



# Full wwPDB NMR Structure Validation Report ⓘ

Oct 11, 2023 – 02:37 PM EDT

PDB ID : 8EOD  
BMRB ID : 51187  
Title : EEVD:Sis1-81 (J domain) bound conformation  
Authors : Matos, C.O.; Pinheiro, G.M.S.; Ramos, C.H.I.; Almeida, F.C.L.  
Deposited on : 2022-10-03

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.35.1

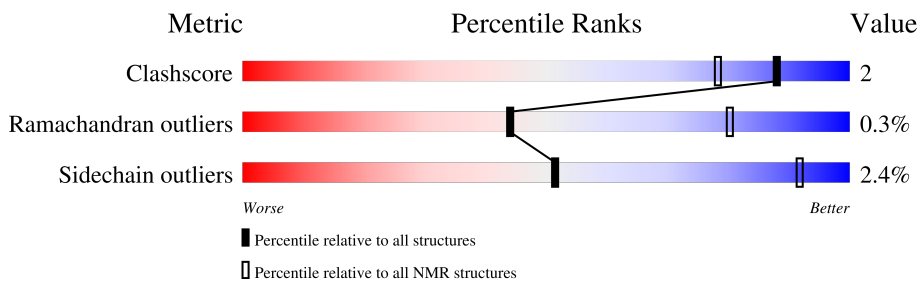
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 88%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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  $\geq 3$ , 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	105	

## 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: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:77 (74)	0.96	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 4 clusters and 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1312 atoms, of which 652 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein SIS1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	84	1312	417	652	110	132	1	0

There are 25 discrepancies between the modelled and reference sequences:

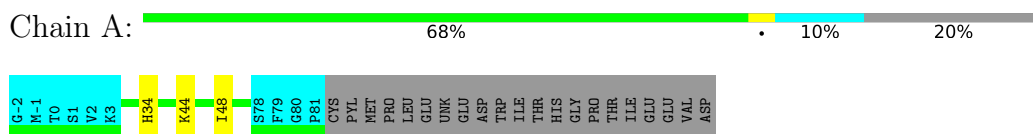
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P25294
A	-1	MET	-	expression tag	UNP P25294
A	0	THR	-	expression tag	UNP P25294
A	1	SER	-	expression tag	UNP P25294
A	82	CYS	-	expression tag	UNP P25294
A	83	PYL	-	expression tag	UNP P25294
A	84	MET	-	expression tag	UNP P25294
A	85	PRO	-	expression tag	UNP P25294
A	86	LEU	-	expression tag	UNP P25294
A	87	GLU	-	expression tag	UNP P25294
A	88	UNK	-	expression tag	UNP P25294
A	89	GLU	-	expression tag	UNP P25294
A	90	ASP	-	expression tag	UNP P25294
A	91	TRP	-	expression tag	UNP P25294
A	92	ILE	-	expression tag	UNP P25294
A	93	THR	-	expression tag	UNP P25294
A	94	HIS	-	expression tag	UNP P25294
A	95	GLY	-	expression tag	UNP P25294
A	96	PRO	-	expression tag	UNP P25294
A	97	THR	-	expression tag	UNP P25294
A	98	ILE	-	expression tag	UNP P25294
A	99	GLU	-	expression tag	UNP P25294
A	100	GLU	-	expression tag	UNP P25294
A	101	VAL	-	expression tag	UNP P25294
A	102	ASP	-	expression tag	UNP P25294

## 4 Residue-property plots [i](#)

### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein SIS1

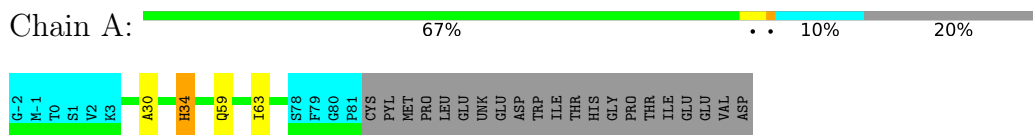


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

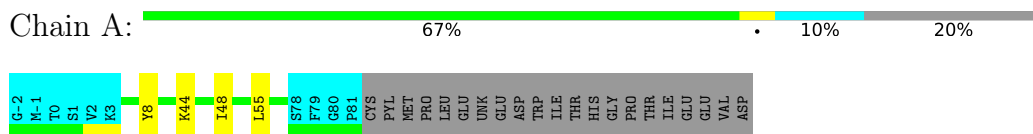
#### 4.2.1 Score per residue for model 1

- Molecule 1: Protein SIS1



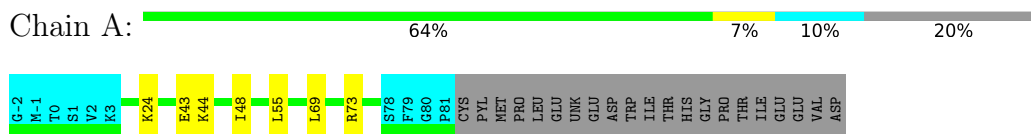
#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Protein SIS1



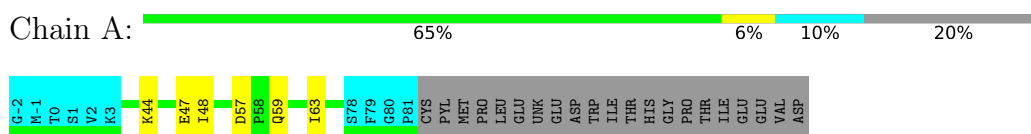
### 4.2.3 Score per residue for model 3

- Molecule 1: Protein SIS1



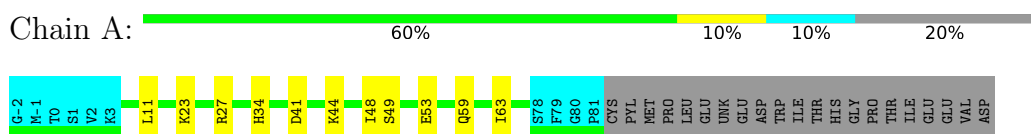
### 4.2.4 Score per residue for model 4

- Molecule 1: Protein SIS1



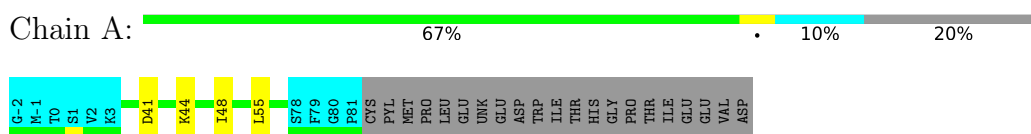
### 4.2.5 Score per residue for model 5

- Molecule 1: Protein SIS1



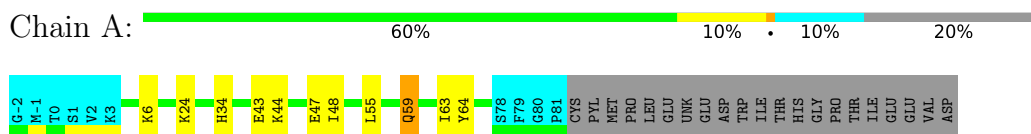
### 4.2.6 Score per residue for model 6

- Molecule 1: Protein SIS1



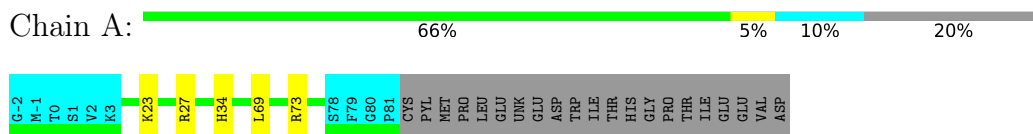
### 4.2.7 Score per residue for model 7

- Molecule 1: Protein SIS1



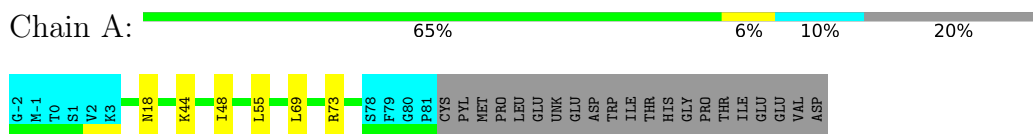
### 4.2.8 Score per residue for model 8

- Molecule 1: Protein SIS1



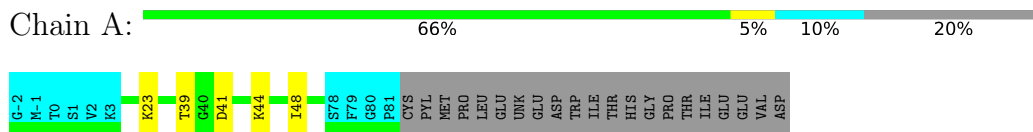
### 4.2.9 Score per residue for model 9

- Molecule 1: Protein SIS1



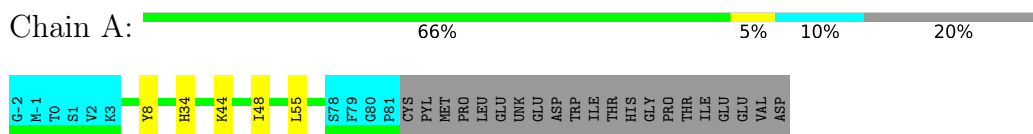
### 4.2.10 Score per residue for model 10

- Molecule 1: Protein SIS1



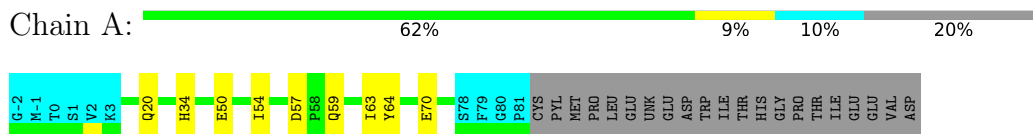
### 4.2.11 Score per residue for model 11

- Molecule 1: Protein SIS1



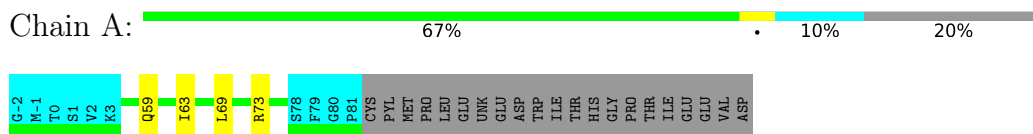
### 4.2.12 Score per residue for model 12

- Molecule 1: Protein SIS1



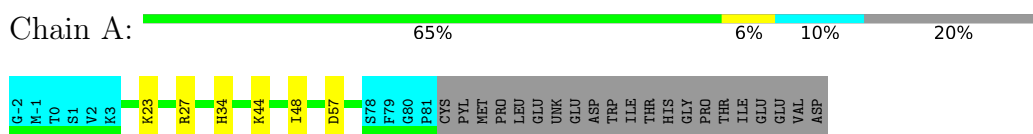
### 4.2.13 Score per residue for model 13

