:160:A:GLU:H	8	0.35
(1,665)	1:149:A:ILE:HG13	1:160:A:GLU:H	8	0.35
(1,661)	1:155:A:VAL:HB	1:94:A:SER:H	1	0.35
(1,637)	1:151:A:THR:HB	1:159:A:THR:HA	14	0.35
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	3	0.35
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	2	0.35
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	2	0.35
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	8	0.35
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	8	0.35
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	16	0.35
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	14	0.35
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	13	0.35
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	16	0.35
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	16	0.35
(1,314)	1:106:A:PRO:HB2	1:107:A:PHE:HD1	18	0.35
(1,314)	1:106:A:PRO:HB2	1:107:A:PHE:HD2	18	0.35
(1,314)	1:106:A:PRO:HB3	1:107:A:PHE:HD1	18	0.35
(1,314)	1:106:A:PRO:HB3	1:107:A:PHE:HD2	18	0.35
(1,308)	1:103:A:MET:HB2	1:104:A:LEU:HB2	5	0.35
(1,308)	1:103:A:MET:HB3	1:104:A:LEU:HB2	5	0.35
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	14	0.35
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	14	0.35
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	14	0.35
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	14	0.35
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:94:A:SER:HA	1:93:A:LEU:H	17	0.35
(1,228)	1:136:A:LYS:HG2	1:132:A:GLU:HB2	8	0.35
(1,228)	1:136:A:LYS:HG2	1:132:A:GLU:HB3	8	0.35
(1,228)	1:136:A:LYS:HG3	1:132:A:GLU:HB2	8	0.35
(1,228)	1:136:A:LYS:HG3	1:132:A:GLU:HB3	8	0.35
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	14	0.35
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	14	0.35
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	10	0.35
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	10	0.35
(1,21)	1:24:A:LEU:HA	1:26:A:GLN:H	19	0.35
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	5	0.35
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	16	0.35
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	9	0.34
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	10	0.34
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG2	11	0.34
(1,2116)	1:113:A:THR:HB	1:101:A:GLU:HG3	11	0.34
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	7	0.34
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	14	0.34
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	15	0.34
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	16	0.34
(1,2054)	1:75:A:MET:HE1	1:3:A:MET:HG2	15	0.34
(1,2054)	1:75:A:MET:HE1	1:3:A:MET:HG3	15	0.34
(1,2054)	1:75:A:MET:HE2	1:3:A:MET:HG2	15	0.34
(1,2054)	1:75:A:MET:HE2	1:3:A:MET:HG3	15	0.34
(1,2054)	1:75:A:MET:HE3	1:3:A:MET:HG2	15	0.34
(1,2054)	1:75:A:MET:HE3	1:3:A:MET:HG3	15	0.34
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	12	0.34
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	12	0.34
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	17	0.34
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	2	0.34
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	3	0.34
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	3	0.34
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	19	0.34
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	19	0.34
(1,1731)	1:77:A:LYS:HD2	1:80:A:GLU:H	1	0.34
(1,1731)	1:77:A:LYS:HD3	1:80:A:GLU:H	1	0.34
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	4	0.34
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	4	0.34
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	15	0.34
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	15	0.34
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	15	0.34
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	3	0.34
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	3	0.34
(1,1682)	1:166:A:PHE:HA	1:137:A:CYS:HB2	8	0.34
(1,1682)	1:166:A:PHE:HA	1:137:A:CYS:HB3	8	0.34
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	3	0.34
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	3	0.34
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	3	0.34
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	3	0.34
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	3	0.34
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	3	0.34
(1,1540)	1:30:A:LYS:HE2	1:31:A:ILE:H	18	0.34
(1,1540)	1:30:A:LYS:HE3	1:31:A:ILE:H	18	0.34
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG12	16	0.34
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG13	16	0.34
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG12	17	0.34
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG13	17	0.34
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG2	12	0.34
(1,1461)	1:42:A:THR:HA	1:44:A:LYS:HG3	12	0.34
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	1	0.34
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	1	0.34
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	1	0.34
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	1	0.34
(1,1425)	1:87:A:TYR:HA	1:86:A:LEU:H	19	0.34
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	9	0.34
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	9	0.34
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	7	0.34
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	9	0.34
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	9	0.34
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	9	0.34
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	1	0.34
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	17	0.34
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	7	0.34
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	10	0.34
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	7	0.34
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	7	0.34
(1,1041)	1:23:A:LYS:H	1:19:A:GLN:HA	14	0.34
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	16	0.34
(1,949)	1:23:A:LYS:HE2	1:19:A:GLN:HA	3	0.34
(1,949)	1:23:A:LYS:HE3	1:19:A:GLN:HA	3	0.34
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	8	0.34
(1,937)	1:113:A:THR:H	1:112:A:SER:HB2	1	0.34
(1,937)	1:113:A:THR:H	1:112:A:SER:HB3	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	2	0.34
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	2	0.34
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	2	0.34
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	2	0.34
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	2	0.34
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	2	0.34
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	13	0.34
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	18	0.34
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	14	0.34
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	17	0.34
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	7	0.34
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	7	0.34
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	15	0.34
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	1	0.34
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	11	0.34
(1,484)	1:109:A:GLN:HB2	1:136:A:LYS:HE2	3	0.34
(1,484)	1:109:A:GLN:HB2	1:136:A:LYS:HE3	3	0.34
(1,484)	1:109:A:GLN:HB3	1:136:A:LYS:HE2	3	0.34
(1,484)	1:109:A:GLN:HB3	1:136:A:LYS:HE3	3	0.34
(1,478)	1:109:A:GLN:HG2	1:110:A:VAL:H	12	0.34
(1,478)	1:109:A:GLN:HG3	1:110:A:VAL:H	12	0.34
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	13	0.34
(1,313)	1:106:A:PRO:HD2	1:108:A:GLY:H	9	0.34
(1,313)	1:106:A:PRO:HD3	1:108:A:GLY:H	9	0.34
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	10	0.34
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	10	0.34
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	10	0.34
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	10	0.34
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	15	0.34
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	15	0.34
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	8	0.34
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	14	0.34
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	10	0.34
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	13	0.34
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	11	0.33
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	11	0.33
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	15	0.33
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	15	0.33
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	15	0.33
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	15	0.33
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	8	0.33
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	3	0.33
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	17	0.33
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	15	0.33
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	10	0.33
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	15	0.33
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	15	0.33
(1,2009)	1:48:A:TYR:HD2	1:9:A:ILE:H	8	0.33
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB2	20	0.33
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB3	20	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	1	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	1	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	1	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	1	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	1	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	1	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	14	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	14	0.33
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	14	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	14	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	14	0.33
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	14	0.33
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	13	0.33
(1,1953)	1:72:A:GLN:HG2	1:10:A:ARG:HG2	17	0.33
(1,1953)	1:72:A:GLN:HG2	1:10:A:ARG:HG3	17	0.33
(1,1953)	1:72:A:GLN:HG3	1:10:A:ARG:HG2	17	0.33
(1,1953)	1:72:A:GLN:HG3	1:10:A:ARG:HG3	17	0.33
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	17	0.33
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	9	0.33
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	9	0.33
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	20	0.33
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	20	0.33
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	2	0.33
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	2	0.33
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	13	0.33
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	1	0.33
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	1	0.33
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	2	0.33
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	2	0.33
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	15	0.33
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	15	0.33
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	10	0.33
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	11	0.33
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	11	0.33
(1,1695)	1:34:A:THR:HB	1:35:A:LYS:HA	11	0.33
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	1	0.33
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	1	0.33
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	2	0.33
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	14	0.33
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	14	0.33
(1,1465)	1:47:A:GLY:H	1:48:A:TYR:H	20	0.33
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	17	0.33
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	17	0.33
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	17	0.33
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	17	0.33
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	12	0.33
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	9	0.33
(1,1355)	1:50:A:PHE:HA	1:8:A:TYR:HB3	18	0.33
(1,1348)	1:17:A:THR:H	1:21:A:LEU:H	11	0.33
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	5	0.33
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	5	0.33
(1,1255)	1:41:A:THR:HG21	1:42:A:THR:HB	8	0.33
(1,1255)	1:41:A:THR:HG22	1:42:A:THR:HB	8	0.33
(1,1255)	1:41:A:THR:HG23	1:42:A:THR:HB	8	0.33
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	5	0.33
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	19	0.33
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	19	0.33
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	10	0.33
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	10	0.33
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	19	0.33
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	4	0.33
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	4	0.33
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	6	0.33
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	6	0.33
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	7	0.33
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	12	0.33
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	9	0.33
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	9	0.33
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	16	0.33
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	16	0.33
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	15	0.33
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	15	0.33
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	15	0.33
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	15	0.33
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	15	0.33
(1,475)	1:138:A:GLU:HG2	1:166:A:PHE:HB2	11	0.33
(1,475)	1:138:A:GLU:HG2	1:166:A:PHE:HB3	11	0.33
(1,475)	1:138:A:GLU:HG3	1:166:A:PHE:HB2	11	0.33
(1,475)	1:138:A:GLU:HG3	1:166:A:PHE:HB3	11	0.33
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	4	0.33
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	4	0.33
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	15	0.33
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	15	0.33
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	15	0.33
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	15	0.33
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	9	0.33
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	9	0.33
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	9	0.33
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	9	0.33
(1,186)	1:115:A:ILE:HD11	1:125:A:GLY:H	11	0.33
(1,186)	1:115:A:ILE:HD12	1:125:A:GLY:H	11	0.33
(1,186)	1:115:A:ILE:HD13	1:125:A:GLY:H	11	0.33
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	2	0.33
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	8	0.33
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	8	0.33
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	18	0.33
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	18	0.33
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	9	0.33
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	2	0.32
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	2	0.32
(1,2158)	1:6:A:ASN:HA	1:50:A:PHE:HB2	2	0.32
(1,2158)	1:6:A:ASN:HA	1:50:A:PHE:HB3	2	0.32
(1,2109)	1:114:A:ARG:HH21	1:112:A:SER:HB2	18	0.32
(1,2109)	1:114:A:ARG:HH21	1:112:A:SER:HB3	18	0.32
(1,2109)	1:114:A:ARG:HH22	1:112:A:SER:HB2	18	0.32
(1,2109)	1:114:A:ARG:HH22	1:112:A:SER:HB3	18	0.32
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	4	0.32
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	5	0.32
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	13	0.32
(1,2071)	1:128:A:PHE:H	1:88:A:ILE:HG12	19	0.32
(1,2071)	1:128:A:PHE:H	1:88:A:ILE:HG13	19	0.32
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	5	0.32
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	2	0.32
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	2	0.32
(1,1957)	1:77:A:LYS:HG2	1:3:A:MET:HA	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:77:A:LYS:HG3	1:3:A:MET:HA	20	0.32
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	8	0.32
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	14	0.32
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	14	0.32
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	20	0.32
(1,1782)	1:37:A:ILE:HB	1:49:A:GLY:H	13	0.32
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG12	3	0.32
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG13	3	0.32
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	4	0.32
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	4	0.32
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	4	0.32
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	4	0.32
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	4	0.32
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	4	0.32
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	15	0.32
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	15	0.32
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	13	0.32
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB2	20	0.32
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB3	20	0.32
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	3	0.32
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	8	0.32
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	1	0.32
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	3	0.32
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	12	0.32
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	18	0.32
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	7	0.32
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	8	0.32
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	8	0.32
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	8	0.32
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	8	0.32
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	8	0.32
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	19	0.32
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	19	0.32
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	13	0.32
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	13	0.32
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	19	0.32
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	19	0.32
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	10	0.32
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	20	0.32
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	20	0.32
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	6	0.32
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	5	0.32
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	16	0.32
(1,937)	1:113:A:THR:H	1:112:A:SER:HB2	12	0.32
(1,937)	1:113:A:THR:H	1:112:A:SER:HB3	12	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	4	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	4	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	4	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	4	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	4	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	4	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	7	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	7	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	7	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	7	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	7	0.32
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	7	0.32
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	11	0.32
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	11	0.32
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	11	0.32
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	11	0.32
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	11	0.32
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	11	0.32
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	8	0.32
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	12	0.32
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	13	0.32
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	7	0.32
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	7	0.32
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	13	0.32
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	13	0.32
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	19	0.32
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	13	0.32
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	18	0.32
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	18	0.32
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	18	0.32
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	18	0.32
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	13	0.32
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	13	0.32
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	15	0.32
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	6	0.32
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	20	0.32
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	13	0.32
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	12	0.32
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	11	0.32
(1,356)	1:136:A:LYS:HG2	1:109:A:GLN:H	18	0.32
(1,356)	1:136:A:LYS:HG3	1:109:A:GLN:H	18	0.32
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	10	0.32
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	10	0.32
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	14	0.32
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	8	0.32
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	8	0.32
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	3	0.32
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	3	0.32
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	4	0.32
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	4	0.32
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	11	0.32
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	14	0.32
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	1	0.32
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	1	0.32
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	13	0.32
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	13	0.32
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	7	0.32
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	7	0.32
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	4	0.32
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	9	0.32
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	9	0.32
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	14	0.32
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	18	0.31
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	5	0.31
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	5	0.31
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	5	0.31
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	6	0.31
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	14	0.31
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	13	0.31
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	19	0.31
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	6	0.31
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	6	0.31
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	6	0.31
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	7	0.31
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	7	0.31
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	7	0.31
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	2	0.31
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	2	0.31
(1,1998)	1:32:A:VAL:HG11	1:33:A:SER:HB2	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1998)	1:32:A:VAL:HG11	1:33:A:SER:HB3	2	0.31
(1,1998)	1:32:A:VAL:HG12	1:33:A:SER:HB2	2	0.31
(1,1998)	1:32:A:VAL:HG12	1:33:A:SER:HB3	2	0.31
(1,1998)	1:32:A:VAL:HG13	1:33:A:SER:HB2	2	0.31
(1,1998)	1:32:A:VAL:HG13	1:33:A:SER:HB3	2	0.31
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	8	0.31
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	9	0.31
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	18	0.31
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	13	0.31
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB2	19	0.31
(1,1903)	1:77:A:LYS:HG2	1:80:A:GLU:HB3	19	0.31
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB2	19	0.31
(1,1903)	1:77:A:LYS:HG3	1:80:A:GLU:HB3	19	0.31
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	14	0.31
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	7	0.31
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	4	0.31
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	4	0.31
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	4	0.31
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	4	0.31
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	8	0.31
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	9	0.31
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	12	0.31
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	12	0.31
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	17	0.31
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	17	0.31
(1,1661)	1:162:A:LEU:HG	1:164:A:CYS:HA	13	0.31
(1,1655)	1:162:A:LEU:HG	1:164:A:CYS:H	18	0.31
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	6	0.31
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	6	0.31
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	6	0.31
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	6	0.31
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	20	0.31
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	6	0.31
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	6	0.31
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	14	0.31
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	14	0.31
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	16	0.31
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	16	0.31
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	16	0.31
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	16	0.31
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	16	0.31
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	5	0.31
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	8	0.31
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	18	0.31
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	18	0.31
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	9	0.31
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	9	0.31
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	9	0.31
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	9	0.31