- Molecule 1: Protein SIS1



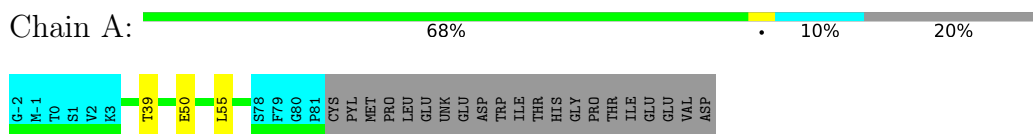
### 4.2.14 Score per residue for model 14

- Molecule 1: Protein SIS1



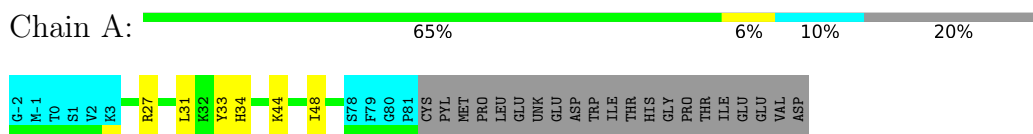
### 4.2.15 Score per residue for model 15

- Molecule 1: Protein SIS1



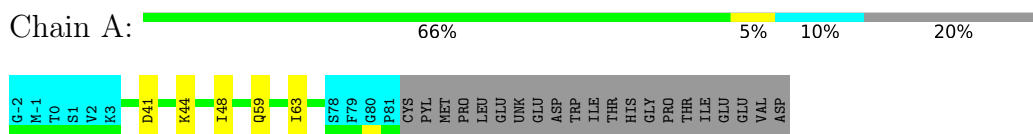
### 4.2.16 Score per residue for model 16

- Molecule 1: Protein SIS1



### 4.2.17 Score per residue for model 17

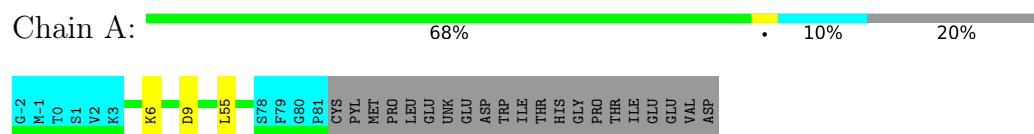
- Molecule 1: Protein SIS1





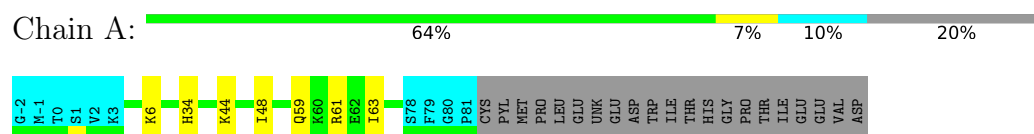
### 4.2.18 Score per residue for model 18

- Molecule 1: Protein SIS1



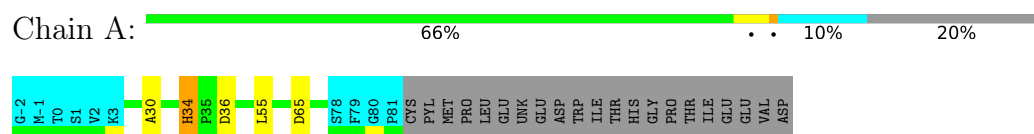
### 4.2.19 Score per residue for model 19

- Molecule 1: Protein SIS1



### 4.2.20 Score per residue for model 20

- Molecule 1: Protein SIS1



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.2
ARIA	structure calculation	2.3

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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

## 6 Model quality i

### 6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	591	580	579	2±1
All	All	11820	11600	11580	44

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:O	1:A:48:ILE:HG13	0.61	1.95	7	13
1:A:57:ASP:OD1	1:A:59:GLN:HG2	0.56	2.00	12	1
1:A:69:LEU:O	1:A:73:ARG:HG3	0.54	2.03	13	4
1:A:11:LEU:O	1:A:11:LEU:HD13	0.50	2.07	5	1
1:A:43:GLU:HG3	1:A:44:LYS:N	0.48	2.23	3	1
1:A:30:ALA:O	1:A:34:HIS:HB3	0.48	2.08	20	2
1:A:8:TYR:CE1	1:A:55:LEU:HD23	0.46	2.45	11	1
1:A:23:LYS:O	1:A:27:ARG:HG2	0.46	2.09	14	2
1:A:6:LYS:O	1:A:9:ASP:HB3	0.46	2.11	18	1
1:A:59:GLN:O	1:A:63:ILE:HG13	0.45	2.11	1	8
1:A:8:TYR:CD1	1:A:55:LEU:HD23	0.44	2.48	2	2
1:A:34:HIS:CE1	1:A:36:ASP:HB2	0.44	2.47	20	1
1:A:33:TYR:CD2	1:A:48:ILE:HD11	0.44	2.48	16	1
1:A:49:SER:O	1:A:53:GLU:HG2	0.43	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:GLU:H	1:A:70:GLU:CD	0.43	2.17	12	1
1:A:43:GLU:O	1:A:47:GLU:HB2	0.42	2.14	7	1
1:A:23:LYS:O	1:A:27:ARG:HG3	0.42	2.15	5	1
1:A:50:GLU:O	1:A:54:ILE:HG13	0.41	2.15	12	1
1:A:27:ARG:O	1:A:31:LEU:HD23	0.41	2.16	16	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	74/105 (70%)	71±1 (96±1%)	2±1 (3±2%)	0±0 (0±1%)	44 80
All	All	1480/2100 (70%)	1427 (96%)	49 (3%)	4 (0%)	44 80

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	41	ASP	4

### 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	62/88 (70%)	60±1 (98±2%)	2±1 (2±2%)	51 92
All	All	1240/1760 (70%)	1210 (98%)	30 (2%)	51 92

All 12 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	34	HIS	10
1	A	55	LEU	7
1	A	24	LYS	2
1	A	57	ASP	2
1	A	39	THR	2
1	A	47	GLU	1
1	A	59	GLN	1
1	A	18	ASN	1
1	A	23	LYS	1
1	A	20	GLN	1
1	A	50	GLU	1
1	A	6	LYS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides 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 i

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_1*

#### 7.1.1 Bookkeeping i

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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

#### 7.1.2 Chemical shift referencing i

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	83	$-0.36 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	74	$0.05 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	76	$-0.21 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	77	$0.81 \pm 0.48$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 882 atoms were assigned a chemical shift out of a possible 1000. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	359/366 (98%)	147/149 (99%)	143/148 (97%)	69/69 (100%)
Sidechain	467/561 (83%)	318/358 (89%)	149/180 (83%)	0/23 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	56/73 (77%)	28/34 (82%)	28/37 (76%)	0/2 (0%)
Overall	882/1000 (88%)	493/541 (91%)	320/365 (88%)	69/94 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 980 atoms were assigned a chemical shift out of a possible 1117. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	402/416 (97%)	166/170 (98%)	159/168 (95%)	77/78 (99%)
Sidechain	514/618 (83%)	350/396 (88%)	164/198 (83%)	0/24 (0%)
Aromatic	64/83 (77%)	32/39 (82%)	32/42 (76%)	0/2 (0%)
Overall	980/1117 (88%)	548/605 (91%)	355/408 (87%)	77/104 (74%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

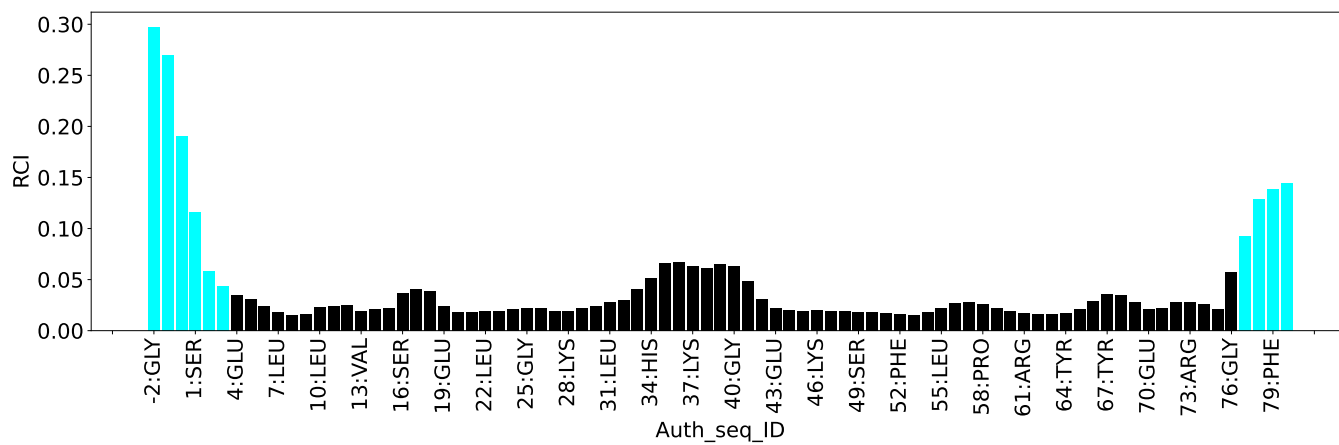
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	52	PHE	CE2	117.51	124.80 – 136.72	-11.1
1	A	75	GLY	CA	59.32	38.93 – 51.79	10.9
1	A	45	PHE	CE2	118.22	124.80 – 136.72	-10.5
1	A	52	PHE	CE1	117.51	124.17 – 137.29	-10.1
1	A	45	PHE	CE1	118.22	124.17 – 137.29	-9.5
1	A	79	PHE	CE2	119.56	124.80 – 136.72	-9.4
1	A	79	PHE	CE1	119.56	124.17 – 137.29	-8.5
1	A	15	PRO	HA	2.48	2.78 – 6.00	-5.9

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2954
Intra-residue ( $ i-j =0$ )	1266
Sequential ( $ i-j =1$ )	659
Medium range ( $ i-j >1$ and $ i-j <5$ )	627
Long range ( $ i-j \geq 5$ )	402
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	28.1
Number of long range restraints per residue <sup>1</sup>	3.8

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

### 8.2 Residual restraint violations

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

#### 8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	88.2	0.2
0.2-0.5 (Medium)	171.5	0.5
>0.5 (Large)	156.2	5.27

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis

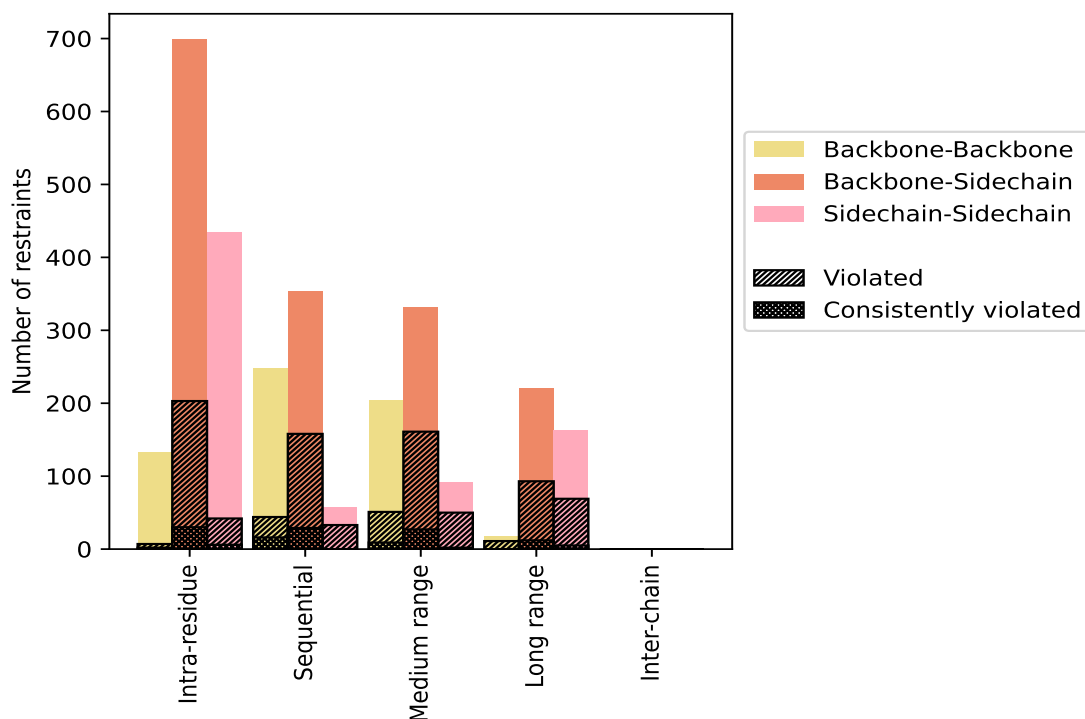
### 9.1 Summary of distance violations

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>1266</b>	<b>42.9</b>	<b>252</b>	<b>19.9</b>	<b>8.5</b>	<b>38</b>	<b>3.0</b>	<b>1.3</b>
Backbone-Backbone	133	4.5	7	5.3	0.2	2	1.5	0.1
Backbone-Sidechain	699	23.7	203	29.0	6.9	30	4.3	1.0
Sidechain-Sidechain	434	14.7	42	9.7	1.4	6	1.4	0.2
<b>Sequential (<math> i-j =1</math>)</b>	<b>659</b>	<b>22.3</b>	<b>235</b>	<b>35.7</b>	<b>8.0</b>	<b>45</b>	<b>6.8</b>	<b>1.5</b>
Backbone-Backbone	248	8.4	44	17.7	1.5	16	6.5	0.5
Backbone-Sidechain	354	12.0	158	44.6	5.3	29	8.2	1.0
Sidechain-Sidechain	57	1.9	33	57.9	1.1	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>627</b>	<b>21.2</b>	<b>262</b>	<b>41.8</b>	<b>8.9</b>	<b>38</b>	<b>6.1</b>	<b>1.3</b>
Backbone-Backbone	204	6.9	51	25.0	1.7	9	4.4	0.3
Backbone-Sidechain	332	11.2	161	48.5	5.5	27	8.1	0.9
Sidechain-Sidechain	91	3.1	50	54.9	1.7	2	2.2	0.1
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>402</b>	<b>13.6</b>	<b>173</b>	<b>43.0</b>	<b>5.9</b>	<b>17</b>	<b>4.2</b>	<b>0.6</b>
Backbone-Backbone	18	0.6	11	61.1	0.4	0	0.0	0.0
Backbone-Sidechain	221	7.5	93	42.1	3.1	12	5.4	0.4
Sidechain-Sidechain	163	5.5	69	42.3	2.3	5	3.1	0.2
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
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
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>2954</b>	<b>100.0</b>	<b>922</b>	<b>31.2</b>	<b>31.2</b>	<b>138</b>	<b>4.7</b>	<b>4.7</b>
Backbone-Backbone	603	20.4	113	18.7	3.8	27	4.5	0.9
Backbone-Sidechain	1606	54.4	615	38.3	20.8	98	6.1	3.3
Sidechain-Sidechain	745	25.2	194	26.0	6.6	13	1.7	0.4

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
1	135	122	98	79	0	434	0.52	3.29	0.46	0.37
2	123	120	121	58	0	422	0.52	2.7	0.42	0.38
3	124	119	108	65	0	416	0.5	3.13	0.4	0.37
4	116	111	110	61	0	398	0.48	3.87	0.41	0.36
5	127	114	114	67	0	422	0.52	4.14	0.45	0.38
6	137	119	108	59	0	423	0.51	2.97	0.41	0.38
7	126	123	123	66	0	438	0.53	3.47	0.48	0.36
8	126	118	120	66	0	430	0.53	3.56	0.43	0.39
9	119	123	99	62	0	403	0.5	2.32	0.38	0.38
10	114	107	99	73	0	393	0.51	3.01	0.42	0.4
11	119	115	106	74	0	414	0.51	4.64	0.48	0.37

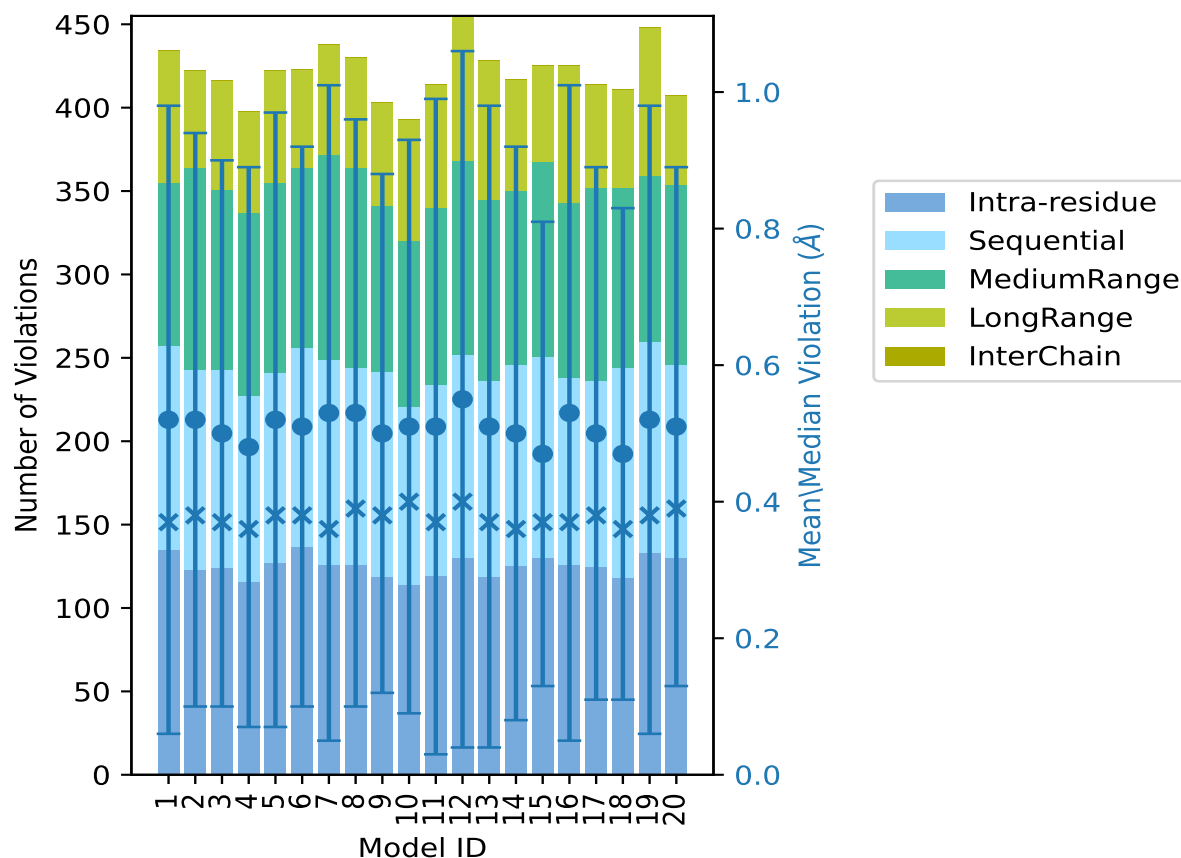
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>					
12	130	122	116	87	0	455	0.55	5.27	0.51	0.4
13	119	117	109	83	0	428	0.51	3.89	0.47	0.37
14	125	121	104	67	0	417	0.5	3.31	0.42	0.36
15	130	121	117	57	0	425	0.47	2.39	0.34	0.37
16	126	112	105	82	0	425	0.53	4.85	0.48	0.37
17	125	111	116	62	0	414	0.5	2.4	0.39	0.38
18	118	126	108	59	0	411	0.47	2.22	0.36	0.36
19	133	127	99	89	0	448	0.52	3.4	0.46	0.38
20	130	116	108	53	0	407	0.51	2.74	0.38	0.39

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

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

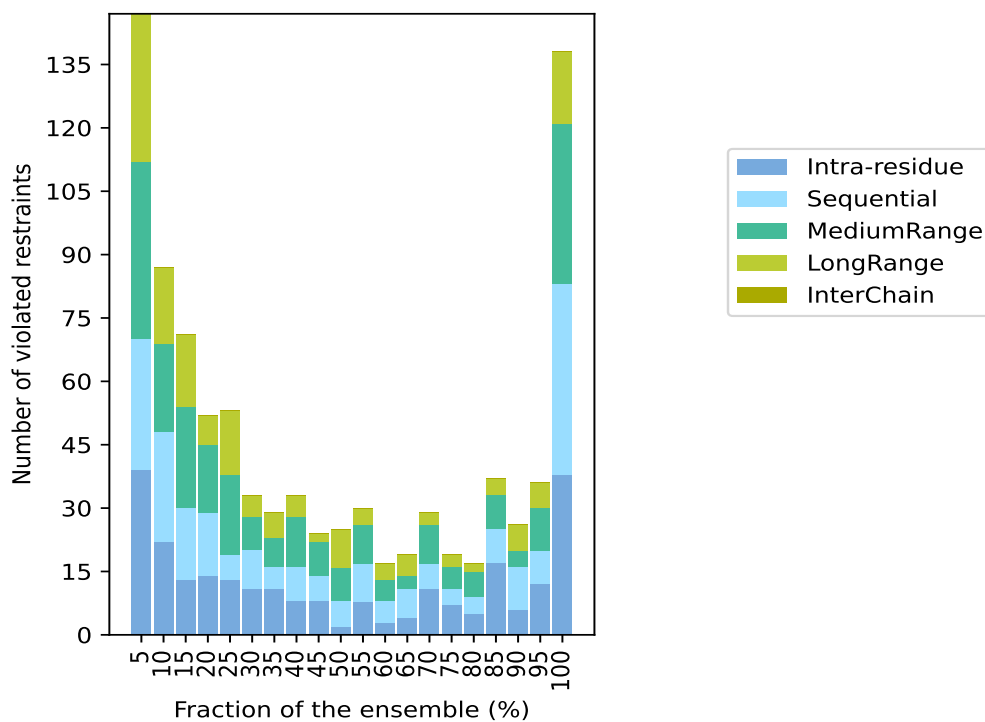
### 9.3 Distance violation statistics for the ensemble