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	1	0.31
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	17	0.31
(1,1335)	1:24:A:LEU:H	1:21:A:LEU:H	6	0.31
(1,1291)	1:48:A:TYR:HD1	1:10:A:ARG:HA	16	0.31
(1,1291)	1:48:A:TYR:HD2	1:10:A:ARG:HA	16	0.31
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	6	0.31
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	6	0.31
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD11	17	0.31
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD12	17	0.31
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD13	17	0.31
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD21	17	0.31
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD22	17	0.31
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD23	17	0.31
(1,1198)	1:138:A:GLU:H	1:139:A:ALA:HA	16	0.31
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	10	0.31
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	10	0.31
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	11	0.31
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	11	0.31
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG2	19	0.31
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG3	19	0.31
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG2	19	0.31
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG3	19	0.31
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG2	19	0.31
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG3	19	0.31
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	20	0.31
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	20	0.31
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	20	0.31
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	20	0.31
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	8	0.31
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	8	0.31
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	13	0.31
(1,937)	1:113:A:THR:H	1:112:A:SER:HB2	3	0.31
(1,937)	1:113:A:THR:H	1:112:A:SER:HB3	3	0.31
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	13	0.31
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	13	0.31
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	8	0.31
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	12	0.31
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	13	0.31
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	4	0.31
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	4	0.31
(1,520)	1:111:A:ILE:HB	1:132:A:GLU:H	18	0.31
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	10	0.31
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	14	0.31
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	16	0.31
(1,313)	1:106:A:PRO:HD2	1:108:A:GLY:H	8	0.31
(1,313)	1:106:A:PRO:HD3	1:108:A:GLY:H	8	0.31
(1,313)	1:106:A:PRO:HD2	1:108:A:GLY:H	17	0.31
(1,313)	1:106:A:PRO:HD3	1:108:A:GLY:H	17	0.31
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	13	0.31
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	18	0.31
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	18	0.31
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	18	0.31
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	18	0.31
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	19	0.31
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	18	0.31
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	8	0.31
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	8	0.31
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	9	0.31
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	9	0.31
(1,68)	1:114:A:ARG:HA	1:97:A:GLU:H	13	0.31
(1,2114)	1:112:A:SER:HG	1:113:A:THR:HA	15	0.3
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	11	0.3
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	16	0.3
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	16	0.3
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	2	0.3
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	17	0.3
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	3	0.3
(1,1801)	1:44:A:LYS:HD2	1:42:A:THR:HB	16	0.3
(1,1801)	1:44:A:LYS:HD3	1:42:A:THR:HB	16	0.3
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	7	0.3
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	7	0.3
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	6	0.3
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	7	0.3
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	2	0.3
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	14	0.3
(1,1669)	1:165:A:LYS:HD2	1:166:A:PHE:H	14	0.3
(1,1669)	1:165:A:LYS:HD3	1:166:A:PHE:H	14	0.3
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	19	0.3
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	2	0.3
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	2	0.3
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	18	0.3
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG11	20	0.3
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG12	20	0.3
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG13	20	0.3
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG21	20	0.3
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG22	20	0.3
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG23	20	0.3
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	17	0.3
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	1	0.3
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	1	0.3
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	1	0.3
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	17	0.3
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	17	0.3
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	17	0.3
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	2	0.3
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	2	0.3
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	2	0.3
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	17	0.3
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	6	0.3
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	9	0.3
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	12	0.3
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	12	0.3
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	12	0.3
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	12	0.3
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB2	8	0.3
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB3	8	0.3
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB2	8	0.3
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB3	8	0.3
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	13	0.3
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	13	0.3
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	19	0.3
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	19	0.3
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	7	0.3
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	7	0.3
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	7	0.3
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	10	0.3
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	13	0.3
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	13	0.3
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	5	0.3
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	20	0.3
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	20	0.3
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD11	6	0.3
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD12	6	0.3
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD13	6	0.3
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD11	6	0.3
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD12	6	0.3
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD13	6	0.3
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD11	6	0.3
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD12	6	0.3
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD13	6	0.3
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	5	0.3
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	9	0.3
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	11	0.3
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	11	0.3
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	11	0.3
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	11	0.3
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	13	0.3
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	11	0.3
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	11	0.3
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	11	0.3
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	11	0.3
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	15	0.3
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	15	0.3
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	3	0.3
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	3	0.3
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	5	0.3
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	5	0.3
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	11	0.3
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	17	0.3
(1,432)	1:86:A:LEU:HA	1:167:A:SER:HA	17	0.3
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	18	0.3
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	11	0.3
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	11	0.3
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	11	0.3
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	12	0.3
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	3	0.3
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:95:A:MET:HB2	1:115:A:ILE:HB	15	0.3
(1,187)	1:95:A:MET:HB3	1:115:A:ILE:HB	15	0.3
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	20	0.3
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	11	0.3
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	15	0.3
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	15	0.3
(1,2154)	1:6:A:ASN:HA	1:5:A:THR:HG1	1	0.29
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	5	0.29
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	19	0.29
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	1	0.29
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	13	0.29
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	19	0.29
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	11	0.29
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	11	0.29
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	4	0.29
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	20	0.29
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	11	0.29
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	9	0.29
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	9	0.29
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	17	0.29
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	17	0.29
(1,1853)	1:31:A:ILE:HB	1:22:A:VAL:HA	19	0.29
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	14	0.29
(1,1801)	1:44:A:LYS:HD2	1:42:A:THR:HB	7	0.29
(1,1801)	1:44:A:LYS:HD3	1:42:A:THR:HB	7	0.29
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	20	0.29
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	20	0.29
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	20	0.29
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG12	17	0.29
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG13	17	0.29
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	5	0.29
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	13	0.29
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	2	0.29
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	2	0.29
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	18	0.29
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	18	0.29
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	17	0.29
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	17	0.29
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	17	0.29
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	17	0.29
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	17	0.29
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:93:A:LEU:HA	1:122:A:THR:HA	18	0.29
(1,1534)	1:64:A:SER:HB2	1:67:A:LYS:HD2	12	0.29
(1,1534)	1:64:A:SER:HB2	1:67:A:LYS:HD3	12	0.29
(1,1534)	1:64:A:SER:HB3	1:67:A:LYS:HD2	12	0.29
(1,1534)	1:64:A:SER:HB3	1:67:A:LYS:HD3	12	0.29
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	7	0.29
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	14	0.29
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	19	0.29
(1,1425)	1:87:A:TYR:HA	1:86:A:LEU:H	18	0.29
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	11	0.29
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	11	0.29
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	11	0.29
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	11	0.29
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB2	17	0.29
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB3	17	0.29
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	2	0.29
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	2	0.29
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	17	0.29
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	17	0.29
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG2	6	0.29
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG3	6	0.29
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	8	0.29
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	8	0.29
(1,1100)	1:60:A:GLN:HA	1:59:A:ALA:H	16	0.29
(1,1090)	1:160:A:GLU:H	1:148:A:PHE:HA	14	0.29
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	4	0.29
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	4	0.29
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	11	0.29
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	12	0.29
(1,937)	1:113:A:THR:H	1:112:A:SER:HB2	18	0.29
(1,937)	1:113:A:THR:H	1:112:A:SER:HB3	18	0.29
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	16	0.29
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	16	0.29
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	16	0.29
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	16	0.29
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	16	0.29
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	16	0.29
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	5	0.29
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	5	0.29
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	5	0.29
(1,693)	1:155:A:VAL:HB	1:94:A:SER:HB2	19	0.29
(1,693)	1:155:A:VAL:HB	1:94:A:SER:HB3	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	12	0.29
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	12	0.29
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	12	0.29
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	12	0.29
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	11	0.29
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	1	0.29
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	1	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	11	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	11	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	11	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	11	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	11	0.29
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	11	0.29
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	2	0.29
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	12	0.29
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	12	0.29
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	20	0.29
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	14	0.29
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	16	0.29
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	3	0.29
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	3	0.29
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	16	0.29
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	16	0.29
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	1	0.29
(1,148)	1:99:A:GLU:HA	1:98:A:GLN:H	17	0.29
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	16	0.29
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	16	0.29
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	17	0.29
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	2	0.29
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	2	0.29
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	4	0.29
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	4	0.29
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	4	0.29
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	4	0.29
(1,86)	1:130:A:ARG:HB2	1:85:A:ASN:HB2	18	0.29
(1,86)	1:130:A:ARG:HB3	1:85:A:ASN:HB2	18	0.29
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	18	0.29
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	19	0.29
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	16	0.28
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	12	0.28
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	14	0.28
(1,2084)	1:90:A:ASN:H	1:89:A:SER:HG	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	6	0.28
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	10	0.28
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	10	0.28
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	20	0.28
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	20	0.28
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	20	0.28
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	1	0.28
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD11	20	0.28
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD12	20	0.28
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD13	20	0.28
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD21	20	0.28
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD22	20	0.28
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD23	20	0.28
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	20	0.28
(1,1979)	1:7:A:LEU:HA	1:75:A:MET:HA	16	0.28
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	20	0.28
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	19	0.28
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	19	0.28
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	11	0.28
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	9	0.28
(1,1593)	1:92:A:PRO:HB2	1:95:A:MET:H	8	0.28
(1,1593)	1:92:A:PRO:HB3	1:95:A:MET:H	8	0.28
(1,1443)	1:80:A:GLU:HG2	1:76:A:ALA:HB1	4	0.28
(1,1443)	1:80:A:GLU:HG2	1:76:A:ALA:HB2	4	0.28
(1,1443)	1:80:A:GLU:HG2	1:76:A:ALA:HB3	4	0.28
(1,1443)	1:80:A:GLU:HG3	1:76:A:ALA:HB1	4	0.28
(1,1443)	1:80:A:GLU:HG3	1:76:A:ALA:HB2	4	0.28
(1,1443)	1:80:A:GLU:HG3	1:76:A:ALA:HB3	4	0.28
(1,1413)	1:78:A:GLN:HB2	1:3:A:MET:HA	16	0.28
(1,1413)	1:78:A:GLN:HB3	1:3:A:MET:HA	16	0.28
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	19	0.28
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	2	0.28
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	2	0.28
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	2	0.28
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	5	0.28
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	14	0.28
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	14	0.28
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	14	0.28
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	2	0.28
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	2	0.28
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	4	0.28
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	9	0.28
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	3	0.28
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	3	0.28
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	3	0.28
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	3	0.28
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	20	0.28
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	20	0.28
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	20	0.28
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	20	0.28
(1,1156)	1:130:A:ARG:HB2	1:86:A:LEU:H	11	0.28
(1,1156)	1:130:A:ARG:HB3	1:86:A:LEU:H	11	0.28
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB2	11	0.28
(1,1136)	1:79:A:GLN:HB2	1:80:A:GLU:HB3	11	0.28
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB2	11	0.28
(1,1136)	1:79:A:GLN:HB3	1:80:A:GLU:HB3	11	0.28
(1,1128)	1:30:A:LYS:HE2	1:54:A:ASP:H	13	0.28
(1,1128)	1:30:A:LYS:HE3	1:54:A:ASP:H	13	0.28
(1,1074)	1:77:A:LYS:HD2	1:80:A:GLU:HG2	4	0.28
(1,1074)	1:77:A:LYS:HD2	1:80:A:GLU:HG3	4	0.28
(1,1074)	1:77:A:LYS:HD3	1:80:A:GLU:HG2	4	0.28
(1,1074)	1:77:A:LYS:HD3	1:80:A:GLU:HG3	4	0.28
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	8	0.28
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	8	0.28
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB2	14	0.28
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB3	14	0.28
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB2	14	0.28
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB3	14	0.28
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	18	0.28
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	11	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	12	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	12	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	12	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	12	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	12	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	12	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	14	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	14	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	14	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	14	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	14	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	14	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	17	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	17	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	17	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	17	0.28
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	17	0.28
(1,898)	1:53:A:PHE:H	1:51:A:VAL:HA	9	0.28
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	3	0.28
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	9	0.28
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	20	0.28
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG21	8	0.28
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG22	8	0.28
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG23	8	0.28
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	13	0.28
(1,815)	1:92:A:PRO:HB2	1:95:A:MET:HA	8	0.28
(1,815)	1:92:A:PRO:HB3	1:95:A:MET:HA	8	0.28
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	11	0.28
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	11	0.28
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	7	0.28
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	4	0.28
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	4	0.28
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	4	0.28
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	4	0.28
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	6	0.28
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	6	0.28
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	6	0.28
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	6	0.28
(1,676)	1:151:A:THR:HA	1:155:A:VAL:HB	8	0.28
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	20	0.28
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	9	0.28
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	17	0.28
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	15	0.28
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	17	0.28
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	9	0.28
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	10	0.28
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	10	0.28
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	4	0.28
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	4	0.28
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	4	0.28
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	4	0.28
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	4	0.28
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	4	0.28
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	17	0.28
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	9	0.28
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	12	0.28
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB2	2	0.28
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB3	2	0.28
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	20	0.28
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	18	0.28
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	19	0.28
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	5	0.28
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	11	0.28
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	11	0.28
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	17	0.28
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	17	0.28
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	11	0.28
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	11	0.28
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	20	0.28
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	20	0.28
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB2	6	0.28
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB3	6	0.28
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB2	6	0.28
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB3	6	0.28
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	5	0.28
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	5	0.28
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	11	0.27
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	15	0.27
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	7	0.27
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	9	0.27
(1,2050)	1:3:A:MET:HE1	1:75:A:MET:HA	12	0.27
(1,2050)	1:3:A:MET:HE2	1:75:A:MET:HA	12	0.27
(1,2050)	1:3:A:MET:HE3	1:75:A:MET:HA	12	0.27
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	11	0.27
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	11	0.27
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	11	0.27
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB2	5	0.27
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB3	5	0.27
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	10	0.27