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, 2032(IR:1014, SQ:424, MR:365, LR:229, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
39	31	42	35	0	147	1	5.0
22	26	21	18	0	87	2	10.0
13	17	24	17	0	71	3	15.0
14	15	16	7	0	52	4	20.0
13	6	19	15	0	53	5	25.0
11	9	8	5	0	33	6	30.0
11	5	7	6	0	29	7	35.0
8	8	12	5	0	33	8	40.0
8	6	8	2	0	24	9	45.0
2	6	8	9	0	25	10	50.0
8	9	9	4	0	30	11	55.0
3	5	5	4	0	17	12	60.0
4	7	3	5	0	19	13	65.0
11	6	9	3	0	29	14	70.0
7	4	5	3	0	19	15	75.0
5	4	6	2	0	17	16	80.0
17	8	8	4	0	37	17	85.0
6	10	4	6	0	26	18	90.0
12	8	10	6	0	36	19	95.0
38	45	38	17	0	138	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

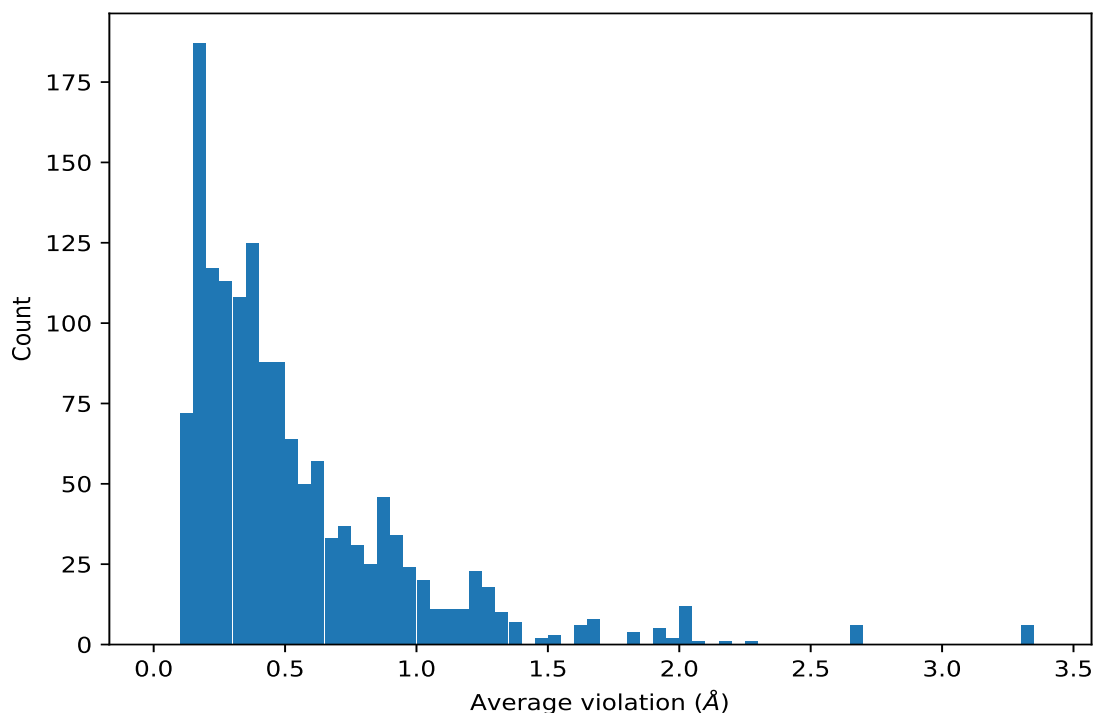
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	20	2.02	0.19	2.01
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	20	2.02	0.19	2.01
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	20	2.02	0.19	2.01
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	20	1.94	1.06	2.18
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	20	1.94	1.06	2.18
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	20	1.94	1.06	2.18
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	20	1.81	0.29	1.85
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	20	1.81	0.29	1.85
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	20	1.81	0.29	1.85
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	20	1.61	0.29	1.66
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	20	1.61	0.29	1.66
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	20	1.61	0.29	1.66
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	20	1.3	0.1	1.28
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	20	1.3	0.1	1.28
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	20	1.3	0.1	1.28
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	20	1.26	0.68	1.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	20	1.26	0.68	1.29
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	20	1.24	0.12	1.27
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	20	1.24	0.12	1.27
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	20	1.24	0.12	1.27
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	20	1.18	0.38	1.1
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	20	1.13	0.18	1.12
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	20	1.13	0.18	1.12
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	20	1.13	0.18	1.12
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	20	1.11	0.12	1.13
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	20	1.11	0.12	1.13
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	20	1.11	0.12	1.13
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	20	1.1	0.24	1.0
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	20	1.06	0.06	1.07
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	20	1.05	0.01	1.05
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	20	1.03	0.28	0.98
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	20	1.03	0.28	0.98
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	20	1.03	0.28	0.98
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	20	1.03	0.38	1.07
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	20	1.01	0.1	1.0
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	20	1.01	0.1	1.0
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	20	1.01	0.1	1.0
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	20	1.01	0.04	1.02
(1,143)	1:29:A:ALA:HA	1:32:A:LYS:HA	20	1.01	0.04	1.02
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	20	1.0	0.19	0.98
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	20	1.0	0.19	0.98
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	20	1.0	0.19	0.98
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	20	0.96	0.29	1.0
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	20	0.96	0.29	1.0
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	20	0.96	0.29	1.0
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	20	0.96	0.05	0.96
(1,369)	1:0:A:THR:HA	1:1:A:SER:HA	20	0.96	0.05	0.96
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	20	0.95	0.09	0.96
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	20	0.94	0.24	0.98
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	20	0.93	0.64	0.58
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	20	0.93	0.09	0.97
(1,122)	1:9:A:ASP:H	1:10:A:LEU:HA	20	0.93	0.09	0.97
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	20	0.89	0.13	0.86
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	20	0.89	0.13	0.86
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	20	0.88	0.11	0.9
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	20	0.88	0.09	0.86
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	20	0.88	0.08	0.85
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	20	0.83	0.1	0.84

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	20	0.83	0.17	0.86
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	20	0.83	0.17	0.86
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	20	0.83	0.17	0.86
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	20	0.83	0.17	0.86
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	20	0.83	0.17	0.86
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	20	0.83	0.17	0.86
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	20	0.78	0.18	0.75
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD11	20	0.76	0.21	0.78
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD12	20	0.76	0.21	0.78
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD13	20	0.76	0.21	0.78
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	20	0.76	0.21	0.78
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	20	0.76	0.21	0.78
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	20	0.76	0.21	0.78
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	20	0.76	0.18	0.73
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	20	0.76	0.14	0.81
(1,374)	1:28:A:LYS:HA	1:28:A:LYS:HB3	20	0.76	0.14	0.81
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	20	0.75	0.13	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	20	0.75	0.13	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	20	0.75	0.13	0.78
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	20	0.75	0.1	0.74
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	20	0.73	0.16	0.74
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	20	0.73	0.08	0.74
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	20	0.72	0.07	0.7
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	20	0.71	0.1	0.7
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	20	0.7	0.1	0.7
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	20	0.69	0.01	0.69
(1,115)	1:46:A:LYS:HA	1:46:A:LYS:HB2	20	0.69	0.01	0.69
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB3	20	0.69	0.11	0.72
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	20	0.69	0.11	0.72
(1,69)	1:30:A:ALA:H	1:32:A:LYS:HB3	20	0.69	0.11	0.72
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	20	0.68	0.0	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	20	0.68	0.0	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	20	0.68	0.0	0.68
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	20	0.68	0.15	0.7
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	20	0.67	0.06	0.68
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	20	0.66	0.14	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	20	0.65	0.01	0.65
(1,19)	1:46:A:LYS:HA	1:46:A:LYS:HB2	20	0.65	0.01	0.65
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	20	0.65	0.11	0.68
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	20	0.65	0.04	0.64
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	20	0.64	0.13	0.64
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	20	0.64	0.04	0.66

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	20	0.64	0.04	0.66
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	20	0.63	0.05	0.63
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	20	0.63	0.05	0.63
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	20	0.62	0.01	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	20	0.62	0.01	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	20	0.62	0.01	0.62
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	20	0.61	0.01	0.61
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	20	0.61	0.27	0.6
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	20	0.6	0.06	0.62
(1,27)	1:48:A:ILE:H	1:50:A:GLU:HB2	20	0.6	0.06	0.62
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	20	0.59	0.21	0.51
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	20	0.59	0.21	0.51
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	20	0.59	0.21	0.51
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	20	0.58	0.07	0.53
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	20	0.58	0.02	0.58
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	20	0.57	0.08	0.58
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	20	0.55	0.09	0.52
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	20	0.54	0.05	0.52
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	20	0.54	0.05	0.52
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	20	0.54	0.05	0.52
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	20	0.53	0.2	0.67
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	20	0.51	0.08	0.51
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	20	0.51	0.08	0.51
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	20	0.51	0.08	0.51
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	20	0.5	0.13	0.5
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	20	0.49	0.09	0.49
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	20	0.49	0.04	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	20	0.48	0.01	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	20	0.48	0.01	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	20	0.48	0.01	0.48
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	20	0.48	0.1	0.53
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	20	0.47	0.04	0.48
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	20	0.46	0.06	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	20	0.46	0.06	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	20	0.46	0.06	0.45
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	20	0.46	0.06	0.45
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	20	0.46	0.06	0.45
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	20	0.46	0.06	0.45
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	20	0.44	0.13	0.44
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	20	0.44	0.11	0.43
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	20	0.44	0.09	0.42
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	20	0.44	0.09	0.42