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	10	0.27
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	10	0.27
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	10	0.27
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	10	0.27
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	10	0.27
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD11	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD12	17	0.27
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD13	17	0.27
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD21	17	0.27
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD22	17	0.27
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD23	17	0.27
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	5	0.27
(1,1958)	1:77:A:LYS:HA	1:3:A:MET:HG2	5	0.27
(1,1958)	1:77:A:LYS:HA	1:3:A:MET:HG3	5	0.27
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	15	0.27
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	5	0.27
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	5	0.27
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	19	0.27
(1,1882)	1:61:A:LYS:HG2	1:28:A:TYR:HB2	4	0.27
(1,1882)	1:61:A:LYS:HG3	1:28:A:TYR:HB2	4	0.27
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	1	0.27
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	18	0.27
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	11	0.27
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	11	0.27
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	20	0.27
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	20	0.27
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	20	0.27
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	7	0.27
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	7	0.27
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	5	0.27
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	5	0.27
(1,1661)	1:162:A:LEU:HG	1:164:A:CYS:HA	3	0.27
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG2	12	0.27
(1,1623)	1:98:A:GLN:HA	1:97:A:GLU:HG3	12	0.27
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	6	0.27
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	6	0.27
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	6	0.27
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	6	0.27
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	6	0.27
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	6	0.27
(1,1581)	1:93:A:LEU:HA	1:122:A:THR:HA	17	0.27
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	8	0.27
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	7	0.27
(1,1317)	1:72:A:GLN:HA	1:67:A:LYS:HA	16	0.27
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	3	0.27
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	3	0.27
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD11	10	0.27
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD12	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD13	10	0.27
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD21	10	0.27
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD22	10	0.27
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD23	10	0.27
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	8	0.27
(1,1179)	1:67:A:LYS:HA	1:73:A:ALA:H	13	0.27
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	11	0.27
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	10	0.27
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	10	0.27
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	10	0.27
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	10	0.27
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	16	0.27
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	16	0.27
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	16	0.27
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	16	0.27
(1,1150)	1:130:A:ARG:HA	1:112:A:SER:H	13	0.27
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	1	0.27
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	8	0.27
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	15	0.27
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	15	0.27
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	18	0.27
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	11	0.27
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	11	0.27
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	6	0.27
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	15	0.27
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	15	0.27
(1,556)	1:136:A:LYS:HD2	1:108:A:GLY:H	18	0.27
(1,556)	1:136:A:LYS:HD3	1:108:A:GLY:H	18	0.27
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	10	0.27
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	10	0.27
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	4	0.27
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB2	7	0.27
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB3	7	0.27
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	16	0.27
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	16	0.27
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE1	2	0.27
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE2	2	0.27
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	16	0.27
(1,187)	1:95:A:MET:HB2	1:115:A:ILE:HB	8	0.27
(1,187)	1:95:A:MET:HB3	1:115:A:ILE:HB	8	0.27
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	9	0.27
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	20	0.27
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	20	0.27
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	8	0.27
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	8	0.27
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	16	0.27
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	16	0.27
(1,60)	1:157:A:ALA:HB1	1:90:A:ASN:HA	16	0.27
(1,60)	1:157:A:ALA:HB2	1:90:A:ASN:HA	16	0.27
(1,60)	1:157:A:ALA:HB3	1:90:A:ASN:HA	16	0.27
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	15	0.27
(1,27)	1:50:A:PHE:HE1	1:52:A:ASP:HB3	1	0.27
(1,27)	1:50:A:PHE:HE2	1:52:A:ASP:HB3	1	0.27
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	8	0.26
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	17	0.26
(1,2149)	1:166:A:PHE:HD1	1:138:A:GLU:H	5	0.26
(1,2108)	1:112:A:SER:HG	1:113:A:THR:H	11	0.26
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	7	0.26
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	7	0.26
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	7	0.26
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	19	0.26
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	19	0.26
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	19	0.26
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG11	11	0.26
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG12	11	0.26
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG13	11	0.26
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG11	11	0.26
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG12	11	0.26
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG13	11	0.26
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	16	0.26
(1,2064)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	18	0.26
(1,2064)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	18	0.26
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	19	0.26
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	19	0.26
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	19	0.26
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	6	0.26
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB2	19	0.26
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB3	19	0.26
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	19	0.26
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	19	0.26
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	4	0.26
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	16	0.26
(1,1782)	1:37:A:ILE:HB	1:49:A:GLY:H	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	13	0.26
(1,1714)	1:165:A:LYS:HB2	1:87:A:TYR:H	18	0.26
(1,1714)	1:165:A:LYS:HB3	1:87:A:TYR:H	18	0.26
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	2	0.26
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	2	0.26
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	14	0.26
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	14	0.26
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	7	0.26
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	7	0.26
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	7	0.26
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	7	0.26
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	7	0.26
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	7	0.26
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	2	0.26
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	15	0.26
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	7	0.26
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	7	0.26
(1,1581)	1:93:A:LEU:HA	1:122:A:THR:HA	9	0.26
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	12	0.26
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	3	0.26
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG2	3	0.26
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG3	3	0.26
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG2	6	0.26
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG3	6	0.26
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD2	3	0.26
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD3	3	0.26
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD2	3	0.26
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD3	3	0.26
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD2	3	0.26
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD3	3	0.26
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD2	3	0.26
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD3	3	0.26
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD2	3	0.26
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD3	3	0.26
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD2	3	0.26
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD3	3	0.26
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD2	11	0.26
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD3	11	0.26
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD2	11	0.26
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD3	11	0.26
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD2	11	0.26
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD3	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD2	11	0.26
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD3	11	0.26
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD2	11	0.26
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD3	11	0.26
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD2	11	0.26
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD3	11	0.26
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	10	0.26
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	13	0.26
(1,1322)	1:166:A:PHE:H	1:167:A:SER:HA	13	0.26
(1,1291)	1:48:A:TYR:HD1	1:10:A:ARG:HA	13	0.26
(1,1291)	1:48:A:TYR:HD2	1:10:A:ARG:HA	13	0.26
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	18	0.26
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	18	0.26
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD11	13	0.26
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD12	13	0.26
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD13	13	0.26
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD21	13	0.26
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD22	13	0.26
(1,1206)	1:49:A:GLY:H	1:21:A:LEU:HD23	13	0.26
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG2	17	0.26
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG3	17	0.26
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	6	0.26
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	17	0.26
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	20	0.26
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	6	0.26
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	6	0.26
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	6	0.26
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	6	0.26
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	12	0.26
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	12	0.26
(1,1041)	1:23:A:LYS:H	1:19:A:GLN:HA	17	0.26
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB2	5	0.26
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB3	5	0.26
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB2	5	0.26
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB3	5	0.26
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	3	0.26
(1,968)	1:27:A:PRO:HG2	1:25:A:CYS:HA	6	0.26
(1,968)	1:27:A:PRO:HG3	1:25:A:CYS:HA	6	0.26
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	2	0.26
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG2	15	0.26
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG3	15	0.26
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	12	0.26
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	9	0.26
(1,703)	1:163:A:LEU:HD11	1:164:A:CYS:H	7	0.26
(1,703)	1:163:A:LEU:HD12	1:164:A:CYS:H	7	0.26
(1,703)	1:163:A:LEU:HD13	1:164:A:CYS:H	7	0.26
(1,703)	1:163:A:LEU:HD21	1:164:A:CYS:H	7	0.26
(1,703)	1:163:A:LEU:HD22	1:164:A:CYS:H	7	0.26
(1,703)	1:163:A:LEU:HD23	1:164:A:CYS:H	7	0.26
(1,653)	1:144:A:PHE:HA	1:146:A:GLY:H	14	0.26
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	2	0.26
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	10	0.26
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	7	0.26
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	2	0.26
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	2	0.26
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	2	0.26
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	2	0.26
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	8	0.26
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	13	0.26
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD11	15	0.26
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD12	15	0.26
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD13	15	0.26
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	10	0.26
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	7	0.26
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	7	0.26
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	7	0.26
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	7	0.26
(1,289)	1:93:A:LEU:HB2	1:95:A:MET:H	8	0.26
(1,289)	1:93:A:LEU:HB3	1:95:A:MET:H	8	0.26
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	5	0.26
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	5	0.26
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	5	0.26
(1,146)	1:96:A:ASP:HB2	1:98:A:GLN:HB2	9	0.26
(1,146)	1:96:A:ASP:HB2	1:98:A:GLN:HB3	9	0.26
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	4	0.26
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG21	12	0.26
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG22	12	0.26
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG23	12	0.26
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	5	0.26
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	5	0.26
(1,102)	1:115:A:ILE:HB	1:124:A:ARG:H	9	0.26
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	10	0.26
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2143)	1:134:A:THR:HA	1:166:A:PHE:HE1	11	0.25
(1,2114)	1:112:A:SER:HG	1:113:A:THR:HA	8	0.25
(1,2106)	1:132:A:GLU:HA	1:111:A:ILE:HA	18	0.25
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	11	0.25
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	11	0.25
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	11	0.25
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	13	0.25
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	18	0.25
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	7	0.25
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	18	0.25
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	14	0.25
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	12	0.25
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	14	0.25
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	19	0.25
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	3	0.25
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	12	0.25
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	12	0.25
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	3	0.25
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	17	0.25
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	14	0.25
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	12	0.25
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	12	0.25
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	1	0.25
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	1	0.25
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	16	0.25
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	16	0.25
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	14	0.25
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	14	0.25
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	8	0.25
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	8	0.25
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	8	0.25
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	8	0.25
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	8	0.25
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	8	0.25
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	3	0.25
(1,1626)	1:39:A:ASP:HA	1:44:A:LYS:H	12	0.25
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	17	0.25
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	17	0.25
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	19	0.25
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	19	0.25
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	8	0.25
(1,1495)	1:58:A:ALA:HA	1:61:A:LYS:HE2	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1495)	1:58:A:ALA:HA	1:61:A:LYS:HE3	9	0.25
(1,1297)	1:39:A:ASP:HA	1:46:A:LYS:HD2	6	0.25
(1,1297)	1:39:A:ASP:HA	1:46:A:LYS:HD3	6	0.25
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	15	0.25
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	15	0.25
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	3	0.25
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	16	0.25
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	11	0.25
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	11	0.25
(1,1132)	1:21:A:LEU:HD11	1:16:A:THR:HB	4	0.25
(1,1132)	1:21:A:LEU:HD12	1:16:A:THR:HB	4	0.25
(1,1132)	1:21:A:LEU:HD13	1:16:A:THR:HB	4	0.25
(1,1132)	1:21:A:LEU:HD21	1:16:A:THR:HB	4	0.25
(1,1132)	1:21:A:LEU:HD22	1:16:A:THR:HB	4	0.25
(1,1132)	1:21:A:LEU:HD23	1:16:A:THR:HB	4	0.25
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	13	0.25
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	2	0.25
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	2	0.25
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	14	0.25
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	14	0.25
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	4	0.25
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	6	0.25
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	9	0.25
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	7	0.25
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	11	0.25
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	11	0.25
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	11	0.25
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	17	0.25
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	12	0.25
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	12	0.25
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	7	0.25
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	5	0.25
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	5	0.25
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	5	0.25
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	5	0.25
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	19	0.25
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	19	0.25
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	16	0.25
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	1	0.25
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	1	0.25
(1,520)	1:111:A:ILE:HB	1:132:A:GLU:H	9	0.25
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	3	0.25
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	9	0.25
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	1	0.25
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	9	0.25
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	9	0.25
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB2	17	0.25
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB3	17	0.25
(1,209)	1:21:A:LEU:HG	1:22:A:VAL:H	2	0.25
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	17	0.25
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	17	0.25
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	17	0.25
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	17	0.25
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	6	0.25
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB2	1	0.25
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB3	1	0.25
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB2	1	0.25
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB3	1	0.25
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	9	0.25
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	9	0.25
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	7	0.25
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	7	0.25
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	14	0.25
(1,28)	1:45:A:CYS:HB2	1:15:A:HIS:HA	3	0.25
(1,28)	1:45:A:CYS:HB3	1:15:A:HIS:HA	3	0.25
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	12	0.24
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	12	0.24
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	9	0.24
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	13	0.24
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	13	0.24
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	13	0.24
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	13	0.24
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	13	0.24
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	13	0.24
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	16	0.24
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	4	0.24
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	4	0.24
(1,2093)	1:161:A:PRO:HD2	1:90:A:ASN:HD21	17	0.24
(1,2093)	1:161:A:PRO:HD2	1:90:A:ASN:HD22	17	0.24
(1,2093)	1:161:A:PRO:HD3	1:90:A:ASN:HD21	17	0.24
(1,2093)	1:161:A:PRO:HD3	1:90:A:ASN:HD22	17	0.24
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	12	0.24
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	2	0.24
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	3	0.24
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	3	0.24
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE21	18	0.24
(1,2031)	1:73:A:ALA:H	1:72:A:GLN:HE22	18	0.24
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	9	0.24
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	9	0.24
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	9	0.24
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	12	0.24
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	12	0.24
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	12	0.24
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	12	0.24
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	12	0.24
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	12	0.24
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	14	0.24
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	12	0.24
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	12	0.24
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD11	1	0.24
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD12	1	0.24
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD13	1	0.24
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD21	1	0.24
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD22	1	0.24
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD23	1	0.24
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	9	0.24
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	20	0.24
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE1	18	0.24
(1,1716)	1:165:A:LYS:HD2	1:87:A:TYR:HE2	18	0.24
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE1	18	0.24
(1,1716)	1:165:A:LYS:HD3	1:87:A:TYR:HE2	18	0.24
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	13	0.24
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	13	0.24
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	12	0.24
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	12	0.24
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	20	0.24
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	17	0.24
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	19	0.24
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	19	0.24
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	19	0.24
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	19	0.24
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	3	0.24
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	3	0.24
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	8	0.24
(1,1255)	1:41:A:THR:HG21	1:42:A:THR:HB	1	0.24
(1,1255)	1:41:A:THR:HG22	1:42:A:THR:HB	1	0.24
(1,1255)	1:41:A:THR:HG23	1:42:A:THR:HB	1	0.24
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	14	0.24
(1,1128)	1:30:A:LYS:HE2	1:54:A:ASP:H	16	0.24
(1,1128)	1:30:A:LYS:HE3	1:54:A:ASP:H	16	0.24
(1,1114)	1:133:A:SER:HA	1:132:A:GLU:HG2	12	0.24
(1,1114)	1:133:A:SER:HA	1:132:A:GLU:HG3	12	0.24
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	9	0.24
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	9	0.24
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	7	0.24
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	12	0.24
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	12	0.24
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	13	0.24
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	18	0.24
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	18	0.24