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	20	0.44	0.09	0.42
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	20	0.44	0.14	0.44
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	20	0.43	0.05	0.42
(1,134)	1:20:A:GLN:HA	1:20:A:GLN:HB2	20	0.43	0.05	0.42
(1,134)	1:22:A:LEU:HA	1:22:A:LEU:HB3	20	0.43	0.05	0.42
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	20	0.41	0.03	0.41
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	20	0.4	0.08	0.4
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	20	0.4	0.09	0.42
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	20	0.39	0.08	0.4
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	20	0.39	0.05	0.4
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	20	0.39	0.03	0.4
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	20	0.38	0.01	0.39
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	20	0.38	0.08	0.36
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	20	0.38	0.08	0.36
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	20	0.38	0.08	0.36
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	20	0.38	0.03	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	20	0.38	0.03	0.38
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	20	0.38	0.02	0.38
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	20	0.38	0.09	0.36
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	20	0.38	0.04	0.38
(1,242)	1:31:A:LEU:HA	1:34:A:HIS:H	20	0.38	0.04	0.38
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	20	0.36	0.19	0.3
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	20	0.36	0.19	0.3
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	20	0.36	0.1	0.36
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	20	0.35	0.09	0.36
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	20	0.35	0.09	0.34
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	20	0.35	0.09	0.34
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	20	0.35	0.09	0.34
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	20	0.35	0.14	0.34
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	20	0.35	0.0	0.35
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	20	0.34	0.21	0.23
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	20	0.34	0.21	0.23
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	20	0.34	0.04	0.35
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	20	0.34	0.04	0.35
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	20	0.33	0.03	0.34
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	20	0.33	0.08	0.32
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	20	0.33	0.09	0.33
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	20	0.33	0.09	0.33
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	20	0.33	0.09	0.33
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	20	0.33	0.12	0.34
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	20	0.33	0.12	0.34
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	20	0.33	0.12	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	20	0.33	0.02	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	20	0.33	0.02	0.33
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	20	0.32	0.1	0.3
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	20	0.32	0.1	0.3
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	20	0.32	0.1	0.3
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	20	0.32	0.06	0.34
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	20	0.32	0.06	0.34
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	20	0.32	0.06	0.32
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	20	0.31	0.05	0.32
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	20	0.31	0.0	0.31
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	20	0.3	0.08	0.28
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	20	0.3	0.04	0.3
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	20	0.3	0.03	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	20	0.3	0.02	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	20	0.3	0.02	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	20	0.3	0.02	0.3
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	20	0.29	0.05	0.3
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	20	0.28	0.01	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	20	0.28	0.01	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	20	0.28	0.0	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	20	0.28	0.0	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	20	0.28	0.0	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	20	0.27	0.01	0.28
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	20	0.27	0.03	0.28
(1,79)	1:6:A:LYS:H	1:9:A:ASP:H	20	0.27	0.03	0.28
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	20	0.26	0.02	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	20	0.26	0.04	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	20	0.26	0.04	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	20	0.26	0.04	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	20	0.26	0.01	0.26
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	20	0.26	0.01	0.26
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	20	0.26	0.03	0.24
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	20	0.25	0.06	0.26
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	20	0.25	0.08	0.25
(1,99)	1:59:A:GLN:H	1:60:A:LYS:HB2	20	0.25	0.08	0.25
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	20	0.23	0.0	0.23
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	20	0.23	0.03	0.23
(1,231)	1:24:A:LYS:HD3	1:24:A:LYS:HE2	20	0.23	0.03	0.22
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	20	0.23	0.03	0.22
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	20	0.23	0.01	0.23
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	20	0.22	0.04	0.22
(1,294)	1:6:A:LYS:HG2	1:6:A:LYS:HD2	20	0.22	0.04	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,294)	1:24:A:LYS:HD3	1:24:A:LYS:HG2	20	0.22	0.04	0.22
(1,294)	1:28:A:LYS:HD3	1:28:A:LYS:HG2	20	0.22	0.04	0.22
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	20	0.22	0.05	0.22
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	20	0.22	0.07	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	20	0.21	0.02	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	20	0.2	0.03	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	20	0.2	0.03	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	20	0.2	0.03	0.21
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	20	0.19	0.05	0.22
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	20	0.18	0.03	0.18
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	20	0.16	0.01	0.16
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	20	0.16	0.02	0.16
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	20	0.13	0.01	0.13
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	20	0.12	0.01	0.11
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	19	1.38	0.41	1.47
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	19	1.38	0.41	1.47
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	19	1.38	0.41	1.47
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	19	1.29	0.27	1.33
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	19	1.23	0.25	1.27
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	19	1.17	0.33	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	19	1.17	0.33	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	19	1.17	0.33	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	19	1.17	0.33	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	19	1.17	0.33	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	19	1.17	0.33	1.0
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	19	1.05	0.36	0.98
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	19	1.05	0.36	0.98
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	19	1.05	0.36	0.98
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	19	1.05	0.36	0.98
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	19	1.01	0.44	1.26
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	19	1.0	0.41	1.15
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	19	0.93	0.38	0.8
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	19	0.93	0.38	0.8
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	19	0.91	0.02	0.91
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	19	0.75	0.3	0.68

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	19	0.75	0.3	0.68
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	19	0.75	0.3	0.68
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	19	0.73	0.24	0.79
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	19	0.73	0.53	0.5
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	19	0.67	0.21	0.67
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	19	0.67	0.37	0.56
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	19	0.6	0.21	0.59
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	19	0.58	0.02	0.59
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	19	0.54	0.34	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	19	0.54	0.34	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	19	0.54	0.34	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	19	0.54	0.34	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	19	0.54	0.34	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	19	0.54	0.34	0.49
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	19	0.51	0.18	0.58
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	19	0.43	0.02	0.43
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	19	0.42	0.18	0.42
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	19	0.42	0.18	0.42
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	19	0.42	0.18	0.42
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	19	0.42	0.06	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	19	0.42	0.06	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	19	0.42	0.06	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	19	0.42	0.06	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	19	0.42	0.06	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	19	0.42	0.06	0.43
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	19	0.39	0.13	0.41
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	19	0.35	0.12	0.35
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	19	0.35	0.12	0.35
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	19	0.35	0.12	0.35
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	19	0.35	0.08	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	19	0.35	0.08	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	19	0.35	0.08	0.34
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	19	0.34	0.14	0.33
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	19	0.34	0.14	0.33
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	19	0.34	0.14	0.33
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	19	0.29	0.07	0.34
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	19	0.29	0.07	0.34
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	19	0.28	0.1	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	19	0.27	0.04	0.28
(1,456)	1:0:A:THR:HB	1:1:A:SER:H	19	0.27	0.04	0.28
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	19	0.25	0.07	0.25
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	19	0.25	0.07	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	19	0.25	0.07	0.25
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	19	0.22	0.07	0.21
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	19	0.22	0.07	0.21
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	19	0.22	0.07	0.21
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	19	0.22	0.06	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	19	0.22	0.0	0.22
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	19	0.2	0.03	0.21
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	19	0.18	0.02	0.18
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	19	0.17	0.04	0.18
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	19	0.15	0.0	0.15
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	18	0.7	0.31	0.64
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	18	0.7	0.31	0.64
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	18	0.7	0.31	0.64
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	18	0.62	0.3	0.61
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	18	0.6	0.27	0.66
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	18	0.56	0.22	0.55
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	18	0.55	0.23	0.55
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	18	0.55	0.23	0.55
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	18	0.55	0.23	0.55
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	18	0.53	0.34	0.42
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	18	0.53	0.34	0.42
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	18	0.53	0.34	0.42
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	18	0.53	0.18	0.56
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	18	0.53	0.18	0.56
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	18	0.53	0.18	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	18	0.51	0.14	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	18	0.51	0.14	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	18	0.51	0.14	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	18	0.51	0.14	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	18	0.51	0.14	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	18	0.51	0.14	0.56
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	18	0.51	0.14	0.56
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	18	0.51	0.14	0.56
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	18	0.42	0.13	0.38
(1,320)	1:77:A:PRO:HD3	1:78:A:SER:H	18	0.42	0.13	0.38
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	18	0.39	0.15	0.38
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	18	0.39	0.15	0.38
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	18	0.36	0.01	0.36
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	18	0.35	0.09	0.37
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	18	0.35	0.09	0.37
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	18	0.35	0.14	0.36
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	18	0.35	0.14	0.36

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	18	0.35	0.14	0.36
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	18	0.33	0.18	0.32
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	18	0.32	0.11	0.32
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB2	18	0.32	0.11	0.32
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	18	0.32	0.11	0.28
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	18	0.32	0.14	0.29
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	18	0.3	0.11	0.29
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	18	0.28	0.11	0.28
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	18	0.23	0.06	0.24
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	18	0.22	0.07	0.19
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	18	0.21	0.05	0.21
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	18	0.21	0.05	0.21
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	18	0.21	0.05	0.21
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	18	0.21	0.1	0.2
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	18	0.19	0.07	0.16
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB2	18	0.19	0.07	0.16
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	18	0.14	0.0	0.14
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	18	0.1	0.0	0.1
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	17	1.24	0.57	1.33
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	17	1.24	0.57	1.33
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	17	1.21	0.46	1.4
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	17	1.06	0.29	1.02
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	17	1.06	0.29	1.02
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	17	0.96	0.55	0.91
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	17	0.96	0.55	0.91
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	17	0.96	0.55	0.91
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	17	0.94	0.01	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	17	0.93	0.03	0.94
(2,47)	1:6:A:LYS:HG3	1:4:A:GLU:HA	17	0.87	0.38	1.01
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	17	0.87	0.38	1.01
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	17	0.87	0.33	0.72
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	17	0.54	0.25	0.52
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	17	0.54	0.25	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	17	0.52	0.01	0.52
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	17	0.51	0.14	0.48
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	17	0.51	0.14	0.48
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	17	0.51	0.14	0.48
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	17	0.49	0.22	0.6
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	17	0.49	0.22	0.6
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	17	0.49	0.22	0.6
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	17	0.49	0.22	0.6
(1,326)	1:78:A:SER:HA	1:79:A:PHE:H	17	0.48	0.14	0.53

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	17	0.48	0.14	0.53
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	17	0.48	0.18	0.53
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	17	0.45	0.16	0.51
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	17	0.45	0.16	0.51
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	17	0.45	0.16	0.51
(1,288)	1:26:A:TYR:HA	1:11:A:LEU:HD21	17	0.45	0.16	0.51
(1,288)	1:26:A:TYR:HA	1:11:A:LEU:HD22	17	0.45	0.16	0.51
(1,288)	1:26:A:TYR:HA	1:11:A:LEU:HD23	17	0.45	0.16	0.51
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	17	0.45	0.01	0.45
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	17	0.43	0.16	0.52
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	17	0.38	0.01	0.38
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	17	0.35	0.01	0.35
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	17	0.32	0.2	0.25
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	17	0.32	0.02	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	17	0.31	0.03	0.32
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	17	0.31	0.1	0.31
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	17	0.3	0.1	0.31
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	17	0.27	0.14	0.26
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	17	0.26	0.08	0.26
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	17	0.23	0.01	0.23
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	17	0.23	0.05	0.23
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	17	0.2	0.06	0.19
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	17	0.2	0.06	0.18
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	17	0.2	0.05	0.19
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	17	0.2	0.05	0.19
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	17	0.2	0.03	0.2
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	17	0.19	0.08	0.17
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	17	0.17	0.02	0.18
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	17	0.15	0.01	0.16
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	17	0.13	0.01	0.13
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	17	0.11	0.0	0.11
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	16	0.81	0.25	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	16	0.81	0.25	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	16	0.81	0.25	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	16	0.81	0.25	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	16	0.81	0.25	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	16	0.81	0.25	0.9
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	16	0.53	0.3	0.66
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	16	0.43	0.12	0.43
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	16	0.4	0.14	0.41
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	16	0.4	0.14	0.41
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	16	0.4	0.14	0.41