(1,1012)	1:43:A:ASN:HB3	1:44:A:LYS:HA	8	0.24
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	16	0.24
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	16	0.24
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	13	0.24
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	14	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	16	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	16	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	16	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	16	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	16	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	16	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	18	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	18	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	18	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	18	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	18	0.24
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	18	0.24
(1,900)	1:32:A:VAL:HB	1:33:A:SER:HA	5	0.24
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	1	0.24
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	16	0.24
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	19	0.24
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	19	0.24
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	12	0.24
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	12	0.24
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	19	0.24
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	17	0.24
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	17	0.24
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	17	0.24
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	17	0.24
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	9	0.24
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	9	0.24
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	9	0.24
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	9	0.24
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	10	0.24
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	10	0.24
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	13	0.24
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	9	0.24
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	9	0.24
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	9	0.24
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	9	0.24
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	9	0.24
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	9	0.24
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	14	0.24
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	14	0.24
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	16	0.24
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	16	0.24
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	5	0.24
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	5	0.24
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	12	0.24
(1,308)	1:103:A:MET:HB2	1:104:A:LEU:HB2	12	0.24
(1,308)	1:103:A:MET:HB3	1:104:A:LEU:HB2	12	0.24
(1,295)	1:97:A:GLU:HB2	1:115:A:ILE:H	3	0.24
(1,295)	1:97:A:GLU:HB3	1:115:A:ILE:H	3	0.24
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	4	0.24
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	4	0.24
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	5	0.24
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	5	0.24
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	17	0.24
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	17	0.24
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	16	0.24
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	14	0.24
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	14	0.24
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	14	0.24
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	14	0.24
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	4	0.24
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	1	0.24
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	1	0.24
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	1	0.24
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	1	0.24
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	15	0.24
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	15	0.24
(1,99)	1:41:A:THR:HB	1:40:A:LYS:H	8	0.24
(1,69)	1:111:A:ILE:HA	1:110:A:VAL:H	4	0.24
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	5	0.24
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	10	0.24
(1,28)	1:45:A:CYS:HB2	1:15:A:HIS:HA	18	0.24
(1,28)	1:45:A:CYS:HB3	1:15:A:HIS:HA	18	0.24
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	6	0.23
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	6	0.23
(1,2167)	1:6:A:ASN:H	1:4:A:GLY:HA2	15	0.23
(1,2167)	1:6:A:ASN:H	1:4:A:GLY:HA3	15	0.23
(1,2130)	1:48:A:TYR:HD1	1:46:A:LYS:H	16	0.23
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	10	0.23
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	10	0.23
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	10	0.23
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	10	0.23
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	8	0.23
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	13	0.23
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	13	0.23
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	13	0.23
(1,2086)	1:126:A:VAL:HG11	1:89:A:SER:HG	2	0.23
(1,2086)	1:126:A:VAL:HG12	1:89:A:SER:HG	2	0.23
(1,2086)	1:126:A:VAL:HG13	1:89:A:SER:HG	2	0.23
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	6	0.23
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	9	0.23
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	9	0.23
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	13	0.23
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB2	15	0.23
(1,2037)	1:10:A:ARG:HG2	1:72:A:GLN:HB3	15	0.23
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB2	15	0.23
(1,2037)	1:10:A:ARG:HG3	1:72:A:GLN:HB3	15	0.23
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	2	0.23
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	2	0.23
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE21	13	0.23
(1,2036)	1:73:A:ALA:HA	1:72:A:GLN:HE22	13	0.23
(1,2009)	1:48:A:TYR:HD2	1:9:A:ILE:H	11	0.23
(1,1997)	1:32:A:VAL:HG11	1:33:A:SER:H	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1997)	1:32:A:VAL:HG12	1:33:A:SER:H	3	0.23
(1,1997)	1:32:A:VAL:HG13	1:33:A:SER:H	3	0.23
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	4	0.23
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	4	0.23
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	4	0.23
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	4	0.23
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	4	0.23
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	4	0.23
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	15	0.23
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	6	0.23
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	6	0.23
(1,1945)	1:50:A:PHE:HE1	1:35:A:LYS:HG2	20	0.23
(1,1945)	1:50:A:PHE:HE1	1:35:A:LYS:HG3	20	0.23
(1,1945)	1:50:A:PHE:HE2	1:35:A:LYS:HG2	20	0.23
(1,1945)	1:50:A:PHE:HE2	1:35:A:LYS:HG3	20	0.23
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	12	0.23
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	10	0.23
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	10	0.23
(1,1901)	1:77:A:LYS:HB2	1:79:A:GLN:HG2	18	0.23
(1,1901)	1:77:A:LYS:HB2	1:79:A:GLN:HG3	18	0.23
(1,1901)	1:77:A:LYS:HB3	1:79:A:GLN:HG2	18	0.23
(1,1901)	1:77:A:LYS:HB3	1:79:A:GLN:HG3	18	0.23
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB2	13	0.23
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB3	13	0.23
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB2	13	0.23
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB3	13	0.23
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	2	0.23
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	17	0.23
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	2	0.23
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	2	0.23
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	7	0.23
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	5	0.23
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	4	0.23
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	18	0.23
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	15	0.23
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	15	0.23
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	7	0.23
(1,1539)	1:33:A:SER:HA	1:34:A:THR:H	18	0.23
(1,1513)	1:115:A:ILE:HD11	1:97:A:GLU:H	16	0.23
(1,1513)	1:115:A:ILE:HD12	1:97:A:GLU:H	16	0.23
(1,1513)	1:115:A:ILE:HD13	1:97:A:GLU:H	16	0.23
(1,1500)	1:40:A:LYS:HG2	1:39:A:ASP:HA	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:40:A:LYS:HG3	1:39:A:ASP:HA	18	0.23
(1,1465)	1:47:A:GLY:H	1:48:A:TYR:H	16	0.23
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	11	0.23
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	11	0.23
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	14	0.23
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	14	0.23
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	13	0.23
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	10	0.23
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	10	0.23
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	1	0.23
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	1	0.23
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	16	0.23
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	16	0.23
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	15	0.23
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	9	0.23
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	9	0.23
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	9	0.23
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	9	0.23
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	1	0.23
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	1	0.23
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	4	0.23
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	4	0.23
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	11	0.23
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	11	0.23
(1,1085)	1:4:A:GLY:HA2	1:77:A:LYS:HA	8	0.23
(1,1085)	1:4:A:GLY:HA3	1:77:A:LYS:HA	8	0.23
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	14	0.23
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	2	0.23
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	11	0.23
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	11	0.23
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	14	0.23
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	14	0.23
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	20	0.23
(1,937)	1:113:A:THR:H	1:112:A:SER:HB2	16	0.23
(1,937)	1:113:A:THR:H	1:112:A:SER:HB3	16	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	10	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	10	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	10	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	10	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	10	0.23
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	10	0.23
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	19	0.23
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	2	0.23
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	2	0.23
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	2	0.23
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	4	0.23
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	4	0.23
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	4	0.23
(1,719)	1:164:A:CYS:HB2	1:88:A:ILE:HG12	7	0.23
(1,719)	1:164:A:CYS:HB2	1:88:A:ILE:HG13	7	0.23
(1,719)	1:164:A:CYS:HB3	1:88:A:ILE:HG12	7	0.23
(1,719)	1:164:A:CYS:HB3	1:88:A:ILE:HG13	7	0.23
(1,716)	1:165:A:LYS:HB2	1:86:A:LEU:HA	4	0.23
(1,716)	1:165:A:LYS:HB3	1:86:A:LEU:HA	4	0.23
(1,676)	1:151:A:THR:HA	1:155:A:VAL:HB	2	0.23
(1,676)	1:151:A:THR:HA	1:155:A:VAL:HB	15	0.23
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	3	0.23
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	16	0.23
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	20	0.23
(1,611)	1:156:A:SER:HA	1:155:A:VAL:H	5	0.23
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	3	0.23
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	2	0.23
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	2	0.23
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	6	0.23
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	6	0.23
(1,522)	1:139:A:ALA:HA	1:143:A:HIS:H	8	0.23
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	9	0.23
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	9	0.23
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	9	0.23
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	9	0.23
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	9	0.23
(1,432)	1:86:A:LEU:HA	1:167:A:SER:HA	10	0.23
(1,366)	1:86:A:LEU:HG	1:84:A:THR:HG21	18	0.23
(1,366)	1:86:A:LEU:HG	1:84:A:THR:HG22	18	0.23
(1,366)	1:86:A:LEU:HG	1:84:A:THR:HG23	18	0.23
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	4	0.23
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	7	0.23
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	10	0.23
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	16	0.23
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	1	0.23
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	1	0.23
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	8	0.23
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:67:A:LYS:HE2	1:64:A:SER:HA	15	0.23
(1,244)	1:67:A:LYS:HE3	1:64:A:SER:HA	15	0.23
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	20	0.23
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	20	0.23
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE1	6	0.23
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE2	6	0.23
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	1	0.23
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	7	0.23
(1,2178)	1:31:A:ILE:HA	1:53:A:PHE:HA	4	0.22
(1,2171)	1:6:A:ASN:HB2	1:5:A:THR:H	14	0.22
(1,2171)	1:6:A:ASN:HB3	1:5:A:THR:H	14	0.22
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	4	0.22
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	16	0.22
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	16	0.22
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	16	0.22
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	16	0.22
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	16	0.22
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	16	0.22
(1,2108)	1:112:A:SER:HG	1:113:A:THR:H	20	0.22
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	20	0.22
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	1	0.22
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	1	0.22
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	1	0.22
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	11	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	7	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	7	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	7	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	13	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	13	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	13	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	14	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	14	0.22
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	14	0.22
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	19	0.22
(1,1976)	1:6:A:ASN:HB2	1:5:A:THR:H	14	0.22
(1,1976)	1:6:A:ASN:HB3	1:5:A:THR:H	14	0.22
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	3	0.22
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	19	0.22
(1,1955)	1:77:A:LYS:HD2	1:79:A:GLN:HB2	6	0.22
(1,1955)	1:77:A:LYS:HD2	1:79:A:GLN:HB3	6	0.22
(1,1955)	1:77:A:LYS:HD3	1:79:A:GLN:HB2	6	0.22
(1,1955)	1:77:A:LYS:HD3	1:79:A:GLN:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	7	0.22
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	1	0.22
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	1	0.22
(1,1816)	1:53:A:PHE:HB2	1:30:A:LYS:H	2	0.22
(1,1816)	1:53:A:PHE:HB3	1:30:A:LYS:H	2	0.22
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	15	0.22
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	18	0.22
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	12	0.22
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	12	0.22
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	13	0.22
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	13	0.22
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	12	0.22
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	12	0.22
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	13	0.22
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	13	0.22
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	4	0.22
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	20	0.22
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	9	0.22
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	9	0.22
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	9	0.22
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	9	0.22
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	4	0.22
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	19	0.22
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	19	0.22
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	19	0.22
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	2	0.22
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	7	0.22
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	7	0.22
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	17	0.22
(1,1020)	1:61:A:LYS:HE2	1:29:A:GLY:HA2	11	0.22
(1,1020)	1:61:A:LYS:HE3	1:29:A:GLY:HA2	11	0.22
(1,991)	1:44:A:LYS:HB2	1:15:A:HIS:HA	1	0.22
(1,991)	1:44:A:LYS:HB3	1:15:A:HIS:HA	1	0.22
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	10	0.22
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	5	0.22
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	5	0.22
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	17	0.22
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	17	0.22
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	17	0.22
(1,942)	1:23:A:LYS:HG2	1:19:A:GLN:HG2	6	0.22
(1,942)	1:23:A:LYS:HG2	1:19:A:GLN:HG3	6	0.22
(1,942)	1:23:A:LYS:HG3	1:19:A:GLN:HG2	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,942)	1:23:A:LYS:HG3	1:19:A:GLN:HG3	6	0.22
(1,719)	1:164:A:CYS:HB2	1:88:A:ILE:HG12	1	0.22
(1,719)	1:164:A:CYS:HB2	1:88:A:ILE:HG13	1	0.22
(1,719)	1:164:A:CYS:HB3	1:88:A:ILE:HG12	1	0.22
(1,719)	1:164:A:CYS:HB3	1:88:A:ILE:HG13	1	0.22
(1,716)	1:165:A:LYS:HB2	1:86:A:LEU:HA	11	0.22
(1,716)	1:165:A:LYS:HB3	1:86:A:LEU:HA	11	0.22
(1,716)	1:165:A:LYS:HB2	1:86:A:LEU:HA	19	0.22
(1,716)	1:165:A:LYS:HB3	1:86:A:LEU:HA	19	0.22
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	2	0.22
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	6	0.22
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	2	0.22
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	20	0.22
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	20	0.22
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	1	0.22
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	1	0.22
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	1	0.22
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	1	0.22
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	1	0.22
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	1	0.22
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	14	0.22
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	11	0.22
(1,408)	1:129:A:ALA:HB1	1:88:A:ILE:HD11	18	0.22
(1,408)	1:129:A:ALA:HB1	1:88:A:ILE:HD12	18	0.22
(1,408)	1:129:A:ALA:HB1	1:88:A:ILE:HD13	18	0.22
(1,408)	1:129:A:ALA:HB2	1:88:A:ILE:HD11	18	0.22
(1,408)	1:129:A:ALA:HB2	1:88:A:ILE:HD12	18	0.22
(1,408)	1:129:A:ALA:HB2	1:88:A:ILE:HD13	18	0.22
(1,408)	1:129:A:ALA:HB3	1:88:A:ILE:HD11	18	0.22
(1,408)	1:129:A:ALA:HB3	1:88:A:ILE:HD12	18	0.22
(1,408)	1:129:A:ALA:HB3	1:88:A:ILE:HD13	18	0.22
(1,398)	1:123:A:SER:HA	1:126:A:VAL:H	1	0.22
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE1	17	0.22
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE2	17	0.22
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	1	0.22
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	2	0.22
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	13	0.22
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	13	0.22
(1,244)	1:67:A:LYS:HE2	1:64:A:SER:HA	9	0.22
(1,244)	1:67:A:LYS:HE3	1:64:A:SER:HA	9	0.22
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	19	0.22
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	20	0.22
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	7	0.22
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	7	0.22
(1,108)	1:115:A:ILE:HG12	1:116:A:LEU:HA	7	0.22
(1,108)	1:115:A:ILE:HG13	1:116:A:LEU:HA	7	0.22
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	3	0.22
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	3	0.22
(1,102)	1:115:A:ILE:HB	1:124:A:ARG:H	16	0.22
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	8	0.22
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	8	0.22
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB2	15	0.22
(1,29)	1:12:A:LEU:H	1:10:A:ARG:HB3	15	0.22
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	6	0.21
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	15	0.21
(1,2130)	1:48:A:TYR:HD1	1:46:A:LYS:H	1	0.21
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	19	0.21
(1,2096)	1:90:A:ASN:H	1:91:A:LEU:H	8	0.21
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	10	0.21
(1,2078)	1:128:A:PHE:HA	1:88:A:ILE:H	14	0.21
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	3	0.21
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	14	0.21
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	15	0.21
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	15	0.21
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	18	0.21
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	19	0.21
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	19	0.21
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	19	0.21
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	19	0.21
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	19	0.21
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	19	0.21
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	20	0.21
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	7	0.21
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	10	0.21
(1,1912)	1:73:A:ALA:HA	1:9:A:ILE:H	6	0.21
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	7	0.21
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	7	0.21
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	13	0.21
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	13	0.21
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	19	0.21
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	19	0.21
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	10	0.21
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG21	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG22	13	0.21
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG23	13	0.21
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	9	0.21
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	9	0.21
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG21	16	0.21
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG22	16	0.21
(1,1608)	1:94:A:SER:HA	1:122:A:THR:HG23	16	0.21
(1,1590)	1:92:A:PRO:HD2	1:160:A:GLU:H	7	0.21
(1,1590)	1:92:A:PRO:HD3	1:160:A:GLU:H	7	0.21
(1,1577)	1:92:A:PRO:HA	1:151:A:THR:HA	7	0.21
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	8	0.21
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	8	0.21
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	4	0.21
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG12	8	0.21
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG13	8	0.21
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	13	0.21
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	4	0.21
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	19	0.21
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	19	0.21
(1,1291)	1:48:A:TYR:HD1	1:10:A:ARG:HA	17	0.21
(1,1291)	1:48:A:TYR:HD2	1:10:A:ARG:HA	17	0.21
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	3	0.21
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	3	0.21
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	12	0.21
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	12	0.21
(1,1255)	1:41:A:THR:HG21	1:42:A:THR:HB	7	0.21
(1,1255)	1:41:A:THR:HG22	1:42:A:THR:HB	7	0.21
(1,1255)	1:41:A:THR:HG23	1:42:A:THR:HB	7	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	1	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	1	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	1	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	1	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	5	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	5	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	5	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	5	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	19	0.21
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	19	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	19	0.21
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	19	0.21
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD1	5	0.21
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD2	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD1	5	0.21
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD2	5	0.21
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	3	0.21
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	17	0.21
(1,958)	1:27:A:PRO:HG2	1:23:A:LYS:HB2	9	0.21
(1,958)	1:27:A:PRO:HG2	1:23:A:LYS:HB3	9	0.21
(1,958)	1:27:A:PRO:HG3	1:23:A:LYS:HB2	9	0.21
(1,958)	1:27:A:PRO:HG3	1:23:A:LYS:HB3	9	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	3	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	3	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	3	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	3	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	3	0.21
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	3	0.21
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	19	0.21
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	8	0.21
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD2	14	0.21
(1,686)	1:156:A:SER:HB2	1:158:A:PRO:HD3	14	0.21
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD2	14	0.21
(1,686)	1:156:A:SER:HB3	1:158:A:PRO:HD3	14	0.21
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	4	0.21
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	9	0.21
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	19	0.21
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG21	15	0.21
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG22	15	0.21
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG23	15	0.21
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	2	0.21
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	2	0.21
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	2	0.21
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	2	0.21
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	20	0.21
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	10	0.21
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	19	0.21
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	6	0.21
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	6	0.21
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	5	0.21
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	5	0.21
(1,522)	1:139:A:ALA:HA	1:143:A:HIS:H	9	0.21
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	17	0.21
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	17	0.21
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	1	0.21
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:84:A:THR:HB	1:85:A:ASN:HA	14	0.21
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	2	0.21
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	20	0.21
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	19	0.21
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	19	0.21
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	20	0.21
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	20	0.21
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	10	0.21
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	10	0.21
(1,196)	1:97:A:GLU:HA	1:115:A:ILE:HG21	3	0.21
(1,196)	1:97:A:GLU:HA	1:115:A:ILE:HG22	3	0.21
(1,196)	1:97:A:GLU:HA	1:115:A:ILE:HG23	3	0.21
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	5	0.21
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	13	0.21
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	2	0.21
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	2	0.21
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	18	0.21
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	18	0.21
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG21	17	0.21
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG22	17	0.21
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG23	17	0.21
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	12	0.21
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	12	0.21
(1,102)	1:115:A:ILE:HB	1:124:A:ARG:H	20	0.21
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	11	0.21
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	11	0.21
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	12	0.21
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	12	0.21
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	6	0.21
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	3	0.2
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	14	0.2
(1,2137)	1:90:A:ASN:HB2	1:163:A:LEU:HB2	19	0.2
(1,2137)	1:90:A:ASN:HB2	1:163:A:LEU:HB3	19	0.2
(1,2137)	1:90:A:ASN:HB3	1:163:A:LEU:HB2	19	0.2
(1,2137)	1:90:A:ASN:HB3	1:163:A:LEU:HB3	19	0.2
(1,2125)	1:35:A:LYS:HB2	1:50:A:PHE:HE1	2	0.2
(1,2125)	1:35:A:LYS:HB3	1:50:A:PHE:HE1	2	0.2
(1,2119)	1:113:A:THR:HG1	1:129:A:ALA:HA	15	0.2
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	2	0.2
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	2	0.2
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	2	0.2
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	6	0.2
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	19	0.2
(1,2069)	1:165:A:LYS:HE2	1:87:A:TYR:HE2	17	0.2
(1,2069)	1:165:A:LYS:HE3	1:87:A:TYR:HE2	17	0.2
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	18	0.2
(1,2046)	1:7:A:LEU:HD11	1:75:A:MET:HA	6	0.2
(1,2046)	1:7:A:LEU:HD12	1:75:A:MET:HA	6	0.2
(1,2046)	1:7:A:LEU:HD13	1:75:A:MET:HA	6	0.2
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	13	0.2
(1,2008)	1:48:A:TYR:HD2	1:10:A:ARG:HE	15	0.2
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB2	2	0.2
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB3	2	0.2
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	14	0.2
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	14	0.2
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	14	0.2
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG21	20	0.2
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG22	20	0.2
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG23	20	0.2
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	6	0.2
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	13	0.2
(1,1939)	1:43:A:ASN:HB3	1:42:A:THR:HA	2	0.2
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	5	0.2
(1,1839)	1:50:A:PHE:HE1	1:34:A:THR:HA	1	0.2
(1,1839)	1:50:A:PHE:HE2	1:34:A:THR:HA	1	0.2
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	11	0.2
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD2	5	0.2
(1,1744)	1:29:A:GLY:HA3	1:61:A:LYS:HD3	5	0.2
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	9	0.2
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	9	0.2
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	16	0.2
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	16	0.2
(1,1673)	1:165:A:LYS:HB2	1:87:A:TYR:HA	18	0.2
(1,1673)	1:165:A:LYS:HB3	1:87:A:TYR:HA	18	0.2
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	13	0.2
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG21	14	0.2
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG22	14	0.2
(1,1635)	1:18:A:ASP:HA	1:16:A:THR:HG23	14	0.2
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	18	0.2
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	18	0.2
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	14	0.2
(1,1540)	1:30:A:LYS:HE2	1:31:A:ILE:H	11	0.2
(1,1540)	1:30:A:LYS:HE3	1:31:A:ILE:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:47:A:GLY:H	1:48:A:TYR:H	1	0.2
(1,1348)	1:17:A:THR:H	1:21:A:LEU:H	13	0.2
(1,1334)	1:146:A:GLY:H	1:163:A:LEU:HA	2	0.2
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	7	0.2
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	7	0.2
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	19	0.2
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB2	12	0.2
(1,1065)	1:136:A:LYS:HE2	1:135:A:GLU:HB3	12	0.2
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB2	12	0.2
(1,1065)	1:136:A:LYS:HE3	1:135:A:GLU:HB3	12	0.2
(1,969)	1:30:A:LYS:HD2	1:31:A:ILE:H	2	0.2
(1,969)	1:30:A:LYS:HD3	1:31:A:ILE:H	2	0.2
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	9	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	17	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	17	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	17	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	17	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	17	0.2
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	17	0.2
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	4	0.2
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	4	0.2
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	4	0.2
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	4	0.2
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	4	0.2
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	4	0.2
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	2	0.2
(1,890)	1:86:A:LEU:HB2	1:88:A:ILE:HA	3	0.2
(1,890)	1:86:A:LEU:HB3	1:88:A:ILE:HA	3	0.2
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	7	0.2
(1,722)	1:61:A:LYS:HB2	1:64:A:SER:H	19	0.2
(1,722)	1:61:A:LYS:HB3	1:64:A:SER:H	19	0.2
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	20	0.2
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	8	0.2
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	8	0.2
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	2	0.2
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	2	0.2
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	7	0.2
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	7	0.2
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	18	0.2
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	10	0.2
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	10	0.2
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	10	0.2
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	11	0.2
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	11	0.2
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	17	0.2
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	17	0.2
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	9	0.2
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	9	0.2
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	8	0.2
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	8	0.2
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	5	0.2
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	5	0.2
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	5	0.2
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	5	0.2
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	16	0.2
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	16	0.2
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	16	0.2
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	16	0.2
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	3	0.2
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	3	0.2
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	7	0.2
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	7	0.2
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	15	0.2
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	15	0.2
(1,121)	1:97:A:GLU:HG2	1:114:A:ARG:HG2	14	0.2
(1,121)	1:97:A:GLU:HG2	1:114:A:ARG:HG3	14	0.2
(1,121)	1:97:A:GLU:HG3	1:114:A:ARG:HG2	14	0.2
(1,121)	1:97:A:GLU:HG3	1:114:A:ARG:HG3	14	0.2
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	6	0.2
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	6	0.2
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	7	0.2
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	7	0.2
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	18	0.2
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	18	0.2
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB2	15	0.2
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB3	15	0.2
(1,60)	1:157:A:ALA:HB1	1:90:A:ASN:HA	9	0.2
(1,60)	1:157:A:ALA:HB2	1:90:A:ASN:HA	9	0.2
(1,60)	1:157:A:ALA:HB3	1:90:A:ASN:HA	9	0.2
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	18	0.2
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	6	0.2
(1,2178)	1:31:A:ILE:HA	1:53:A:PHE:HA	18	0.19
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD21	2	0.19
(1,2136)	1:163:A:LEU:HD21	1:90:A:ASN:HD22	2	0.19
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD21	2	0.19
(1,2136)	1:163:A:LEU:HD22	1:90:A:ASN:HD22	2	0.19
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD21	2	0.19
(1,2136)	1:163:A:LEU:HD23	1:90:A:ASN:HD22	2	0.19
(1,2109)	1:114:A:ARG:HH21	1:112:A:SER:HB2	3	0.19
(1,2109)	1:114:A:ARG:HH21	1:112:A:SER:HB3	3	0.19
(1,2109)	1:114:A:ARG:HH22	1:112:A:SER:HB2	3	0.19
(1,2109)	1:114:A:ARG:HH22	1:112:A:SER:HB3	3	0.19
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	9	0.19
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	3	0.19
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	8	0.19
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	17	0.19
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	3	0.19
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	9	0.19
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	7	0.19
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	7	0.19
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	7	0.19
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	7	0.19
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	7	0.19
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	7	0.19
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	7	0.19
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	1	0.19
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	15	0.19
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	17	0.19
(1,1961)	1:19:A:GLN:HG2	1:22:A:VAL:HB	9	0.19
(1,1961)	1:19:A:GLN:HG3	1:22:A:VAL:HB	9	0.19
(1,1905)	1:16:A:THR:HG21	1:21:A:LEU:HA	2	0.19
(1,1905)	1:16:A:THR:HG22	1:21:A:LEU:HA	2	0.19
(1,1905)	1:16:A:THR:HG23	1:21:A:LEU:HA	2	0.19
(1,1901)	1:77:A:LYS:HB2	1:79:A:GLN:HG2	9	0.19
(1,1901)	1:77:A:LYS:HB2	1:79:A:GLN:HG3	9	0.19
(1,1901)	1:77:A:LYS:HB3	1:79:A:GLN:HG2	9	0.19
(1,1901)	1:77:A:LYS:HB3	1:79:A:GLN:HG3	9	0.19
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB2	6	0.19
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB3	6	0.19
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB2	6	0.19
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB3	6	0.19
(1,1891)	1:43:A:ASN:HA	1:38:A:LEU:HA	20	0.19
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB2	18	0.19
(1,1827)	1:77:A:LYS:HA	1:80:A:GLU:HB3	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1749)	1:66:A:LEU:HB2	1:67:A:LYS:HG2	12	0.19
(1,1749)	1:66:A:LEU:HB2	1:67:A:LYS:HG3	12	0.19
(1,1749)	1:66:A:LEU:HB3	1:67:A:LYS:HG2	12	0.19
(1,1749)	1:66:A:LEU:HB3	1:67:A:LYS:HG3	12	0.19
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	18	0.19
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	18	0.19
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	20	0.19
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	20	0.19
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	7	0.19
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	3	0.19
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	3	0.19
(1,1538)	1:30:A:LYS:HG2	1:31:A:ILE:H	20	0.19
(1,1538)	1:30:A:LYS:HG3	1:31:A:ILE:H	20	0.19
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	13	0.19
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG2	1	0.19
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG3	1	0.19
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	7	0.19
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	7	0.19
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	7	0.19
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	7	0.19
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG21	16	0.19
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG22	16	0.19
(1,1395)	1:52:A:ASP:HB2	1:31:A:ILE:HG23	16	0.19
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	4	0.19
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	4	0.19
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD2	11	0.19
(1,1290)	1:11:A:GLY:H	1:10:A:ARG:HD3	11	0.19
(1,1271)	1:71:A:VAL:HG11	1:12:A:LEU:HA	18	0.19
(1,1271)	1:71:A:VAL:HG12	1:12:A:LEU:HA	18	0.19
(1,1271)	1:71:A:VAL:HG13	1:12:A:LEU:HA	18	0.19
(1,1271)	1:71:A:VAL:HG21	1:12:A:LEU:HA	18	0.19
(1,1271)	1:71:A:VAL:HG22	1:12:A:LEU:HA	18	0.19
(1,1271)	1:71:A:VAL:HG23	1:12:A:LEU:HA	18	0.19
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	10	0.19
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD11	9	0.19
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD12	9	0.19
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD13	9	0.19
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD21	9	0.19
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD22	9	0.19
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD23	9	0.19
(1,1156)	1:130:A:ARG:HB2	1:86:A:LEU:H	18	0.19
(1,1156)	1:130:A:ARG:HB3	1:86:A:LEU:H	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	16	0.19
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	8	0.19
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	8	0.19
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	18	0.19
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	18	0.19
(1,1052)	1:15:A:HIS:HB3	1:16:A:THR:HA	9	0.19
(1,1052)	1:15:A:HIS:HB3	1:16:A:THR:HA	17	0.19
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	16	0.19
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	18	0.19
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	18	0.19
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	19	0.19
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	2	0.19
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	2	0.19
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	15	0.19
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	15	0.19
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	2	0.19
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	2	0.19
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	2	0.19
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	2	0.19
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	2	0.19
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	2	0.19
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	2	0.19
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	15	0.19
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG2	14	0.19
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG3	14	0.19
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	20	0.19
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	20	0.19
(1,764)	1:23:A:LYS:HD2	1:20:A:ASP:H	12	0.19
(1,764)	1:23:A:LYS:HD3	1:20:A:ASP:H	12	0.19
(1,722)	1:61:A:LYS:HB2	1:64:A:SER:H	10	0.19
(1,722)	1:61:A:LYS:HB3	1:64:A:SER:H	10	0.19
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	18	0.19
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	7	0.19
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	7	0.19
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	17	0.19
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	17	0.19
(1,678)	1:150:A:LYS:HG2	1:151:A:THR:HB	3	0.19
(1,678)	1:150:A:LYS:HG3	1:151:A:THR:HB	3	0.19
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	16	0.19
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	16	0.19
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	16	0.19
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,518)	1:111:A:ILE:HA	1:132:A:GLU:H	13	0.19
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG2	5	0.19
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG3	5	0.19
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	5	0.19
(1,475)	1:138:A:GLU:HG2	1:166:A:PHE:HB2	15	0.19
(1,475)	1:138:A:GLU:HG2	1:166:A:PHE:HB3	15	0.19
(1,475)	1:138:A:GLU:HG3	1:166:A:PHE:HB2	15	0.19
(1,475)	1:138:A:GLU:HG3	1:166:A:PHE:HB3	15	0.19
(1,398)	1:123:A:SER:HA	1:126:A:VAL:H	14	0.19
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE1	4	0.19
(1,381)	1:115:A:ILE:HA	1:128:A:PHE:HE2	4	0.19
(1,347)	1:95:A:MET:HA	1:94:A:SER:H	13	0.19
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	13	0.19
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	6	0.19
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	19	0.19
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	9	0.19
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	9	0.19
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	9	0.19
(1,174)	1:115:A:ILE:HD11	1:124:A:ARG:H	17	0.19
(1,174)	1:115:A:ILE:HD12	1:124:A:ARG:H	17	0.19
(1,174)	1:115:A:ILE:HD13	1:124:A:ARG:H	17	0.19
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	13	0.19
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	13	0.19
(1,102)	1:115:A:ILE:HB	1:124:A:ARG:H	7	0.19
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	1	0.19
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	1	0.19
(1,33)	1:60:A:GLN:HG2	1:61:A:LYS:HA	10	0.19
(1,33)	1:60:A:GLN:HG3	1:61:A:LYS:HA	10	0.19
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	3	0.19
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	3	0.19
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	3	0.19
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	3	0.19
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	3	0.19
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	3	0.19
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	14	0.18
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	14	0.18
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	14	0.18
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	14	0.18
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	12	0.18
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	11	0.18
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	6	0.18
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	6	0.18
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	6	0.18
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	6	0.18
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	6	0.18
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	13	0.18
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	10	0.18
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	10	0.18
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	5	0.18
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	19	0.18
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	15	0.18
(1,1661)	1:162:A:LEU:HG	1:164:A:CYS:HA	18	0.18
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD11	10	0.18
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD12	10	0.18
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD13	10	0.18
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD21	10	0.18
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD22	10	0.18
(1,1643)	1:72:A:GLN:H	1:66:A:LEU:HD23	10	0.18
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	8	0.18
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	2	0.18
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	2	0.18
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	6	0.18
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	6	0.18
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	1	0.18
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	6	0.18
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	13	0.18
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	15	0.18
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	9	0.18
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	5	0.18
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	5	0.18
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	10	0.18
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	10	0.18
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	14	0.18
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	14	0.18
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	14	0.18
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG2	20	0.18
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG3	20	0.18
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	10	0.18
(1,1169)	1:129:A:ALA:HA	1:112:A:SER:H	6	0.18
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	12	0.18
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	12	0.18
(1,1148)	1:32:A:VAL:HB	1:33:A:SER:HB2	13	0.18
(1,1148)	1:32:A:VAL:HB	1:33:A:SER:HB3	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	19	0.18
(1,1128)	1:30:A:LYS:HE2	1:54:A:ASP:H	8	0.18
(1,1128)	1:30:A:LYS:HE3	1:54:A:ASP:H	8	0.18
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	5	0.18
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	5	0.18
(1,1104)	1:85:A:ASN:HB3	1:129:A:ALA:H	10	0.18
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG2	16	0.18
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG3	16	0.18
(1,1052)	1:15:A:HIS:HB3	1:16:A:THR:HA	15	0.18
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	12	0.18
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	8	0.18
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	8	0.18
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	8	0.18
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	8	0.18
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	8	0.18
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	8	0.18
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	14	0.18
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	14	0.18
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	2	0.18
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	5	0.18
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	5	0.18
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	11	0.18
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	11	0.18
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	13	0.18
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	13	0.18
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	16	0.18
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	16	0.18
(1,693)	1:155:A:VAL:HB	1:94:A:SER:HB2	7	0.18
(1,693)	1:155:A:VAL:HB	1:94:A:SER:HB3	7	0.18
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	4	0.18
(1,649)	1:148:A:PHE:HA	1:147:A:LYS:H	16	0.18
(1,647)	1:148:A:PHE:HA	1:149:A:ILE:HB	14	0.18
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	12	0.18
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	17	0.18
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	11	0.18
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	4	0.18
(1,608)	1:158:A:PRO:HB2	1:160:A:GLU:H	1	0.18
(1,608)	1:158:A:PRO:HB3	1:160:A:GLU:H	1	0.18
(1,387)	1:116:A:LEU:HA	1:124:A:ARG:HD2	7	0.18
(1,387)	1:116:A:LEU:HA	1:124:A:ARG:HD3	7	0.18
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	4	0.18
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	7	0.18
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	12	0.18
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	12	0.18
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	12	0.18
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	12	0.18
(1,244)	1:67:A:LYS:HE2	1:64:A:SER:HA	16	0.18
(1,244)	1:67:A:LYS:HE3	1:64:A:SER:HA	16	0.18
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	12	0.18
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	12	0.18
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE1	16	0.18
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE2	16	0.18