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	16	0.39	0.13	0.4
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	16	0.36	0.09	0.36
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	16	0.3	0.13	0.28
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	16	0.28	0.08	0.31
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	16	0.28	0.08	0.31
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	16	0.27	0.09	0.26
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	16	0.27	0.09	0.26
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	16	0.27	0.09	0.26
(2,1963)	1:55:A:LEU:HD11	1:55:A:LEU:H	16	0.27	0.09	0.26
(2,1963)	1:55:A:LEU:HD12	1:55:A:LEU:H	16	0.27	0.09	0.26
(2,1963)	1:55:A:LEU:HD13	1:55:A:LEU:H	16	0.27	0.09	0.26
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	16	0.27	0.09	0.27
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	16	0.24	0.07	0.22
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	16	0.21	0.09	0.18
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	16	0.21	0.09	0.16
(1,338)	1:52:A:PHE:H	1:48:A:ILE:HA	16	0.21	0.09	0.16
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	16	0.19	0.04	0.21
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	16	0.19	0.05	0.18
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	16	0.19	0.06	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	16	0.19	0.06	0.19
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	16	0.14	0.03	0.13
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	15	1.03	0.14	1.09
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	15	0.83	0.11	0.86
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	15	0.76	0.13	0.75
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	15	0.72	0.22	0.71
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	15	0.61	0.24	0.58
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	15	0.53	0.1	0.56
(1,44)	1:2:A:VAL:H	1:1:A:SER:HB3	15	0.53	0.1	0.56
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	15	0.53	0.0	0.53
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	15	0.53	0.16	0.59
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	15	0.52	0.28	0.58
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	15	0.48	0.16	0.47
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	15	0.48	0.16	0.47
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	15	0.48	0.16	0.47
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	15	0.48	0.18	0.49

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	15	0.48	0.18	0.49
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	15	0.48	0.18	0.49
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	15	0.38	0.13	0.36
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	15	0.38	0.13	0.36
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	15	0.38	0.13	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	15	0.38	0.13	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	15	0.38	0.13	0.4
(1,178)	1:26:A:TYR:HA	1:11:A:LEU:HD21	15	0.38	0.13	0.4
(1,178)	1:26:A:TYR:HA	1:11:A:LEU:HD22	15	0.38	0.13	0.4
(1,178)	1:26:A:TYR:HA	1:11:A:LEU:HD23	15	0.38	0.13	0.4
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	15	0.33	0.05	0.33
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	15	0.31	0.18	0.26
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	15	0.26	0.07	0.28
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	15	0.26	0.07	0.28
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	15	0.15	0.01	0.15
(1,309)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	15	0.15	0.01	0.15
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	15	0.15	0.03	0.14
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	15	0.12	0.01	0.12
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	14	2.06	0.19	2.01
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	14	0.95	0.4	1.15
(1,483)	1:53:A:GLU:HG2	1:53:A:GLU:H	14	0.95	0.4	1.15
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	14	0.9	0.61	0.7
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	14	0.9	0.61	0.7
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	14	0.9	0.61	0.7
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	14	0.85	0.19	0.85
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	14	0.68	0.32	0.81
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	14	0.61	0.04	0.62
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	14	0.55	0.04	0.55
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	14	0.53	0.25	0.48
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	14	0.53	0.25	0.48
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	14	0.53	0.25	0.48
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	14	0.48	0.21	0.44
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	14	0.48	0.21	0.44
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	14	0.47	0.08	0.46
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	14	0.43	0.04	0.44
(1,136)	1:6:A:LYS:HG2	1:6:A:LYS:HA	14	0.38	0.19	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	14	0.38	0.19	0.34
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	14	0.37	0.08	0.37
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	14	0.37	0.17	0.34
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	14	0.37	0.17	0.34
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	14	0.32	0.21	0.26
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	14	0.32	0.14	0.26
(1,332)	1:70:A:GLU:HA	1:73:A:ARG:HG3	14	0.32	0.14	0.26
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB3	14	0.32	0.14	0.26
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	14	0.31	0.11	0.28
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	14	0.3	0.11	0.3
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	14	0.3	0.11	0.3
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	14	0.29	0.12	0.3
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	14	0.29	0.12	0.3
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	14	0.29	0.12	0.3
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	14	0.29	0.13	0.26
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	14	0.29	0.13	0.26
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	14	0.29	0.13	0.26
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	14	0.27	0.12	0.26
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	14	0.27	0.12	0.26
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	14	0.27	0.12	0.26
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	14	0.23	0.13	0.18
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	14	0.23	0.06	0.22
(1,357)	1:50:A:GLU:HA	1:53:A:GLU:HB2	14	0.23	0.06	0.22
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	14	0.21	0.06	0.22
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	14	0.17	0.05	0.16
(2,2408)	1:24:A:LYS:HB2	1:24:A:LYS:H	14	0.17	0.05	0.16
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	14	0.17	0.04	0.18
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	14	0.17	0.04	0.18
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	14	0.17	0.04	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	14	0.16	0.03	0.16
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	14	0.16	0.03	0.16
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	14	0.15	0.03	0.15
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	14	0.13	0.03	0.13
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	13	0.86	0.74	0.37
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	13	0.56	0.22	0.47

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	13	0.56	0.22	0.47
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	13	0.56	0.22	0.47
(1,135)	1:48:A:ILE:HA	1:48:A:ILE:HD11	13	0.56	0.22	0.47
(1,135)	1:48:A:ILE:HA	1:48:A:ILE:HD12	13	0.56	0.22	0.47
(1,135)	1:48:A:ILE:HA	1:48:A:ILE:HD13	13	0.56	0.22	0.47
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB2	13	0.49	0.37	0.42
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	13	0.49	0.37	0.42
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	13	0.48	0.3	0.35
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	13	0.48	0.3	0.35
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	13	0.48	0.3	0.35
(1,398)	1:63:A:ILE:HG21	1:73:A:ARG:H	13	0.48	0.3	0.35
(1,398)	1:63:A:ILE:HG22	1:73:A:ARG:H	13	0.48	0.3	0.35
(1,398)	1:63:A:ILE:HG23	1:73:A:ARG:H	13	0.48	0.3	0.35
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	13	0.43	0.0	0.43
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	13	0.4	0.22	0.41
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	13	0.38	0.18	0.32
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	13	0.38	0.18	0.32
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	13	0.38	0.18	0.32
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	13	0.35	0.15	0.35
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	13	0.35	0.15	0.35
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	13	0.35	0.15	0.35
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	13	0.35	0.15	0.35
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	13	0.35	0.15	0.35
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	13	0.35	0.15	0.35
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	13	0.3	0.05	0.29
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	13	0.3	0.05	0.29
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	13	0.3	0.05	0.29
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	13	0.29	0.11	0.26
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	13	0.28	0.11	0.25
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	13	0.28	0.11	0.25
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	13	0.28	0.11	0.25
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	13	0.26	0.06	0.29
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	13	0.24	0.09	0.2
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	13	0.24	0.09	0.2
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	13	0.22	0.03	0.23
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	13	0.18	0.06	0.16
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	13	0.17	0.05	0.14
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	13	0.17	0.05	0.14
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	13	0.14	0.04	0.12
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	13	0.14	0.02	0.13
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	13	0.14	0.02	0.13
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	13	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	13	0.13	0.02	0.13
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	12	0.82	0.38	0.88
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	12	0.82	0.38	0.88
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	12	0.72	0.19	0.74
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	12	0.71	0.19	0.74
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	12	0.63	0.19	0.64
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	12	0.57	0.28	0.5
(1,47)	1:2:A:VAL:HB	1:65:A:ASP:H	12	0.57	0.28	0.5
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	12	0.5	0.42	0.24
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	12	0.43	0.43	0.29
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	12	0.43	0.17	0.38
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	12	0.43	0.17	0.38
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	12	0.41	0.26	0.36
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	12	0.39	0.44	0.3
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	12	0.39	0.44	0.3
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	12	0.39	0.44	0.3
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	12	0.36	0.18	0.29
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HB3	12	0.36	0.18	0.29
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	12	0.31	0.21	0.28
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	12	0.28	0.1	0.26
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	12	0.2	0.14	0.13
(1,437)	1:19:A:GLU:HB3	1:19:A:GLU:HA	12	0.2	0.14	0.13
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	12	0.18	0.05	0.18
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	12	0.16	0.04	0.16
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	12	0.12	0.02	0.11
(1,197)	1:34:A:HIS:H	1:34:A:HIS:HA	12	0.12	0.02	0.11
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	11	1.48	0.31	1.55
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	11	1.18	0.34	1.33
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	11	1.18	0.34	1.33
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	11	1.18	0.34	1.33
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	11	1.14	0.28	1.19
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	11	1.1	0.57	0.78
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	11	1.1	0.57	0.78
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	11	1.1	0.57	0.78
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	11	1.09	0.39	1.22
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	11	0.96	0.67	1.34
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	11	0.85	0.01	0.85
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	11	0.84	0.09	0.87
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	11	0.74	0.23	0.76
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	11	0.71	0.41	0.66
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE3	11	0.7	0.42	0.44
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE3	11	0.7	0.42	0.44