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	18	0.18
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	18	0.18
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	4	0.18
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	4	0.18
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	17	0.18
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	17	0.18
(1,60)	1:157:A:ALA:HB1	1:90:A:ASN:HA	12	0.18
(1,60)	1:157:A:ALA:HB2	1:90:A:ASN:HA	12	0.18
(1,60)	1:157:A:ALA:HB3	1:90:A:ASN:HA	12	0.18
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	4	0.17
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	10	0.17
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	17	0.17
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	18	0.17
(1,2086)	1:126:A:VAL:HG11	1:89:A:SER:HG	16	0.17
(1,2086)	1:126:A:VAL:HG12	1:89:A:SER:HG	16	0.17
(1,2086)	1:126:A:VAL:HG13	1:89:A:SER:HG	16	0.17
(1,2046)	1:7:A:LEU:HD11	1:75:A:MET:HA	8	0.17
(1,2046)	1:7:A:LEU:HD12	1:75:A:MET:HA	8	0.17
(1,2046)	1:7:A:LEU:HD13	1:75:A:MET:HA	8	0.17
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	13	0.17
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	13	0.17
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	17	0.17
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	10	0.17
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	9	0.17
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	9	0.17
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	9	0.17
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	9	0.17
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	9	0.17
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	9	0.17
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	18	0.17
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	18	0.17
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	7	0.17
(1,1883)	1:29:A:GLY:HA3	1:28:A:TYR:H	9	0.17
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	4	0.17
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	4	0.17
(1,1816)	1:53:A:PHE:HB2	1:30:A:LYS:H	5	0.17
(1,1816)	1:53:A:PHE:HB3	1:30:A:LYS:H	5	0.17
(1,1801)	1:44:A:LYS:HD2	1:42:A:THR:HB	15	0.17
(1,1801)	1:44:A:LYS:HD3	1:42:A:THR:HB	15	0.17
(1,1726)	1:75:A:MET:HA	1:8:A:TYR:HB2	1	0.17
(1,1711)	1:144:A:PHE:HB2	1:146:A:GLY:H	14	0.17
(1,1711)	1:144:A:PHE:HB3	1:146:A:GLY:H	14	0.17
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	15	0.17
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	15	0.17
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	7	0.17
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	7	0.17
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	7	0.17
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	7	0.17
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	7	0.17
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	7	0.17
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	19	0.17
(1,1498)	1:40:A:LYS:HA	1:39:A:ASP:HB2	20	0.17
(1,1498)	1:40:A:LYS:HA	1:39:A:ASP:HB3	20	0.17
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	5	0.17
(1,1485)	1:20:A:ASP:HB2	1:17:A:THR:HB	17	0.17
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	14	0.17
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	18	0.17
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	5	0.17
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	9	0.17
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	9	0.17
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	20	0.17
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB2	16	0.17
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB3	16	0.17
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG2	18	0.17
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG3	18	0.17
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	13	0.17
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	13	0.17
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	13	0.17
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	13	0.17
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	14	0.17
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	14	0.17
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	14	0.17
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	18	0.17
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	18	0.17
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	18	0.17
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	18	0.17
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	20	0.17
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	20	0.17
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	12	0.17
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	12	0.17
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	13	0.17
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	13	0.17
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG2	14	0.17
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG3	14	0.17
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG2	14	0.17
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG3	14	0.17
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG2	14	0.17
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG3	14	0.17
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	4	0.17
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	3	0.17
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	3	0.17
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	12	0.17
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	19	0.17
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	12	0.17
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	16	0.17
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	11	0.17
(1,884)	1:39:A:ASP:HA	1:38:A:LEU:H	19	0.17
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	11	0.17
(1,820)	1:90:A:ASN:HA	1:163:A:LEU:H	18	0.17
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	13	0.17
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	13	0.17
(1,722)	1:61:A:LYS:HB2	1:64:A:SER:H	13	0.17
(1,722)	1:61:A:LYS:HB3	1:64:A:SER:H	13	0.17
(1,705)	1:160:A:GLU:HA	1:149:A:ILE:H	14	0.17
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	2	0.17
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	14	0.17
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	7	0.17
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	7	0.17
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	7	0.17
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	7	0.17
(1,615)	1:153:A:PRO:HD2	1:150:A:LYS:HE2	18	0.17
(1,615)	1:153:A:PRO:HD2	1:150:A:LYS:HE3	18	0.17
(1,615)	1:153:A:PRO:HD3	1:150:A:LYS:HE2	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:153:A:PRO:HD3	1:150:A:LYS:HE3	18	0.17
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	9	0.17
(1,450)	1:136:A:LYS:HA	1:140:A:VAL:HB	2	0.17
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	12	0.17
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	5	0.17
(1,347)	1:95:A:MET:HA	1:94:A:SER:H	8	0.17
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	8	0.17
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	8	0.17
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	5	0.17
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	5	0.17
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	3	0.17
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB2	2	0.17
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB3	2	0.17
(1,237)	1:114:A:ARG:HB2	1:129:A:ALA:HA	19	0.17
(1,237)	1:114:A:ARG:HB3	1:129:A:ALA:HA	19	0.17
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	7	0.17
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	7	0.17
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE1	14	0.17
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE2	14	0.17
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	12	0.17
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG2	7	0.17
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG3	7	0.17
(1,99)	1:41:A:THR:HB	1:40:A:LYS:H	20	0.17
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	3	0.17
(1,58)	1:141:A:ILE:HB	1:143:A:HIS:H	11	0.17
(1,28)	1:45:A:CYS:HB2	1:15:A:HIS:HA	2	0.17
(1,28)	1:45:A:CYS:HB3	1:15:A:HIS:HA	2	0.17
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	17	0.17
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	1	0.16
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	17	0.16
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	6	0.16
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	6	0.16
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	6	0.16
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	6	0.16
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	15	0.16
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	8	0.16
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	1	0.16
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	15	0.16
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	8	0.16
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	8	0.16
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	8	0.16
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	4	0.16
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	15	0.16
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	15	0.16
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	15	0.16
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	15	0.16
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	15	0.16
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	15	0.16
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB1	17	0.16
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB2	17	0.16
(1,1986)	1:8:A:TYR:HE1	1:76:A:ALA:HB3	17	0.16
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB1	17	0.16
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB2	17	0.16
(1,1986)	1:8:A:TYR:HE2	1:76:A:ALA:HB3	17	0.16
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	19	0.16
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	2	0.16
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	2	0.16
(1,1963)	1:8:A:TYR:HB2	1:74:A:GLN:HA	3	0.16
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD11	10	0.16
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD12	10	0.16
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD13	10	0.16
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD21	10	0.16
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD22	10	0.16
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD23	10	0.16
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	12	0.16
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB2	8	0.16
(1,1896)	1:76:A:ALA:HA	1:80:A:GLU:HB3	8	0.16
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	20	0.16
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	20	0.16
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	6	0.16
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	6	0.16
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	18	0.16
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	18	0.16
(1,1816)	1:53:A:PHE:HB2	1:30:A:LYS:H	7	0.16
(1,1816)	1:53:A:PHE:HB3	1:30:A:LYS:H	7	0.16
(1,1775)	1:81:A:GLN:HG2	1:78:A:GLN:H	1	0.16
(1,1775)	1:81:A:GLN:HG3	1:78:A:GLN:H	1	0.16
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	10	0.16
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	8	0.16
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	8	0.16
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	3	0.16
(1,1676)	1:166:A:PHE:HA	1:85:A:ASN:H	16	0.16
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	5	0.16
(1,1665)	1:164:A:CYS:HB2	1:86:A:LEU:HB2	14	0.16
(1,1665)	1:164:A:CYS:HB2	1:86:A:LEU:HB3	14	0.16
(1,1665)	1:164:A:CYS:HB3	1:86:A:LEU:HB2	14	0.16
(1,1665)	1:164:A:CYS:HB3	1:86:A:LEU:HB3	14	0.16
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	9	0.16
(1,1575)	1:90:A:ASN:HA	1:162:A:LEU:HA	18	0.16
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	5	0.16
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	7	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG11	1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG12	1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG13	1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG21	1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG22	1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG23	1	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG11	14	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG12	14	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG13	14	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG21	14	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG22	14	0.16
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG23	14	0.16
(1,1465)	1:47:A:GLY:H	1:48:A:TYR:H	18	0.16
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	7	0.16
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	7	0.16
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	7	0.16
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	7	0.16
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	18	0.16
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	18	0.16
(1,1304)	1:37:A:ILE:HG12	1:46:A:LYS:HB2	4	0.16
(1,1304)	1:37:A:ILE:HG12	1:46:A:LYS:HB3	4	0.16
(1,1304)	1:37:A:ILE:HG13	1:46:A:LYS:HB2	4	0.16
(1,1304)	1:37:A:ILE:HG13	1:46:A:LYS:HB3	4	0.16
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	11	0.16
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	11	0.16
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG2	16	0.16
(1,1184)	1:72:A:GLN:HA	1:10:A:ARG:HG3	16	0.16
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	4	0.16
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	2	0.16
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	2	0.16
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	2	0.16
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	2	0.16
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	4	0.16
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	4	0.16
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	4	0.16
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	15	0.16
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	15	0.16
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	15	0.16
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	15	0.16
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	1	0.16
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	1	0.16
(1,1137)	1:83:A:PRO:HD2	1:84:A:THR:HB	6	0.16
(1,1137)	1:83:A:PRO:HD3	1:84:A:THR:HB	6	0.16
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	19	0.16
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	19	0.16
(1,1092)	1:20:A:ASP:H	1:16:A:THR:HA	5	0.16
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	14	0.16
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	14	0.16
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG21	16	0.16
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG22	16	0.16
(1,1037)	1:18:A:ASP:H	1:16:A:THR:HG23	16	0.16
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	6	0.16
(1,1012)	1:43:A:ASN:HB3	1:44:A:LYS:HA	3	0.16
(1,1012)	1:43:A:ASN:HB3	1:44:A:LYS:HA	15	0.16
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB2	15	0.16
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB3	15	0.16
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB2	15	0.16
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB3	15	0.16
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	7	0.16
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	11	0.16
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	9	0.16
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	9	0.16
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	8	0.16
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	8	0.16
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	8	0.16
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	8	0.16
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	8	0.16
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	8	0.16
(1,906)	1:73:A:ALA:HA	1:9:A:ILE:HB	4	0.16
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	17	0.16
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	2	0.16
(1,722)	1:61:A:LYS:HB2	1:64:A:SER:H	17	0.16
(1,722)	1:61:A:LYS:HB3	1:64:A:SER:H	17	0.16
(1,658)	1:144:A:PHE:HB2	1:164:A:CYS:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:144:A:PHE:HB3	1:164:A:CYS:H	8	0.16
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	2	0.16
(1,614)	1:162:A:LEU:HG	1:90:A:ASN:HB2	2	0.16
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD11	12	0.16
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD12	12	0.16
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD13	12	0.16
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD21	12	0.16
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD22	12	0.16
(1,570)	1:122:A:THR:HB	1:93:A:LEU:HD23	12	0.16
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG2	19	0.16
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG3	19	0.16
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	2	0.16
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	6	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	7	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	7	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	7	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	7	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	14	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	14	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	14	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	14	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	20	0.16
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	20	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	20	0.16
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	20	0.16
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	4	0.16
(1,460)	1:114:A:ARG:HB2	1:115:A:ILE:H	16	0.16
(1,460)	1:114:A:ARG:HB3	1:115:A:ILE:H	16	0.16
(1,405)	1:129:A:ALA:HB1	1:112:A:SER:H	5	0.16
(1,405)	1:129:A:ALA:HB2	1:112:A:SER:H	5	0.16
(1,405)	1:129:A:ALA:HB3	1:112:A:SER:H	5	0.16
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA2	17	0.16
(1,390)	1:119:A:SER:HA	1:121:A:GLY:HA3	17	0.16
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	5	0.16
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	13	0.16
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG12	6	0.16
(1,335)	1:79:A:GLN:HA	1:111:A:ILE:HG13	6	0.16
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	3	0.16
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	16	0.16
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	16	0.16
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	8	0.16
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	2	0.16
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	2	0.16
(1,287)	1:104:A:LEU:HA	1:103:A:MET:H	3	0.16
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	14	0.16
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	14	0.16
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	2	0.16
(1,175)	1:115:A:ILE:HB	1:125:A:GLY:H	18	0.16
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	2	0.16
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	2	0.16
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	5	0.16
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	5	0.16
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	14	0.16
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	14	0.16
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	9	0.16
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG2	15	0.16
(1,123)	1:102:A:ASN:HA	1:103:A:MET:HG3	15	0.16
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG21	13	0.16
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG22	13	0.16
(1,118)	1:45:A:CYS:HA	1:37:A:ILE:HG23	13	0.16
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	6	0.16
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	6	0.16
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	20	0.16
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	20	0.16
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	3	0.16
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	8	0.16
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	14	0.16
(1,2144)	1:134:A:THR:HB	1:166:A:PHE:HZ	14	0.15
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	14	0.15
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	14	0.15
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	14	0.15
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG21	20	0.15
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG22	20	0.15
(1,2099)	1:132:A:GLU:H	1:110:A:VAL:HG23	20	0.15
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	1	0.15
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	12	0.15
(1,2084)	1:90:A:ASN:H	1:89:A:SER:HG	14	0.15
(1,2079)	1:88:A:ILE:H	1:129:A:ALA:H	20	0.15
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	4	0.15
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	4	0.15
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	4	0.15
(1,2009)	1:48:A:TYR:HD2	1:9:A:ILE:H	6	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD11	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD12	13	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD13	13	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD21	13	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD22	13	0.15
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD23	13	0.15
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	16	0.15
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	1	0.15
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	19	0.15
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB2	19	0.15
(1,1928)	1:143:A:HIS:H	1:145:A:ASN:HB3	19	0.15
(1,1926)	1:71:A:VAL:HB	1:67:A:LYS:H	1	0.15
(1,1908)	1:71:A:VAL:HA	1:11:A:GLY:HA2	19	0.15
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	13	0.15
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	13	0.15
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	8	0.15
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	18	0.15
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	18	0.15
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG21	18	0.15
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG22	18	0.15
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG23	18	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	4	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	4	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	5	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	5	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	10	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	10	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	20	0.15
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	20	0.15
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	9	0.15
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	9	0.15
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	9	0.15
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	9	0.15
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	9	0.15
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	9	0.15
(1,1539)	1:33:A:SER:HA	1:34:A:THR:H	3	0.15
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	16	0.15
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD2	12	0.15
(1,1376)	1:22:A:VAL:HG11	1:27:A:PRO:HD3	12	0.15
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD2	12	0.15
(1,1376)	1:22:A:VAL:HG12	1:27:A:PRO:HD3	12	0.15
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD2	12	0.15
(1,1376)	1:22:A:VAL:HG13	1:27:A:PRO:HD3	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD2	12	0.15
(1,1376)	1:22:A:VAL:HG21	1:27:A:PRO:HD3	12	0.15
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD2	12	0.15
(1,1376)	1:22:A:VAL:HG22	1:27:A:PRO:HD3	12	0.15
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD2	12	0.15
(1,1376)	1:22:A:VAL:HG23	1:27:A:PRO:HD3	12	0.15
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	1	0.15
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	1	0.15
(1,1247)	1:5:A:THR:H	1:56:A:PRO:HA	2	0.15
(1,1195)	1:47:A:GLY:H	1:37:A:ILE:HB	1	0.15
(1,1177)	1:56:A:PRO:HB2	1:3:A:MET:H	14	0.15
(1,1177)	1:56:A:PRO:HB3	1:3:A:MET:H	14	0.15
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	6	0.15
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	6	0.15
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	6	0.15
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	6	0.15
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	13	0.15
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	13	0.15
(1,1150)	1:130:A:ARG:HA	1:112:A:SER:H	1	0.15
(1,1150)	1:130:A:ARG:HA	1:112:A:SER:H	6	0.15
(1,1150)	1:130:A:ARG:HA	1:112:A:SER:H	15	0.15
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	17	0.15
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	17	0.15
(1,1049)	1:17:A:THR:HB	1:18:A:ASP:HA	11	0.15
(1,1043)	1:23:A:LYS:HA	1:25:A:CYS:H	2	0.15
(1,991)	1:44:A:LYS:HB2	1:15:A:HIS:HA	2	0.15
(1,991)	1:44:A:LYS:HB3	1:15:A:HIS:HA	2	0.15
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	1	0.15
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	10	0.15
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	10	0.15
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	10	0.15
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	10	0.15
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	10	0.15
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	10	0.15
(1,889)	1:85:A:ASN:HA	1:130:A:ARG:H	5	0.15
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	6	0.15
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	6	0.15
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD11	14	0.15
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD12	14	0.15
(1,866)	1:62:A:ALA:HB1	1:9:A:ILE:HD13	14	0.15
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD11	14	0.15
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD12	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,866)	1:62:A:ALA:HB2	1:9:A:ILE:HD13	14	0.15
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD11	14	0.15
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD12	14	0.15
(1,866)	1:62:A:ALA:HB3	1:9:A:ILE:HD13	14	0.15
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	8	0.15
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG2	1	0.15
(1,829)	1:84:A:THR:HB	1:83:A:PRO:HG3	1	0.15
(1,781)	1:71:A:VAL:HG11	1:10:A:ARG:HG2	20	0.15
(1,781)	1:71:A:VAL:HG11	1:10:A:ARG:HG3	20	0.15
(1,781)	1:71:A:VAL:HG12	1:10:A:ARG:HG2	20	0.15
(1,781)	1:71:A:VAL:HG12	1:10:A:ARG:HG3	20	0.15
(1,781)	1:71:A:VAL:HG13	1:10:A:ARG:HG2	20	0.15
(1,781)	1:71:A:VAL:HG13	1:10:A:ARG:HG3	20	0.15
(1,781)	1:71:A:VAL:HG21	1:10:A:ARG:HG2	20	0.15
(1,781)	1:71:A:VAL:HG21	1:10:A:ARG:HG3	20	0.15
(1,781)	1:71:A:VAL:HG22	1:10:A:ARG:HG2	20	0.15
(1,781)	1:71:A:VAL:HG22	1:10:A:ARG:HG3	20	0.15
(1,781)	1:71:A:VAL:HG23	1:10:A:ARG:HG2	20	0.15
(1,781)	1:71:A:VAL:HG23	1:10:A:ARG:HG3	20	0.15
(1,729)	1:61:A:LYS:HB2	1:65:A:ALA:H	14	0.15
(1,729)	1:61:A:LYS:HB3	1:65:A:ALA:H	14	0.15
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	8	0.15
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	8	0.15
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	8	0.15
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	5	0.15
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	20	0.15
(1,701)	1:159:A:THR:HA	1:149:A:ILE:HG21	8	0.15
(1,701)	1:159:A:THR:HA	1:149:A:ILE:HG22	8	0.15
(1,701)	1:159:A:THR:HA	1:149:A:ILE:HG23	8	0.15
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	16	0.15
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	15	0.15
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	15	0.15
(1,684)	1:158:A:PRO:HA	1:159:A:THR:HB	5	0.15
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	7	0.15
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	18	0.15
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	5	0.15
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	14	0.15
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	15	0.15
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	15	0.15
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	15	0.15
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	15	0.15
(1,613)	1:155:A:VAL:HA	1:154:A:GLY:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	5	0.15
(1,520)	1:111:A:ILE:HB	1:132:A:GLU:H	13	0.15
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG2	14	0.15
(1,501)	1:111:A:ILE:HB	1:79:A:GLN:HG3	14	0.15
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	20	0.15
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	4	0.15
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	4	0.15
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	4	0.15
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	4	0.15
(1,432)	1:86:A:LEU:HA	1:167:A:SER:HA	13	0.15
(1,425)	1:110:A:VAL:HA	1:111:A:ILE:HA	17	0.15
(1,405)	1:129:A:ALA:HB1	1:112:A:SER:H	9	0.15
(1,405)	1:129:A:ALA:HB2	1:112:A:SER:H	9	0.15
(1,405)	1:129:A:ALA:HB3	1:112:A:SER:H	9	0.15
(1,405)	1:129:A:ALA:HB1	1:112:A:SER:H	17	0.15
(1,405)	1:129:A:ALA:HB2	1:112:A:SER:H	17	0.15
(1,405)	1:129:A:ALA:HB3	1:112:A:SER:H	17	0.15
(1,398)	1:123:A:SER:HA	1:126:A:VAL:H	5	0.15
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	9	0.15
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD11	16	0.15
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD12	16	0.15
(1,371)	1:95:A:MET:HA	1:115:A:ILE:HD13	16	0.15
(1,352)	1:86:A:LEU:HG	1:85:A:ASN:H	10	0.15
(1,327)	1:17:A:THR:H	1:18:A:ASP:HA	18	0.15
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	4	0.15
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	4	0.15
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	2	0.15
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	12	0.15
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	2	0.15
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	2	0.15
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	2	0.15
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	2	0.15
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	19	0.15
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	19	0.15
(1,50)	1:51:A:VAL:HA	1:35:A:LYS:H	9	0.15
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	1	0.15
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	5	0.15
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	12	0.15
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	16	0.15
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	8	0.14
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	8	0.14
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	8	0.14
(1,2087)	1:91:A:LEU:H	1:89:A:SER:HG	7	0.14
(1,2086)	1:126:A:VAL:HG11	1:89:A:SER:HG	17	0.14
(1,2086)	1:126:A:VAL:HG12	1:89:A:SER:HG	17	0.14
(1,2086)	1:126:A:VAL:HG13	1:89:A:SER:HG	17	0.14
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	10	0.14
(1,2019)	1:6:A:ASN:HA	1:51:A:VAL:H	4	0.14
(1,2009)	1:48:A:TYR:HD2	1:9:A:ILE:H	15	0.14
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB2	8	0.14
(1,2003)	1:33:A:SER:H	1:52:A:ASP:HB3	8	0.14
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	1	0.14
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	1	0.14
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	1	0.14
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG21	5	0.14
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG22	5	0.14
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG23	5	0.14
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	12	0.14
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD11	3	0.14
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD12	3	0.14
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD13	3	0.14
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD21	3	0.14
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD22	3	0.14
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD23	3	0.14
(1,1982)	1:8:A:TYR:H	1:74:A:GLN:H	6	0.14
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	18	0.14
(1,1884)	1:61:A:LYS:HD2	1:29:A:GLY:HA2	3	0.14
(1,1884)	1:61:A:LYS:HD3	1:29:A:GLY:HA2	3	0.14
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	12	0.14
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	12	0.14
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	14	0.14
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	14	0.14
(1,1816)	1:53:A:PHE:HB2	1:30:A:LYS:H	14	0.14
(1,1816)	1:53:A:PHE:HB3	1:30:A:LYS:H	14	0.14
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	13	0.14
(1,1763)	1:49:A:GLY:H	1:37:A:ILE:HD11	2	0.14
(1,1763)	1:49:A:GLY:H	1:37:A:ILE:HD12	2	0.14
(1,1763)	1:49:A:GLY:H	1:37:A:ILE:HD13	2	0.14
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	15	0.14
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	15	0.14
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	1	0.14
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	1	0.14
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	20	0.14
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	8	0.14
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	8	0.14
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	9	0.14
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	9	0.14
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB1	14	0.14
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB2	14	0.14
(1,1629)	1:77:A:LYS:HG2	1:76:A:ALA:HB3	14	0.14
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB1	14	0.14
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB2	14	0.14
(1,1629)	1:77:A:LYS:HG3	1:76:A:ALA:HB3	14	0.14
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	16	0.14
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	16	0.14
(1,1602)	1:93:A:LEU:HD11	1:155:A:VAL:H	5	0.14
(1,1602)	1:93:A:LEU:HD12	1:155:A:VAL:H	5	0.14
(1,1602)	1:93:A:LEU:HD13	1:155:A:VAL:H	5	0.14
(1,1602)	1:93:A:LEU:HD21	1:155:A:VAL:H	5	0.14
(1,1602)	1:93:A:LEU:HD22	1:155:A:VAL:H	5	0.14
(1,1602)	1:93:A:LEU:HD23	1:155:A:VAL:H	5	0.14
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB2	12	0.14
(1,1576)	1:90:A:ASN:HA	1:163:A:LEU:HB3	12	0.14
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	11	0.14
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	19	0.14
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	14	0.14
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	14	0.14
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	8	0.14
(1,1482)	1:41:A:THR:HB	1:40:A:LYS:HB2	8	0.14
(1,1482)	1:41:A:THR:HB	1:40:A:LYS:HB3	8	0.14
(1,1407)	1:74:A:GLN:HG2	1:8:A:TYR:HB2	10	0.14
(1,1407)	1:74:A:GLN:HG3	1:8:A:TYR:HB2	10	0.14
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	7	0.14
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	8	0.14
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	7	0.14
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	20	0.14
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	11	0.14
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB2	12	0.14
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB3	12	0.14
(1,1183)	1:159:A:THR:H	1:151:A:THR:HA	10	0.14
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB2	11	0.14
(1,1162)	1:136:A:LYS:HB2	1:135:A:GLU:HB3	11	0.14
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB2	11	0.14
(1,1162)	1:136:A:LYS:HB3	1:135:A:GLU:HB3	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	3	0.14
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	3	0.14
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	4	0.14
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	4	0.14
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	10	0.14
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	10	0.14
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	3	0.14
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	3	0.14
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB2	5	0.14
(1,1095)	1:64:A:SER:H	1:60:A:GLN:HB3	5	0.14
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG2	3	0.14
(1,1087)	1:133:A:SER:H	1:135:A:GLU:HG3	3	0.14
(1,1072)	1:77:A:LYS:HB2	1:4:A:GLY:H	15	0.14
(1,1072)	1:77:A:LYS:HB3	1:4:A:GLY:H	15	0.14
(1,1069)	1:86:A:LEU:HA	1:129:A:ALA:H	15	0.14
(1,1041)	1:23:A:LYS:H	1:19:A:GLN:HA	16	0.14
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	11	0.14
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	11	0.14
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB2	16	0.14
(1,1033)	1:80:A:GLU:HG2	1:79:A:GLN:HB3	16	0.14
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB2	16	0.14
(1,1033)	1:80:A:GLU:HG3	1:79:A:GLN:HB3	16	0.14
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	19	0.14
(1,1012)	1:43:A:ASN:HB3	1:44:A:LYS:HA	12	0.14
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	6	0.14
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	6	0.14
(1,944)	1:63:A:VAL:HB	1:65:A:ALA:H	1	0.14
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	16	0.14
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	16	0.14
(1,880)	1:88:A:ILE:HD11	1:89:A:SER:H	11	0.14
(1,880)	1:88:A:ILE:HD12	1:89:A:SER:H	11	0.14
(1,880)	1:88:A:ILE:HD13	1:89:A:SER:H	11	0.14
(1,861)	1:23:A:LYS:HB2	1:24:A:LEU:HG	14	0.14
(1,861)	1:23:A:LYS:HB3	1:24:A:LEU:HG	14	0.14
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	13	0.14
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	19	0.14
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	1	0.14
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	1	0.14
(1,722)	1:61:A:LYS:HB2	1:64:A:SER:H	11	0.14
(1,722)	1:61:A:LYS:HB3	1:64:A:SER:H	11	0.14
(1,716)	1:165:A:LYS:HB2	1:86:A:LEU:HA	18	0.14
(1,716)	1:165:A:LYS:HB3	1:86:A:LEU:HA	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	19	0.14
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	11	0.14
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	12	0.14
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	8	0.14
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	8	0.14
(1,645)	1:148:A:PHE:HA	1:160:A:GLU:HA	9	0.14
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	14	0.14
(1,614)	1:162:A:LEU:HG	1:90:A:ASN:HB2	11	0.14
(1,561)	1:136:A:LYS:HA	1:138:A:GLU:HB2	16	0.14
(1,561)	1:136:A:LYS:HA	1:138:A:GLU:HB3	16	0.14
(1,556)	1:136:A:LYS:HD2	1:108:A:GLY:H	19	0.14
(1,556)	1:136:A:LYS:HD3	1:108:A:GLY:H	19	0.14
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	4	0.14
(1,522)	1:139:A:ALA:HA	1:143:A:HIS:H	3	0.14
(1,521)	1:111:A:ILE:HB	1:130:A:ARG:HA	13	0.14
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	5	0.14
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	5	0.14
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	5	0.14
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	5	0.14
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	11	0.14
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	11	0.14
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	11	0.14
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	11	0.14
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	16	0.14
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	16	0.14
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	16	0.14
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	16	0.14
(1,462)	1:115:A:ILE:HB	1:127:A:GLY:H	12	0.14
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	3	0.14
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG21	6	0.14
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG22	6	0.14
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG23	6	0.14
(1,340)	1:84:A:THR:HB	1:85:A:ASN:HA	15	0.14
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	5	0.14
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	5	0.14
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	5	0.14
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	5	0.14
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	10	0.14
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	10	0.14
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	10	0.14
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	10	0.14
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	5	0.14
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	10	0.14
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	10	0.14
(1,258)	1:80:A:GLU:HA	1:82:A:ASP:HB2	10	0.14
(1,258)	1:80:A:GLU:HA	1:82:A:ASP:HB3	10	0.14
(1,244)	1:67:A:LYS:HE2	1:64:A:SER:HA	19	0.14
(1,244)	1:67:A:LYS:HE3	1:64:A:SER:HA	19	0.14
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	13	0.14
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	13	0.14
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	9	0.14
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	9	0.14
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	3	0.14
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	3	0.14
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	5	0.14
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	5	0.14
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	2	0.14
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	2	0.14
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE1	20	0.14
(1,105)	1:129:A:ALA:HA	1:128:A:PHE:HE2	20	0.14
(1,102)	1:115:A:ILE:HB	1:124:A:ARG:H	10	0.14
(1,99)	1:41:A:THR:HB	1:40:A:LYS:H	11	0.14
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG2	2	0.14
(1,91)	1:113:A:THR:HB	1:114:A:ARG:HG3	2	0.14
(1,50)	1:51:A:VAL:HA	1:35:A:LYS:H	11	0.14
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	2	0.14
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	6	0.14
(1,2178)	1:31:A:ILE:HA	1:53:A:PHE:HA	17	0.13
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	5	0.13
(1,2163)	1:6:A:ASN:H	1:81:A:GLN:HE21	4	0.13
(1,2163)	1:6:A:ASN:H	1:81:A:GLN:HE22	4	0.13
(1,2100)	1:110:A:VAL:HG21	1:131:A:MET:HG2	5	0.13
(1,2100)	1:110:A:VAL:HG21	1:131:A:MET:HG3	5	0.13
(1,2100)	1:110:A:VAL:HG22	1:131:A:MET:HG2	5	0.13
(1,2100)	1:110:A:VAL:HG22	1:131:A:MET:HG3	5	0.13
(1,2100)	1:110:A:VAL:HG23	1:131:A:MET:HG2	5	0.13
(1,2100)	1:110:A:VAL:HG23	1:131:A:MET:HG3	5	0.13
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG11	20	0.13
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG12	20	0.13
(1,2098)	1:109:A:GLN:HE21	1:110:A:VAL:HG13	20	0.13
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG11	20	0.13
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG12	20	0.13
(1,2098)	1:109:A:GLN:HE22	1:110:A:VAL:HG13	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2081)	1:88:A:ILE:H	1:128:A:PHE:H	14	0.13
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	5	0.13
(1,2067)	1:87:A:TYR:HH	1:126:A:VAL:HB	16	0.13
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD11	16	0.13
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD12	16	0.13
(1,2060)	1:131:A:MET:H	1:86:A:LEU:HD13	16	0.13
(1,2048)	1:8:A:TYR:HD1	1:75:A:MET:HA	11	0.13
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	12	0.13
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	12	0.13
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	12	0.13
(1,2001)	1:33:A:SER:H	1:34:A:THR:H	2	0.13
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	5	0.13
(1,1988)	1:10:A:ARG:HG2	1:72:A:GLN:HG2	17	0.13
(1,1988)	1:10:A:ARG:HG2	1:72:A:GLN:HG3	17	0.13
(1,1988)	1:10:A:ARG:HG3	1:72:A:GLN:HG2	17	0.13
(1,1988)	1:10:A:ARG:HG3	1:72:A:GLN:HG3	17	0.13
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	1	0.13
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	12	0.13
(1,1983)	1:8:A:TYR:H	1:74:A:GLN:HA	13	0.13
(1,1980)	1:7:A:LEU:HA	1:8:A:TYR:H	11	0.13
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	10	0.13
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	14	0.13
(1,1942)	1:38:A:LEU:HA	1:44:A:LYS:H	16	0.13
(1,1939)	1:43:A:ASN:HB3	1:42:A:THR:HA	14	0.13
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	9	0.13
(1,1905)	1:16:A:THR:HG21	1:21:A:LEU:HA	4	0.13
(1,1905)	1:16:A:THR:HG22	1:21:A:LEU:HA	4	0.13
(1,1905)	1:16:A:THR:HG23	1:21:A:LEU:HA	4	0.13
(1,1891)	1:43:A:ASN:HA	1:38:A:LEU:HA	6	0.13
(1,1769)	1:56:A:PRO:HG2	1:4:A:GLY:HA2	9	0.13
(1,1769)	1:56:A:PRO:HG2	1:4:A:GLY:HA3	9	0.13
(1,1769)	1:56:A:PRO:HG3	1:4:A:GLY:HA2	9	0.13
(1,1769)	1:56:A:PRO:HG3	1:4:A:GLY:HA3	9	0.13
(1,1742)	1:43:A:ASN:HB3	1:42:A:THR:HB	3	0.13
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	1	0.13
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	1	0.13
(1,1707)	1:44:A:LYS:HA	1:38:A:LEU:HB2	6	0.13
(1,1707)	1:44:A:LYS:HA	1:38:A:LEU:HB3	6	0.13
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	10	0.13
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	10	0.13
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	13	0.13
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	14	0.13
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	14	0.13
(1,1686)	1:164:A:CYS:HA	1:88:A:ILE:H	4	0.13
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	3	0.13
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	3	0.13
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB2	20	0.13
(1,1653)	1:146:A:GLY:HA2	1:162:A:LEU:HB3	20	0.13
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB2	20	0.13
(1,1653)	1:146:A:GLY:HA3	1:162:A:LEU:HB3	20	0.13
(1,1651)	1:45:A:CYS:H	1:38:A:LEU:HG	1	0.13
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB2	14	0.13
(1,1636)	1:17:A:THR:HB	1:18:A:ASP:HB3	14	0.13
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	1	0.13
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	1	0.13
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB2	6	0.13
(1,1609)	1:94:A:SER:HA	1:92:A:PRO:HB3	6	0.13
(1,1590)	1:92:A:PRO:HD2	1:160:A:GLU:H	16	0.13
(1,1590)	1:92:A:PRO:HD3	1:160:A:GLU:H	16	0.13
(1,1569)	1:89:A:SER:HA	1:90:A:ASN:HB2	19	0.13
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	3	0.13
(1,1545)	1:16:A:THR:HG21	1:24:A:LEU:HG	20	0.13
(1,1545)	1:16:A:THR:HG22	1:24:A:LEU:HG	20	0.13
(1,1545)	1:16:A:THR:HG23	1:24:A:LEU:HG	20	0.13
(1,1540)	1:30:A:LYS:HE2	1:31:A:ILE:H	5	0.13
(1,1540)	1:30:A:LYS:HE3	1:31:A:ILE:H	5	0.13
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	14	0.13
(1,1500)	1:40:A:LYS:HG2	1:39:A:ASP:HA	9	0.13
(1,1500)	1:40:A:LYS:HG3	1:39:A:ASP:HA	9	0.13
(1,1495)	1:58:A:ALA:HA	1:61:A:LYS:HE2	17	0.13
(1,1495)	1:58:A:ALA:HA	1:61:A:LYS:HE3	17	0.13
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	10	0.13
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE2	16	0.13
(1,1430)	1:89:A:SER:HB2	1:165:A:LYS:HE3	16	0.13
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE2	16	0.13
(1,1430)	1:89:A:SER:HB3	1:165:A:LYS:HE3	16	0.13
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB2	6	0.13
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB3	6	0.13
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	7	0.13
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	10	0.13
(1,1384)	1:32:A:VAL:HA	1:30:A:LYS:HE2	2	0.13
(1,1384)	1:32:A:VAL:HA	1:30:A:LYS:HE3	2	0.13
(1,1378)	1:26:A:GLN:HB2	1:29:A:GLY:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1378)	1:26:A:GLN:HB3	1:29:A:GLY:H	12	0.13
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	3	0.13
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	17	0.13
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB2	3	0.13
(1,1367)	1:22:A:VAL:H	1:26:A:GLN:HB3	3	0.13
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	5	0.13
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	5	0.13
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB2	6	0.13
(1,1316)	1:59:A:ALA:HA	1:61:A:LYS:HB3	6	0.13
(1,1299)	1:63:A:VAL:HB	1:61:A:LYS:H	19	0.13
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG2	20	0.13
(1,1278)	1:138:A:GLU:H	1:135:A:GLU:HG3	20	0.13
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB2	15	0.13
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB3	15	0.13
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	18	0.13
(1,1153)	1:131:A:MET:HB2	1:138:A:GLU:H	7	0.13
(1,1153)	1:131:A:MET:HB3	1:138:A:GLU:H	7	0.13
(1,1137)	1:83:A:PRO:HD2	1:84:A:THR:HB	15	0.13
(1,1137)	1:83:A:PRO:HD3	1:84:A:THR:HB	15	0.13
(1,1131)	1:20:A:ASP:HA	1:17:A:THR:H	18	0.13
(1,1114)	1:133:A:SER:HA	1:132:A:GLU:HG2	1	0.13
(1,1114)	1:133:A:SER:HA	1:132:A:GLU:HG3	1	0.13
(1,1072)	1:77:A:LYS:HB2	1:4:A:GLY:H	8	0.13
(1,1072)	1:77:A:LYS:HB3	1:4:A:GLY:H	8	0.13
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	3	0.13
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	3	0.13
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	16	0.13
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	16	0.13
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	18	0.13
(1,1018)	1:61:A:LYS:HB2	1:65:A:ALA:HB1	10	0.13
(1,1018)	1:61:A:LYS:HB2	1:65:A:ALA:HB2	10	0.13
(1,1018)	1:61:A:LYS:HB2	1:65:A:ALA:HB3	10	0.13
(1,1018)	1:61:A:LYS:HB3	1:65:A:ALA:HB1	10	0.13
(1,1018)	1:61:A:LYS:HB3	1:65:A:ALA:HB2	10	0.13
(1,1018)	1:61:A:LYS:HB3	1:65:A:ALA:HB3	10	0.13
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	18	0.13
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	18	0.13
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	18	0.13
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	18	0.13
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	18	0.13
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	18	0.13
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD2	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD3	16	0.13
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD2	20	0.13
(1,912)	1:73:A:ALA:H	1:67:A:LYS:HD3	20	0.13
(1,900)	1:32:A:VAL:HB	1:33:A:SER:HA	11	0.13
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB2	5	0.13
(1,881)	1:85:A:ASN:HB3	1:128:A:PHE:HB3	5	0.13
(1,854)	1:22:A:VAL:HB	1:19:A:GLN:HA	3	0.13
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	6	0.13
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	7	0.13
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	7	0.13
(1,671)	1:151:A:THR:HB	1:155:A:VAL:HB	16	0.13
(1,636)	1:140:A:VAL:HB	1:139:A:ALA:H	8	0.13
(1,611)	1:156:A:SER:HA	1:155:A:VAL:H	4	0.13
(1,611)	1:156:A:SER:HA	1:155:A:VAL:H	14	0.13
(1,585)	1:141:A:ILE:HD11	1:164:A:CYS:HB2	11	0.13
(1,585)	1:141:A:ILE:HD11	1:164:A:CYS:HB3	11	0.13
(1,585)	1:141:A:ILE:HD12	1:164:A:CYS:HB2	11	0.13
(1,585)	1:141:A:ILE:HD12	1:164:A:CYS:HB3	11	0.13
(1,585)	1:141:A:ILE:HD13	1:164:A:CYS:HB2	11	0.13
(1,585)	1:141:A:ILE:HD13	1:164:A:CYS:HB3	11	0.13
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB2	11	0.13
(1,576)	1:136:A:LYS:HD2	1:107:A:PHE:HB3	11	0.13
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB2	11	0.13
(1,576)	1:136:A:LYS:HD3	1:107:A:PHE:HB3	11	0.13
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	6	0.13
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	11	0.13
(1,521)	1:111:A:ILE:HB	1:130:A:ARG:HA	1	0.13
(1,497)	1:110:A:VAL:HB	1:112:A:SER:H	1	0.13
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	15	0.13
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	15	0.13
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	15	0.13
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	15	0.13
(1,435)	1:132:A:GLU:HA	1:111:A:ILE:H	19	0.13
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	7	0.13
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	15	0.13
(1,364)	1:81:A:GLN:HA	1:80:A:GLU:H	15	0.13
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	20	0.13
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	20	0.13
(1,311)	1:106:A:PRO:HB2	1:103:A:MET:HA	19	0.13
(1,311)	1:106:A:PRO:HB3	1:103:A:MET:HA	19	0.13
(1,299)	1:111:A:ILE:HB	1:132:A:GLU:HA	14	0.13
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD1	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:104:A:LEU:HB2	1:107:A:PHE:HD2	14	0.13
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	17	0.13
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	17	0.13
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	1	0.13
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	1	0.13
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	2	0.13
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	2	0.13
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD2	14	0.13
(1,166)	1:103:A:MET:HB2	1:106:A:PRO:HD3	14	0.13
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD2	14	0.13
(1,166)	1:103:A:MET:HB3	1:106:A:PRO:HD3	14	0.13
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	6	0.13
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	6	0.13
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	8	0.13
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	8	0.13
(1,112)	1:124:A:ARG:HD2	1:116:A:LEU:H	15	0.13
(1,112)	1:124:A:ARG:HD3	1:116:A:LEU:H	15	0.13
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG2	6	0.13
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG3	6	0.13
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB2	6	0.13