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,116)	1:33:A:TYR:HD1	1:44:A:LYS:HE3	11	0.7	0.42	0.44
(1,116)	1:33:A:TYR:HD2	1:44:A:LYS:HE3	11	0.7	0.42	0.44
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE2	11	0.7	0.42	0.44
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE2	11	0.7	0.42	0.44
(1,116)	1:33:A:TYR:HD1	1:44:A:LYS:HE2	11	0.7	0.42	0.44
(1,116)	1:33:A:TYR:HD2	1:44:A:LYS:HE2	11	0.7	0.42	0.44
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	11	0.69	0.01	0.68
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	11	0.65	0.18	0.69
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	11	0.63	0.24	0.76
(1,157)	1:27:A:ARG:HD2	1:27:A:ARG:HA	11	0.6	0.34	0.51
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	11	0.6	0.34	0.51
(1,157)	1:27:A:ARG:HD3	1:27:A:ARG:HA	11	0.6	0.34	0.51
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	11	0.56	0.44	0.4
(2,2343)	1:31:A:LEU:HB2	1:34:A:HIS:HD2	11	0.56	0.44	0.4
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	11	0.53	0.15	0.57
(1,128)	1:-1:A:MET:HB3	1:-1:A:MET:H	11	0.53	0.15	0.57
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	11	0.51	0.32	0.44
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	11	0.4	0.09	0.38
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	11	0.4	0.09	0.38
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	11	0.4	0.09	0.38
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	11	0.28	0.07	0.28
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	11	0.27	0.14	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	11	0.27	0.14	0.22
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	11	0.24	0.11	0.22
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	11	0.22	0.07	0.21
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	11	0.22	0.09	0.21
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	11	0.2	0.07	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	11	0.2	0.07	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	11	0.2	0.07	0.2
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	11	0.16	0.04	0.18
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	11	0.14	0.01	0.13
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	11	0.14	0.03	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	11	0.12	0.01	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	11	0.12	0.01	0.12
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	11	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	10	2.02	1.1	2.18
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	10	2.02	1.1	2.18
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	10	1.51	0.96	1.61
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	10	1.51	0.96	1.61
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	10	1.51	0.96	1.61
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	10	1.09	0.83	0.9
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	10	0.98	0.37	1.1
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	10	0.88	0.32	1.02
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	10	0.86	0.23	0.94
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	10	0.86	0.23	0.94
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	10	0.86	0.23	0.94
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	10	0.72	0.29	0.86
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	10	0.72	0.29	0.86
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	10	0.72	0.29	0.86
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	10	0.68	0.59	0.48
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE2	10	0.68	0.59	0.48
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	10	0.61	0.62	0.34
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	10	0.56	0.51	0.25
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	10	0.55	0.59	0.35
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	10	0.55	0.59	0.35
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	10	0.44	0.17	0.43
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	10	0.44	0.17	0.43
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	10	0.44	0.17	0.43
(1,380)	1:54:A:ILE:HD11	1:73:A:ARG:HD3	10	0.44	0.17	0.43
(1,380)	1:54:A:ILE:HD12	1:73:A:ARG:HD3	10	0.44	0.17	0.43
(1,380)	1:54:A:ILE:HD13	1:73:A:ARG:HD3	10	0.44	0.17	0.43
(1,304)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	10	0.39	0.01	0.39
(1,304)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	10	0.39	0.01	0.39
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	10	0.36	0.21	0.36
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	10	0.3	0.17	0.26
(1,91)	1:26:A:TYR:H	1:29:A:ALA:HB1	10	0.3	0.17	0.26
(1,91)	1:26:A:TYR:H	1:29:A:ALA:HB2	10	0.3	0.17	0.26
(1,91)	1:26:A:TYR:H	1:29:A:ALA:HB3	10	0.3	0.17	0.26
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	10	0.28	0.11	0.26
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	10	0.28	0.11	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	10	0.28	0.11	0.26
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	10	0.26	0.13	0.24
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	10	0.26	0.13	0.24
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	10	0.24	0.09	0.24
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	10	0.23	0.09	0.24
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	10	0.23	0.09	0.24
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	10	0.23	0.09	0.24
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	10	0.22	0.07	0.2
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	10	0.21	0.05	0.2
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	10	0.21	0.06	0.22
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	10	0.2	0.07	0.19
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	10	0.16	0.02	0.15
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	9	2.25	0.75	2.22
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	9	0.78	0.39	0.77
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	9	0.77	0.18	0.79
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	9	0.52	0.02	0.52
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	9	0.5	0.16	0.53
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD11	9	0.45	0.35	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD12	9	0.45	0.35	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD13	9	0.45	0.35	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	9	0.45	0.35	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	9	0.45	0.35	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	9	0.45	0.35	0.28
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	9	0.4	0.16	0.37
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	9	0.4	0.16	0.37
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE2	9	0.4	0.16	0.37
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE2	9	0.4	0.16	0.37
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	9	0.39	0.29	0.16
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	9	0.38	0.02	0.38
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	9	0.38	0.18	0.41
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	9	0.38	0.18	0.41
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	9	0.38	0.18	0.41
(2,458)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	9	0.36	0.12	0.29
(2,458)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	9	0.36	0.12	0.29
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	9	0.35	0.12	0.4
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	9	0.27	0.09	0.27
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	9	0.25	0.17	0.23
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	9	0.25	0.03	0.25
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	9	0.25	0.11	0.21
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	9	0.22	0.06	0.21
(1,246)	1:60:A:LYS:HE3	1:60:A:LYS:HB2	9	0.22	0.06	0.21
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	9	0.19	0.08	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	9	0.18	0.07	0.16
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	9	0.18	0.07	0.16
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	9	0.17	0.07	0.14
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	9	0.14	0.04	0.13
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	9	0.14	0.03	0.13
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	9	0.13	0.01	0.13
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	8	3.33	1.58	3.59
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	8	3.33	1.58	3.59
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	8	3.33	1.58	3.59
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE3	8	3.33	1.58	3.59
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE3	8	3.33	1.58	3.59
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE3	8	3.33	1.58	3.59
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	8	2.17	1.04	2.14
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	8	1.67	0.97	1.81
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	8	1.33	0.56	1.3
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	8	1.33	0.56	1.3
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	8	1.25	0.78	0.89
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	8	0.97	0.47	0.96
(2,694)	1:37:A:LYS:HD3	1:38:A:PRO:HD3	8	0.97	0.47	0.96
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	8	0.81	0.29	0.88
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	8	0.68	0.05	0.67
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	8	0.63	0.2	0.7
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	8	0.61	0.36	0.57
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	8	0.6	0.18	0.64
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	8	0.59	0.29	0.48
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	8	0.59	0.29	0.48
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	8	0.59	0.29	0.48
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	8	0.58	0.03	0.58
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	8	0.55	0.15	0.57
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	8	0.53	0.12	0.5
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	8	0.49	0.03	0.5
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	8	0.47	0.13	0.43
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	8	0.47	0.25	0.41
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	8	0.47	0.25	0.41
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	8	0.47	0.25	0.41
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	8	0.43	0.22	0.36
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB1	8	0.41	0.18	0.44
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB2	8	0.41	0.18	0.44
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB3	8	0.41	0.18	0.44
(1,429)	1:6:A:LYS:HG2	1:7:A:LEU:H	8	0.41	0.18	0.44
(1,429)	1:6:A:LYS:HG3	1:7:A:LEU:H	8	0.41	0.18	0.44
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	8	0.4	0.03	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,173)	1:70:A:GLU:HB2	1:70:A:GLU:HG2	8	0.34	0.01	0.35
(1,173)	1:21:A:GLU:HB3	1:21:A:GLU:HG3	8	0.34	0.01	0.35
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	8	0.32	0.21	0.22
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	8	0.27	0.15	0.22
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	8	0.27	0.15	0.22
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE2	8	0.27	0.15	0.22
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE2	8	0.27	0.15	0.22
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	8	0.25	0.07	0.28
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	8	0.25	0.07	0.28
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	8	0.19	0.07	0.18
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	8	0.19	0.07	0.18
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	8	0.19	0.07	0.18
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	8	0.19	0.07	0.18
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	8	0.19	0.07	0.18
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	8	0.19	0.07	0.18
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	8	0.18	0.06	0.16
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	8	0.16	0.06	0.13
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	8	0.16	0.06	0.13
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	8	0.16	0.06	0.13
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	8	0.16	0.05	0.15
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	8	0.15	0.04	0.14
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	8	0.15	0.04	0.14
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	8	0.15	0.04	0.14
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	8	0.15	0.05	0.14
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	8	0.14	0.03	0.15
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	8	0.12	0.01	0.11
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD3	7	2.66	1.17	3.27
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD3	7	2.66	1.17	3.27
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD3	7	2.66	1.17	3.27
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD2	7	2.66	1.17	3.27
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD2	7	2.66	1.17	3.27
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD2	7	2.66	1.17	3.27
(1,50)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	1.29	0.08	1.34
(1,50)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	7	1.29	0.08	1.34
(1,50)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	7	1.29	0.08	1.34
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	7	1.05	0.77	0.95
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	7	1.01	1.14	0.42
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	7	1.01	1.14	0.42
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	7	1.01	1.14	0.42
(1,119)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	0.93	0.08	0.98
(1,119)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	7	0.93	0.08	0.98
(1,119)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	7	0.93	0.08	0.98