(1,75)	1:138:A:GLU:HA	1:166:A:PHE:HB3	6	0.13
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	4	0.13
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	7	0.13
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	10	0.13
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	15	0.13
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	17	0.13
(1,2178)	1:31:A:ILE:HA	1:53:A:PHE:HA	1	0.12
(1,2178)	1:31:A:ILE:HA	1:53:A:PHE:HA	3	0.12
(1,2167)	1:6:A:ASN:H	1:4:A:GLY:HA2	16	0.12
(1,2167)	1:6:A:ASN:H	1:4:A:GLY:HA3	16	0.12
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	2	0.12
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	4	0.12
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	7	0.12
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	5	0.12
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	20	0.12
(1,2139)	1:163:A:LEU:HG	1:164:A:CYS:HA	4	0.12
(1,2114)	1:112:A:SER:HG	1:113:A:THR:HA	17	0.12
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	3	0.12
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	14	0.12
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	20	0.12
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB1	3	0.12
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2039)	1:74:A:GLN:H	1:73:A:ALA:HB3	3	0.12
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG2	4	0.12
(1,2033)	1:10:A:ARG:HE	1:72:A:GLN:HG3	4	0.12
(1,2011)	1:48:A:TYR:HD2	1:11:A:GLY:H	5	0.12
(1,2010)	1:48:A:TYR:HD2	1:10:A:ARG:H	3	0.12
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	17	0.12
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	17	0.12
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	17	0.12
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG21	17	0.12
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG22	17	0.12
(1,1994)	1:31:A:ILE:HA	1:32:A:VAL:HG23	17	0.12
(1,1989)	1:10:A:ARG:HA	1:49:A:GLY:H	2	0.12
(1,1978)	1:6:A:ASN:HA	1:7:A:LEU:H	5	0.12
(1,1978)	1:6:A:ASN:HA	1:7:A:LEU:H	10	0.12
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	1	0.12
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	11	0.12
(1,1953)	1:72:A:GLN:HG2	1:10:A:ARG:HG2	6	0.12
(1,1953)	1:72:A:GLN:HG2	1:10:A:ARG:HG3	6	0.12
(1,1953)	1:72:A:GLN:HG3	1:10:A:ARG:HG2	6	0.12
(1,1953)	1:72:A:GLN:HG3	1:10:A:ARG:HG3	6	0.12
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD11	7	0.12
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD12	7	0.12
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD13	7	0.12
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD21	7	0.12
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD22	7	0.12
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD23	7	0.12
(1,1899)	1:75:A:MET:HA	1:74:A:GLN:H	17	0.12
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	11	0.12
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	11	0.12
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB2	19	0.12
(1,1867)	1:54:A:ASP:HA	1:30:A:LYS:HB3	19	0.12
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	13	0.12
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG12	19	0.12
(1,1730)	1:73:A:ALA:HA	1:9:A:ILE:HG13	19	0.12
(1,1715)	1:159:A:THR:HB	1:151:A:THR:H	1	0.12
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	4	0.12
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	4	0.12
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	6	0.12
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	6	0.12
(1,1702)	1:66:A:LEU:HB2	1:72:A:GLN:H	8	0.12
(1,1702)	1:66:A:LEU:HB3	1:72:A:GLN:H	8	0.12
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	6	0.12
(1,1569)	1:89:A:SER:HA	1:90:A:ASN:HB2	12	0.12
(1,1565)	1:89:A:SER:HB2	1:90:A:ASN:HA	17	0.12
(1,1565)	1:89:A:SER:HB3	1:90:A:ASN:HA	17	0.12
(1,1546)	1:31:A:ILE:HA	1:54:A:ASP:H	18	0.12
(1,1534)	1:64:A:SER:HB2	1:67:A:LYS:HD2	10	0.12
(1,1534)	1:64:A:SER:HB2	1:67:A:LYS:HD3	10	0.12
(1,1534)	1:64:A:SER:HB3	1:67:A:LYS:HD2	10	0.12
(1,1534)	1:64:A:SER:HB3	1:67:A:LYS:HD3	10	0.12
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	9	0.12
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	15	0.12
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	7	0.12
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	7	0.12
(1,1519)	1:46:A:LYS:HD2	1:47:A:GLY:H	15	0.12
(1,1519)	1:46:A:LYS:HD3	1:47:A:GLY:H	15	0.12
(1,1517)	1:4:A:GLY:H	1:5:A:THR:HA	9	0.12
(1,1465)	1:47:A:GLY:H	1:48:A:TYR:H	17	0.12
(1,1425)	1:87:A:TYR:HA	1:86:A:LEU:H	10	0.12
(1,1423)	1:87:A:TYR:HB2	1:128:A:PHE:HA	9	0.12
(1,1423)	1:87:A:TYR:HB3	1:128:A:PHE:HA	9	0.12
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB2	10	0.12
(1,1418)	1:81:A:GLN:HB2	1:82:A:ASP:HB3	10	0.12
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB2	10	0.12
(1,1418)	1:81:A:GLN:HB3	1:82:A:ASP:HB3	10	0.12
(1,1408)	1:9:A:ILE:HA	1:10:A:ARG:H	7	0.12
(1,1408)	1:9:A:ILE:HA	1:10:A:ARG:H	11	0.12
(1,1408)	1:9:A:ILE:HA	1:10:A:ARG:H	19	0.12
(1,1406)	1:75:A:MET:HA	1:8:A:TYR:H	9	0.12
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	17	0.12
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	2	0.12
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	13	0.12
(1,1384)	1:32:A:VAL:HA	1:30:A:LYS:HE2	20	0.12
(1,1384)	1:32:A:VAL:HA	1:30:A:LYS:HE3	20	0.12
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	2	0.12
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	10	0.12
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	18	0.12
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	5	0.12
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB2	18	0.12
(1,1202)	1:54:A:ASP:H	1:53:A:PHE:HB3	18	0.12
(1,1109)	1:132:A:GLU:HB2	1:110:A:VAL:H	3	0.12
(1,1109)	1:132:A:GLU:HB3	1:110:A:VAL:H	3	0.12
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1073)	1:73:A:ALA:HB1	1:72:A:GLN:HG3	12	0.12
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG2	12	0.12
(1,1073)	1:73:A:ALA:HB2	1:72:A:GLN:HG3	12	0.12
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG2	12	0.12
(1,1073)	1:73:A:ALA:HB3	1:72:A:GLN:HG3	12	0.12
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE2	9	0.12
(1,1053)	1:54:A:ASP:HA	1:30:A:LYS:HE3	9	0.12
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA2	1	0.12
(1,1004)	1:81:A:GLN:HA	1:4:A:GLY:HA3	1	0.12
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB2	19	0.12
(1,996)	1:23:A:LYS:HG2	1:19:A:GLN:HB3	19	0.12
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB2	19	0.12
(1,996)	1:23:A:LYS:HG3	1:19:A:GLN:HB3	19	0.12
(1,900)	1:32:A:VAL:HB	1:33:A:SER:HA	20	0.12
(1,789)	1:22:A:VAL:HG11	1:23:A:LYS:HG2	13	0.12
(1,789)	1:22:A:VAL:HG11	1:23:A:LYS:HG3	13	0.12
(1,789)	1:22:A:VAL:HG12	1:23:A:LYS:HG2	13	0.12
(1,789)	1:22:A:VAL:HG12	1:23:A:LYS:HG3	13	0.12
(1,789)	1:22:A:VAL:HG13	1:23:A:LYS:HG2	13	0.12
(1,789)	1:22:A:VAL:HG13	1:23:A:LYS:HG3	13	0.12
(1,789)	1:22:A:VAL:HG21	1:23:A:LYS:HG2	13	0.12
(1,789)	1:22:A:VAL:HG21	1:23:A:LYS:HG3	13	0.12
(1,789)	1:22:A:VAL:HG22	1:23:A:LYS:HG2	13	0.12
(1,789)	1:22:A:VAL:HG22	1:23:A:LYS:HG3	13	0.12
(1,789)	1:22:A:VAL:HG23	1:23:A:LYS:HG2	13	0.12
(1,789)	1:22:A:VAL:HG23	1:23:A:LYS:HG3	13	0.12
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB1	7	0.12
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB2	7	0.12
(1,726)	1:151:A:THR:HA	1:157:A:ALA:HB3	7	0.12
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	18	0.12
(1,702)	1:163:A:LEU:HA	1:90:A:ASN:HB2	12	0.12
(1,696)	1:157:A:ALA:HA	1:92:A:PRO:HA	1	0.12
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD2	14	0.12
(1,694)	1:156:A:SER:HA	1:158:A:PRO:HD3	14	0.12
(1,684)	1:158:A:PRO:HA	1:159:A:THR:HB	14	0.12
(1,670)	1:153:A:PRO:HB2	1:155:A:VAL:H	17	0.12
(1,670)	1:153:A:PRO:HB3	1:155:A:VAL:H	17	0.12
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG21	3	0.12
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG22	3	0.12
(1,666)	1:149:A:ILE:HB	1:159:A:THR:HG23	3	0.12
(1,635)	1:141:A:ILE:HB	1:139:A:ALA:H	11	0.12
(1,628)	1:140:A:VAL:HB	1:143:A:HIS:HB2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:140:A:VAL:HB	1:143:A:HIS:HB3	8	0.12
(1,620)	1:155:A:VAL:HA	1:94:A:SER:H	6	0.12
(1,585)	1:141:A:ILE:HD11	1:164:A:CYS:HB2	18	0.12
(1,585)	1:141:A:ILE:HD11	1:164:A:CYS:HB3	18	0.12
(1,585)	1:141:A:ILE:HD12	1:164:A:CYS:HB2	18	0.12
(1,585)	1:141:A:ILE:HD12	1:164:A:CYS:HB3	18	0.12
(1,585)	1:141:A:ILE:HD13	1:164:A:CYS:HB2	18	0.12
(1,585)	1:141:A:ILE:HD13	1:164:A:CYS:HB3	18	0.12
(1,548)	1:136:A:LYS:HD2	1:109:A:GLN:H	18	0.12
(1,548)	1:136:A:LYS:HD3	1:109:A:GLN:H	18	0.12
(1,544)	1:122:A:THR:HB	1:121:A:GLY:H	12	0.12
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG2	19	0.12
(1,534)	1:137:A:CYS:HA	1:138:A:GLU:HG3	19	0.12
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB2	6	0.12
(1,479)	1:106:A:PRO:HB2	1:107:A:PHE:HB3	6	0.12
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB2	6	0.12
(1,479)	1:106:A:PRO:HB3	1:107:A:PHE:HB3	6	0.12
(1,460)	1:114:A:ARG:HB2	1:115:A:ILE:H	18	0.12
(1,460)	1:114:A:ARG:HB3	1:115:A:ILE:H	18	0.12
(1,425)	1:110:A:VAL:HA	1:111:A:ILE:HA	3	0.12
(1,425)	1:110:A:VAL:HA	1:111:A:ILE:HA	12	0.12
(1,425)	1:110:A:VAL:HA	1:111:A:ILE:HA	15	0.12
(1,382)	1:115:A:ILE:HB	1:128:A:PHE:H	11	0.12
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	19	0.12
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	19	0.12
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB2	1	0.12
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB3	1	0.12
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB2	16	0.12
(1,277)	1:110:A:VAL:HB	1:131:A:MET:HB3	16	0.12
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	11	0.12
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	11	0.12
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	17	0.12
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	17	0.12
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	3	0.12
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	3	0.12
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	7	0.12
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	7	0.12
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG2	18	0.12
(1,204)	1:113:A:THR:HA	1:114:A:ARG:HG3	18	0.12
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE1	7	0.12
(1,203)	1:113:A:THR:HA	1:128:A:PHE:HE2	7	0.12
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	2	0.12
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	2	0.12
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	2	0.12
(1,133)	1:106:A:PRO:HB2	1:108:A:GLY:H	19	0.12
(1,133)	1:106:A:PRO:HB3	1:108:A:GLY:H	19	0.12
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD2	17	0.12
(1,106)	1:113:A:THR:HA	1:114:A:ARG:HD3	17	0.12
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	13	0.12
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	19	0.12
(1,6)	1:41:A:THR:HA	1:40:A:LYS:H	12	0.12
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	6	0.12
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	6	0.12
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	6	0.12
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	6	0.12
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	6	0.12
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	6	0.12
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG12	11	0.12
(1,5)	1:73:A:ALA:HB1	1:9:A:ILE:HG13	11	0.12
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG12	11	0.12
(1,5)	1:73:A:ALA:HB2	1:9:A:ILE:HG13	11	0.12
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG12	11	0.12
(1,5)	1:73:A:ALA:HB3	1:9:A:ILE:HG13	11	0.12
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	1	0.11
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	10	0.11
(1,2164)	1:6:A:ASN:H	1:7:A:LEU:H	12	0.11
(1,2162)	1:6:A:ASN:H	1:5:A:THR:H	8	0.11
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	16	0.11
(1,2140)	1:90:A:ASN:H	1:163:A:LEU:HB2	15	0.11
(1,2140)	1:90:A:ASN:H	1:163:A:LEU:HB3	15	0.11
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB2	8	0.11
(1,2133)	1:90:A:ASN:HD21	1:163:A:LEU:HB3	8	0.11
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB2	8	0.11
(1,2133)	1:90:A:ASN:HD22	1:163:A:LEU:HB3	8	0.11
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB2	9	0.11
(1,2110)	1:130:A:ARG:HB2	1:112:A:SER:HB3	9	0.11
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB2	9	0.11
(1,2110)	1:130:A:ARG:HB3	1:112:A:SER:HB3	9	0.11
(1,2104)	1:132:A:GLU:H	1:111:A:ILE:H	16	0.11
(1,2085)	1:89:A:SER:HG	1:126:A:VAL:HA	9	0.11
(1,2076)	1:128:A:PHE:H	1:88:A:ILE:HB	12	0.11
(1,2054)	1:75:A:MET:HE1	1:3:A:MET:HG2	6	0.11
(1,2054)	1:75:A:MET:HE1	1:3:A:MET:HG3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2054)	1:75:A:MET:HE2	1:3:A:MET:HG2	6	0.11
(1,2054)	1:75:A:MET:HE2	1:3:A:MET:HG3	6	0.11
(1,2054)	1:75:A:MET:HE3	1:3:A:MET:HG2	6	0.11
(1,2054)	1:75:A:MET:HE3	1:3:A:MET:HG3	6	0.11
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG2	6	0.11
(1,2035)	1:73:A:ALA:HA	1:72:A:GLN:HG3	6	0.11
(1,2001)	1:33:A:SER:H	1:34:A:THR:H	18	0.11
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD11	19	0.11
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD12	19	0.11
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD13	19	0.11
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD21	19	0.11
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD22	19	0.11
(1,1984)	1:8:A:TYR:H	1:7:A:LEU:HD23	19	0.11
(1,1980)	1:7:A:LEU:HA	1:8:A:TYR:H	6	0.11
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	13	0.11
(1,1960)	1:20:A:ASP:HB2	1:17:A:THR:HA	3	0.11
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD11	13	0.11
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD12	13	0.11
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD13	13	0.11
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD21	13	0.11
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD22	13	0.11
(1,1947)	1:37:A:ILE:HB	1:38:A:LEU:HD23	13	0.11
(1,1915)	1:4:A:GLY:H	1:81:A:GLN:H	16	0.11
(1,1902)	1:77:A:LYS:HG2	1:4:A:GLY:H	13	0.11
(1,1902)	1:77:A:LYS:HG3	1:4:A:GLY:H	13	0.11
(1,1899)	1:75:A:MET:HA	1:74:A:GLN:H	15	0.11
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB2	7	0.11
(1,1898)	1:75:A:MET:HG2	1:60:A:GLN:HB3	7	0.11
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB2	7	0.11
(1,1898)	1:75:A:MET:HG3	1:60:A:GLN:HB3	7	0.11
(1,1891)	1:43:A:ASN:HA	1:38:A:LEU:HA	16	0.11
(1,1817)	1:42:A:THR:HA	1:41:A:THR:H	11	0.11
(1,1765)	1:43:A:ASN:HA	1:41:A:THR:H	10	0.11
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB2	3	0.11
(1,1724)	1:58:A:ALA:HA	1:60:A:GLN:HB3	3	0.11
(1,1723)	1:40:A:LYS:HA	1:42:A:THR:H	15	0.11
(1,1703)	1:67:A:LYS:HB2	1:65:A:ALA:H	11	0.11
(1,1703)	1:67:A:LYS:HB3	1:65:A:ALA:H	11	0.11
(1,1689)	1:41:A:THR:HG21	1:43:A:ASN:H	4	0.11
(1,1689)	1:41:A:THR:HG22	1:43:A:ASN:H	4	0.11
(1,1689)	1:41:A:THR:HG23	1:43:A:ASN:H	4	0.11
(1,1686)	1:164:A:CYS:HA	1:88:A:ILE:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB2	9	0.11
(1,1680)	1:141:A:ILE:HA	1:143:A:HIS:HB3	9	0.11
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB2	3	0.11
(1,1675)	1:167:A:SER:HA	1:165:A:LYS:HB3	3	0.11
(1,1637)	1:44:A:LYS:HA	1:38:A:LEU:HA	16	0.11
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG2	3	0.11
(1,1611)	1:94:A:SER:HA	1:92:A:PRO:HG3	3	0.11
(1,1569)	1:89:A:SER:HA	1:90:A:ASN:HB2	13	0.11
(1,1539)	1:33:A:SER:HA	1:34:A:THR:H	2	0.11
(1,1522)	1:52:A:ASP:HA	1:51:A:VAL:HB	17	0.11
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG12	12	0.11
(1,1516)	1:87:A:TYR:H	1:141:A:ILE:HG13	12	0.11
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG11	7	0.11
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG12	7	0.11
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG13	7	0.11
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG21	7	0.11
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG22	7	0.11
(1,1508)	1:115:A:ILE:HB	1:126:A:VAL:HG23	7	0.11
(1,1457)	1:125:A:GLY:H	1:126:A:VAL:HA	2	0.11
(1,1408)	1:9:A:ILE:HA	1:10:A:ARG:H	16	0.11
(1,1402)	1:31:A:ILE:HA	1:52:A:ASP:H	18	0.11
(1,1385)	1:29:A:GLY:HA2	1:28:A:TYR:H	11	0.11
(1,1378)	1:26:A:GLN:HB2	1:29:A:GLY:H	20	0.11
(1,1378)	1:26:A:GLN:HB3	1:29:A:GLY:H	20	0.11
(1,1374)	1:85:A:ASN:HB2	1:128:A:PHE:HA	18	0.11
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	4	0.11
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	6	0.11
(1,1368)	1:49:A:GLY:H	1:10:A:ARG:H	14	0.11
(1,1362)	1:73:A:ALA:HA	1:10:A:ARG:H	8	0.11
(1,1352)	1:61:A:LYS:HD2	1:28:A:TYR:HA	4	0.11
(1,1352)	1:61:A:LYS:HD3	1:28:A:TYR:HA	4	0.11
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	3	0.11
(1,1173)	1:74:A:GLN:H	1:75:A:MET:H	4	0.11
(1,1169)	1:129:A:ALA:HA	1:112:A:SER:H	9	0.11
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD1	2	0.11
(1,1149)	1:130:A:ARG:HB2	1:128:A:PHE:HD2	2	0.11
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD1	2	0.11
(1,1149)	1:130:A:ARG:HB3	1:128:A:PHE:HD2	2	0.11
(1,1128)	1:30:A:LYS:HE2	1:54:A:ASP:H	6	0.11
(1,1128)	1:30:A:LYS:HE3	1:54:A:ASP:H	6	0.11
(1,1115)	1:136:A:LYS:HD2	1:140:A:VAL:H	15	0.11
(1,1115)	1:136:A:LYS:HD3	1:140:A:VAL:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB2	3	0.11
(1,1113)	1:133:A:SER:HA	1:131:A:MET:HB3	3	0.11
(1,1085)	1:4:A:GLY:HA2	1:77:A:LYS:HA	11	0.11
(1,1085)	1:4:A:GLY:HA3	1:77:A:LYS:HA	11	0.11
(1,1060)	1:78:A:GLN:HB2	1:2:A:ALA:HA	16	0.11
(1,1060)	1:78:A:GLN:HB3	1:2:A:ALA:HA	16	0.11
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	7	0.11
(1,1025)	1:4:A:GLY:HA2	1:56:A:PRO:HA	7	0.11
(1,1025)	1:4:A:GLY:HA3	1:56:A:PRO:HA	7	0.11
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	1	0.11
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	1	0.11
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB2	7	0.11
(1,977)	1:53:A:PHE:HA	1:30:A:LYS:HB3	7	0.11
(1,969)	1:30:A:LYS:HD2	1:31:A:ILE:H	18	0.11
(1,969)	1:30:A:LYS:HD3	1:31:A:ILE:H	18	0.11
(1,968)	1:27:A:PRO:HG2	1:25:A:CYS:HA	19	0.11
(1,968)	1:27:A:PRO:HG3	1:25:A:CYS:HA	19	0.11
(1,958)	1:27:A:PRO:HG2	1:23:A:LYS:HB2	10	0.11
(1,958)	1:27:A:PRO:HG2	1:23:A:LYS:HB3	10	0.11
(1,958)	1:27:A:PRO:HG3	1:23:A:LYS:HB2	10	0.11
(1,958)	1:27:A:PRO:HG3	1:23:A:LYS:HB3	10	0.11
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG11	14	0.11
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG12	14	0.11
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG13	14	0.11
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG21	14	0.11
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG22	14	0.11
(1,922)	1:24:A:LEU:H	1:22:A:VAL:HG23	14	0.11
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG11	13	0.11
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG12	13	0.11
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG13	13	0.11
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG21	13	0.11
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG22	13	0.11
(1,921)	1:25:A:CYS:H	1:22:A:VAL:HG23	13	0.11
(1,900)	1:32:A:VAL:HB	1:33:A:SER:HA	8	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG21	1	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG22	1	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG23	1	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG21	13	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG22	13	0.11
(1,875)	1:88:A:ILE:HB	1:113:A:THR:HG23	13	0.11
(1,828)	1:42:A:THR:H	1:43:A:ASN:HB2	16	0.11
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB2	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:92:A:PRO:HA	1:123:A:SER:HB3	3	0.11
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	12	0.11
(1,704)	1:159:A:THR:HB	1:160:A:GLU:HA	15	0.11
(1,684)	1:158:A:PRO:HA	1:159:A:THR:HB	2	0.11
(1,668)	1:164:A:CYS:HB2	1:144:A:PHE:HA	16	0.11
(1,668)	1:164:A:CYS:HB3	1:144:A:PHE:HA	16	0.11
(1,667)	1:149:A:ILE:HB	1:150:A:LYS:HA	11	0.11
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD2	4	0.11
(1,662)	1:150:A:LYS:HG2	1:153:A:PRO:HD3	4	0.11
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD2	4	0.11
(1,662)	1:150:A:LYS:HG3	1:153:A:PRO:HD3	4	0.11
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	2	0.11
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	2	0.11
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	2	0.11
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	2	0.11
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	19	0.11
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	19	0.11
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	19	0.11
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	19	0.11
(1,600)	1:163:A:LEU:HG	1:165:A:LYS:HA	11	0.11
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD2	19	0.11
(1,583)	1:140:A:VAL:HB	1:136:A:LYS:HD3	19	0.11
(1,543)	1:125:A:GLY:HA2	1:124:A:ARG:H	20	0.11
(1,543)	1:125:A:GLY:HA3	1:124:A:ARG:H	20	0.11
(1,520)	1:111:A:ILE:HB	1:132:A:GLU:H	1	0.11
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	1	0.11
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	1	0.11
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG2	14	0.11
(1,504)	1:111:A:ILE:HA	1:79:A:GLN:HG3	14	0.11
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB2	11	0.11
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB3	11	0.11
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB2	19	0.11
(1,445)	1:133:A:SER:HA	1:136:A:LYS:HB3	19	0.11
(1,442)	1:134:A:THR:HA	1:133:A:SER:H	18	0.11
(1,405)	1:129:A:ALA:HB1	1:112:A:SER:H	6	0.11
(1,405)	1:129:A:ALA:HB2	1:112:A:SER:H	6	0.11
(1,405)	1:129:A:ALA:HB3	1:112:A:SER:H	6	0.11
(1,300)	1:114:A:ARG:HG2	1:113:A:THR:H	10	0.11
(1,300)	1:114:A:ARG:HG3	1:113:A:THR:H	10	0.11
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG2	20	0.11
(1,292)	1:103:A:MET:HB2	1:106:A:PRO:HG3	20	0.11
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,292)	1:103:A:MET:HB3	1:106:A:PRO:HG3	20	0.11
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	12	0.11
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	12	0.11
(1,274)	1:106:A:PRO:HG2	1:104:A:LEU:HA	20	0.11
(1,274)	1:106:A:PRO:HG3	1:104:A:LEU:HA	20	0.11
(1,252)	1:39:A:ASP:HA	1:43:A:ASN:H	20	0.11
(1,243)	1:67:A:LYS:HB2	1:71:A:VAL:H	17	0.11
(1,243)	1:67:A:LYS:HB3	1:71:A:VAL:H	17	0.11
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB2	2	0.11
(1,239)	1:113:A:THR:HB	1:112:A:SER:HB3	2	0.11
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB2	11	0.11
(1,165)	1:98:A:GLN:HG2	1:99:A:GLU:HB3	11	0.11
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB2	11	0.11
(1,165)	1:98:A:GLN:HG3	1:99:A:GLU:HB3	11	0.11
(1,128)	1:93:A:LEU:HG	1:155:A:VAL:HB	19	0.11
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB2	9	0.11
(1,122)	1:99:A:GLU:HB2	1:102:A:ASN:HB3	9	0.11
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB2	9	0.11
(1,122)	1:99:A:GLU:HB3	1:102:A:ASN:HB3	9	0.11
(1,111)	1:120:A:SER:HB2	1:122:A:THR:H	9	0.11
(1,111)	1:120:A:SER:HB3	1:122:A:THR:H	9	0.11
(1,68)	1:114:A:ARG:HA	1:97:A:GLU:H	9	0.11
(1,27)	1:50:A:PHE:HE1	1:52:A:ASP:HB3	6	0.11
(1,27)	1:50:A:PHE:HE2	1:52:A:ASP:HB3	6	0.11
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	9	0.11
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	11	0.11
(1,19)	1:33:A:SER:HA	1:34:A:THR:HA	20	0.11
(1,2179)	1:31:A:ILE:HA	1:30:A:LYS:HA	20	0.1
(1,2153)	1:165:A:LYS:HB2	1:87:A:TYR:HD2	12	0.1
(1,2153)	1:165:A:LYS:HB3	1:87:A:TYR:HD2	12	0.1
(1,2152)	1:87:A:TYR:H	1:165:A:LYS:H	18	0.1
(1,2145)	1:138:A:GLU:HA	1:166:A:PHE:HD1	6	0.1
(1,2126)	1:35:A:LYS:H	1:50:A:PHE:HE1	11	0.1
(1,2009)	1:48:A:TYR:HD2	1:9:A:ILE:H	9	0.1
(1,2001)	1:33:A:SER:H	1:34:A:THR:H	13	0.1
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	13	0.1
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	13	0.1
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	13	0.1
(1,1999)	1:32:A:VAL:HG21	1:53:A:PHE:HA	15	0.1
(1,1999)	1:32:A:VAL:HG22	1:53:A:PHE:HA	15	0.1
(1,1999)	1:32:A:VAL:HG23	1:53:A:PHE:HA	15	0.1
(1,1980)	1:7:A:LEU:HA	1:8:A:TYR:H	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	1:7:A:LEU:HA	1:8:A:TYR:H	20	0.1
(1,1978)	1:6:A:ASN:HA	1:7:A:LEU:H	2	0.1
(1,1970)	1:55:A:SER:HB3	1:54:A:ASP:HA	16	0.1
(1,1891)	1:43:A:ASN:HA	1:38:A:LEU:HA	19	0.1
(1,1686)	1:164:A:CYS:HA	1:88:A:ILE:H	18	0.1
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG21	5	0.1
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG22	5	0.1
(1,1645)	1:145:A:ASN:H	1:141:A:ILE:HG23	5	0.1
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG2	20	0.1
(1,1506)	1:43:A:ASN:HA	1:44:A:LYS:HG3	20	0.1
(1,1488)	1:130:A:ARG:H	1:112:A:SER:HA	14	0.1
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB2	11	0.1
(1,1415)	1:79:A:GLN:HA	1:77:A:LYS:HB3	11	0.1
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD11	5	0.1
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD12	5	0.1
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD13	5	0.1
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD21	5	0.1
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD22	5	0.1
(1,1243)	1:74:A:GLN:H	1:66:A:LEU:HD23	5	0.1
(1,1169)	1:129:A:ALA:HA	1:112:A:SER:H	15	0.1
(1,1156)	1:130:A:ARG:HB2	1:86:A:LEU:H	5	0.1
(1,1156)	1:130:A:ARG:HB3	1:86:A:LEU:H	5	0.1
(1,1064)	1:128:A:PHE:HA	1:87:A:TYR:H	9	0.1
(1,1052)	1:15:A:HIS:HB3	1:16:A:THR:HA	11	0.1
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB2	18	0.1
(1,1040)	1:22:A:VAL:H	1:19:A:GLN:HB3	18	0.1
(1,1029)	1:74:A:GLN:H	1:10:A:ARG:H	4	0.1
(1,991)	1:44:A:LYS:HB2	1:15:A:HIS:HA	5	0.1
(1,991)	1:44:A:LYS:HB3	1:15:A:HIS:HA	5	0.1
(1,982)	1:55:A:SER:HB2	1:54:A:ASP:HA	4	0.1
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	9	0.1
(1,837)	1:86:A:LEU:H	1:85:A:ASN:HB3	14	0.1
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB2	10	0.1
(1,624)	1:145:A:ASN:HB2	1:144:A:PHE:HB3	10	0.1
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB2	10	0.1
(1,624)	1:145:A:ASN:HB3	1:144:A:PHE:HB3	10	0.1
(1,621)	1:147:A:LYS:HA	1:146:A:GLY:H	17	0.1
(1,415)	1:116:A:LEU:HA	1:128:A:PHE:HE1	9	0.1
(1,415)	1:116:A:LEU:HA	1:128:A:PHE:HE2	9	0.1
(1,368)	1:103:A:MET:HA	1:104:A:LEU:HB2	14	0.1
(1,352)	1:86:A:LEU:HG	1:85:A:ASN:H	8	0.1
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG21	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG22	16	0.1
(1,343)	1:85:A:ASN:HB3	1:84:A:THR:HG23	16	0.1
(1,331)	1:81:A:GLN:HB2	1:78:A:GLN:H	4	0.1
(1,331)	1:81:A:GLN:HB3	1:78:A:GLN:H	4	0.1
(1,323)	1:73:A:ALA:H	1:74:A:GLN:H	16	0.1
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB2	16	0.1
(1,273)	1:104:A:LEU:HB2	1:107:A:PHE:HB3	16	0.1
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG2	15	0.1
(1,104)	1:111:A:ILE:HA	1:109:A:GLN:HG3	15	0.1
(1,99)	1:41:A:THR:HB	1:40:A:LYS:H	10	0.1
(1,21)	1:24:A:LEU:HA	1:26:A:GLN:H	6	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found