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	7	0.6	0.3	0.54
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	7	0.58	0.3	0.62
(1,12)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	0.54	0.08	0.59
(1,12)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	7	0.54	0.08	0.59
(1,12)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	7	0.54	0.08	0.59
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	7	0.54	0.15	0.51
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	7	0.53	0.28	0.54
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	7	0.52	0.35	0.34
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	7	0.48	0.28	0.34
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	7	0.45	0.0	0.45
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE2	7	0.44	0.17	0.4
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE2	7	0.44	0.17	0.4
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE2	7	0.44	0.17	0.4
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE3	7	0.44	0.17	0.4
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE3	7	0.44	0.17	0.4
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE3	7	0.44	0.17	0.4
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	7	0.43	0.0	0.43
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	7	0.39	0.33	0.21
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	7	0.39	0.33	0.21
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	7	0.39	0.33	0.21
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	7	0.38	0.14	0.35
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	7	0.34	0.0	0.34
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE2	7	0.31	0.12	0.29
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE3	7	0.31	0.12	0.29
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	7	0.3	0.14	0.21
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	7	0.25	0.1	0.22
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	7	0.24	0.06	0.25
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	7	0.17	0.03	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	7	0.17	0.03	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	7	0.17	0.03	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	7	0.17	0.03	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	7	0.17	0.03	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	7	0.17	0.03	0.18
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	7	0.16	0.05	0.15
(1,103)	1:59:A:GLN:HA	1:59:A:GLN:HG3	7	0.16	0.04	0.15
(1,103)	1:62:A:GLU:HA	1:62:A:GLU:HG2	7	0.16	0.04	0.15
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	7	0.16	0.04	0.14
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	7	0.16	0.03	0.15
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	7	0.12	0.01	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	7	0.12	0.01	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	7	0.12	0.01	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	7	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	6	1.95	0.82	2.15
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	6	1.95	0.82	2.15
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	6	1.26	0.69	1.42
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	6	1.26	0.69	1.42
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	6	1.23	0.76	1.32
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	6	1.23	0.76	1.32
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	6	1.01	0.35	1.04
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	6	0.93	0.32	0.92
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	6	0.69	0.47	0.48
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	6	0.69	0.04	0.7
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	6	0.62	0.19	0.66
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	6	0.62	0.19	0.66
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	6	0.62	0.19	0.66
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	6	0.61	0.06	0.61
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	6	0.59	0.02	0.6
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	6	0.53	0.3	0.37
(2,2401)	1:53:A:GLU:HG2	1:56:A:ASN:HB2	6	0.43	0.27	0.37
(2,2401)	1:53:A:GLU:HG3	1:56:A:ASN:HB2	6	0.43	0.27	0.37
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	6	0.4	0.14	0.38
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	6	0.39	0.21	0.32
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	6	0.39	0.21	0.32
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	6	0.39	0.21	0.32
(2,567)	1:24:A:LYS:HE2	1:24:A:LYS:H	6	0.39	0.13	0.36
(2,567)	1:24:A:LYS:HE3	1:24:A:LYS:H	6	0.39	0.13	0.36
(1,75)	1:5:A:THR:HG21	1:15:A:PRO:HG2	6	0.38	0.15	0.32
(1,75)	1:5:A:THR:HG22	1:15:A:PRO:HG2	6	0.38	0.15	0.32
(1,75)	1:5:A:THR:HG23	1:15:A:PRO:HG2	6	0.38	0.15	0.32
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	6	0.38	0.15	0.32
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	6	0.38	0.15	0.32
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	6	0.38	0.15	0.32
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD3	6	0.37	0.07	0.4
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD2	6	0.37	0.07	0.4
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	6	0.34	0.12	0.34
(1,110)	1:50:A:GLU:HG2	1:54:A:ILE:HB	6	0.34	0.16	0.29
(1,110)	1:4:A:GLU:HG3	1:3:A:LYS:HD2	6	0.34	0.16	0.29
(1,110)	1:4:A:GLU:HG3	1:3:A:LYS:HD3	6	0.34	0.16	0.29
(1,8)	1:43:A:GLU:HA	1:43:A:GLU:HG2	6	0.33	0.23	0.24
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG2	6	0.33	0.23	0.24
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG3	6	0.33	0.23	0.24
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	6	0.28	0.06	0.29
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	6	0.25	0.08	0.24
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	6	0.23	0.05	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	6	0.23	0.05	0.22
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	6	0.23	0.05	0.22
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	6	0.23	0.05	0.22
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	6	0.23	0.05	0.22
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	6	0.23	0.05	0.22
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	6	0.22	0.07	0.25
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	6	0.19	0.05	0.2
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	6	0.19	0.07	0.18
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	6	0.17	0.05	0.18
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	6	0.17	0.05	0.18
(1,43)	1:72:A:ALA:H	1:69:A:LEU:HA	6	0.17	0.03	0.17
(1,43)	1:64:A:TYR:HA	1:72:A:ALA:H	6	0.17	0.03	0.17
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	6	0.17	0.02	0.16
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	6	0.16	0.02	0.17
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	6	0.16	0.03	0.16
(1,250)	1:51:A:ALA:HB1	1:10:A:LEU:H	6	0.14	0.02	0.15
(1,250)	1:51:A:ALA:HB2	1:10:A:LEU:H	6	0.14	0.02	0.15
(1,250)	1:51:A:ALA:HB3	1:10:A:LEU:H	6	0.14	0.02	0.15
(1,250)	1:72:A:ALA:HB1	1:71:A:ALA:H	6	0.14	0.02	0.15
(1,250)	1:72:A:ALA:HB2	1:71:A:ALA:H	6	0.14	0.02	0.15
(1,250)	1:72:A:ALA:HB3	1:71:A:ALA:H	6	0.14	0.02	0.15
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	6	0.13	0.02	0.12
(2,2348)	1:45:A:PHE:HD1	1:34:A:HIS:HD2	5	1.94	0.71	1.45
(2,2348)	1:45:A:PHE:HD2	1:34:A:HIS:HD2	5	1.94	0.71	1.45
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD1	5	1.67	0.57	1.57
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD2	5	1.67	0.57	1.57
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD1	5	1.67	0.57	1.57
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD2	5	1.67	0.57	1.57
(2,1188)	1:2:A:VAL:HB	1:65:A:ASP:HA	5	1.39	1.02	1.21
(2,906)	1:8:A:TYR:HB2	1:52:A:PHE:HA	5	1.32	0.27	1.13
(2,641)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	5	1.2	1.19	0.3
(2,641)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	5	1.2	1.19	0.3
(2,641)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	5	1.2	1.19	0.3
(2,2018)	1:59:A:GLN:H	1:59:A:GLN:HG3	5	0.99	0.37	1.16
(2,2115)	1:66:A:GLN:HB3	1:66:A:GLN:H	5	0.94	0.01	0.93
(2,27)	1:2:A:VAL:HB	1:65:A:ASP:HA	5	0.94	1.02	0.76
(2,907)	1:8:A:TYR:HB3	1:52:A:PHE:HA	5	0.87	0.37	0.7
(2,1133)	1:66:A:GLN:HB3	1:63:A:ILE:HA	5	0.86	0.14	0.84
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE2	5	0.83	0.37	0.67
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE2	5	0.83	0.37	0.67
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE2	5	0.83	0.37	0.67
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE3	5	0.83	0.37	0.67

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE3	5	0.83	0.37	0.67
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE3	5	0.83	0.37	0.67
(2,1494)	1:8:A:TYR:H	1:52:A:PHE:HA	5	0.7	0.28	0.61
(2,50)	1:4:A:GLU:H	1:6:A:LYS:HB3	5	0.63	0.45	0.38
(2,1796)	1:34:A:HIS:HB2	1:34:A:HIS:H	5	0.62	0.01	0.61
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD11	5	0.61	0.61	0.35
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD12	5	0.61	0.61	0.35
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD13	5	0.61	0.61	0.35
(1,244)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	5	0.61	0.18	0.65
(1,244)	1:4:A:GLU:HG2	1:3:A:LYS:HD3	5	0.61	0.18	0.65
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD2	5	0.56	0.45	0.23
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD3	5	0.56	0.45	0.23
(2,238)	1:22:A:LEU:HD21	1:15:A:PRO:HA	5	0.56	0.33	0.57
(2,238)	1:22:A:LEU:HD22	1:15:A:PRO:HA	5	0.56	0.33	0.57
(2,238)	1:22:A:LEU:HD23	1:15:A:PRO:HA	5	0.56	0.33	0.57
(2,1375)	1:78:A:SER:HA	1:78:A:SER:HB3	5	0.52	0.0	0.52
(2,1053)	1:58:A:PRO:HA	1:58:A:PRO:HG3	5	0.47	0.01	0.48
(2,274)	1:16:A:SER:HA	1:16:A:SER:HB3	5	0.47	0.01	0.47
(2,1407)	1:33:A:TYR:HD1	1:41:A:ASP:H	5	0.44	0.38	0.29
(2,1407)	1:33:A:TYR:HD2	1:41:A:ASP:H	5	0.44	0.38	0.29
(2,1933)	1:52:A:PHE:H	1:8:A:TYR:HA	5	0.43	0.21	0.36
(1,188)	1:38:A:PRO:HB2	1:38:A:PRO:HD3	5	0.37	0.01	0.37
(1,188)	1:58:A:PRO:HD3	1:58:A:PRO:HB2	5	0.37	0.01	0.37
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD11	5	0.36	0.45	0.13
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD12	5	0.36	0.45	0.13
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD13	5	0.36	0.45	0.13
(2,1831)	1:45:A:PHE:HB2	1:42:A:THR:H	5	0.35	0.13	0.38
(2,1484)	1:55:A:LEU:HD21	1:8:A:TYR:H	5	0.34	0.25	0.19
(2,1484)	1:55:A:LEU:HD22	1:8:A:TYR:H	5	0.34	0.25	0.19
(2,1484)	1:55:A:LEU:HD23	1:8:A:TYR:H	5	0.34	0.25	0.19
(2,627)	1:31:A:LEU:HA	1:34:A:HIS:HB2	5	0.32	0.11	0.32
(1,24)	1:37:A:LYS:HE3	1:34:A:HIS:H	5	0.31	0.11	0.27
(1,24)	1:37:A:LYS:HE2	1:34:A:HIS:H	5	0.31	0.11	0.27
(2,14)	1:2:A:VAL:HA	1:4:A:GLU:HG3	5	0.28	0.17	0.24
(2,2450)	1:58:A:PRO:HD3	1:57:A:ASP:H	5	0.24	0.06	0.22
(2,688)	1:40:A:GLY:H	1:38:A:PRO:HA	5	0.24	0.08	0.22
(1,205)	1:72:A:ALA:H	1:63:A:ILE:HB	5	0.23	0.07	0.21
(2,1211)	1:66:A:GLN:HB3	1:66:A:GLN:H	5	0.22	0.02	0.21
(1,249)	1:60:A:LYS:HG3	1:57:A:ASP:HB3	5	0.21	0.1	0.15
(1,249)	1:23:A:LYS:HE2	1:23:A:LYS:HG2	5	0.21	0.1	0.15
(1,121)	1:64:A:TYR:HD1	1:65:A:ASP:H	5	0.21	0.09	0.18
(1,121)	1:64:A:TYR:HD2	1:65:A:ASP:H	5	0.21	0.09	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,68)	1:72:A:ALA:HB1	1:76:A:GLY:H	5	0.2	0.07	0.18
(1,68)	1:72:A:ALA:HB2	1:76:A:GLY:H	5	0.2	0.07	0.18
(1,68)	1:72:A:ALA:HB3	1:76:A:GLY:H	5	0.2	0.07	0.18
(2,1991)	1:52:A:PHE:HA	1:56:A:ASN:H	5	0.19	0.07	0.18
(2,869)	1:50:A:GLU:HA	1:50:A:GLU:HG3	5	0.18	0.03	0.18
(1,245)	1:58:A:PRO:HB2	1:58:A:PRO:HA	5	0.17	0.02	0.18
(1,245)	1:43:A:GLU:HA	1:46:A:LYS:HB2	5	0.17	0.02	0.18
(2,1531)	1:7:A:LEU:HD21	1:10:A:LEU:H	5	0.17	0.09	0.14
(2,1531)	1:7:A:LEU:HD22	1:10:A:LEU:H	5	0.17	0.09	0.14
(2,1531)	1:7:A:LEU:HD23	1:10:A:LEU:H	5	0.17	0.09	0.14
(2,1553)	1:10:A:LEU:HB3	1:12:A:GLY:H	5	0.17	0.02	0.16
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG21	5	0.17	0.02	0.16
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG22	5	0.17	0.02	0.16
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG23	5	0.17	0.02	0.16
(1,57)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	5	0.16	0.02	0.17
(1,57)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	5	0.16	0.02	0.17
(1,57)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	5	0.16	0.02	0.17
(2,2211)	1:64:A:TYR:HE1	1:72:A:ALA:H	5	0.16	0.05	0.15
(2,2211)	1:64:A:TYR:HE2	1:72:A:ALA:H	5	0.16	0.05	0.15
(2,1173)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	5	0.16	0.03	0.16
(2,1173)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	5	0.16	0.03	0.16
(2,1173)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	5	0.16	0.03	0.16
(2,610)	1:30:A:ALA:HA	1:33:A:TYR:H	5	0.13	0.03	0.12
(2,706)	1:58:A:PRO:HA	1:58:A:PRO:HG3	5	0.13	0.01	0.14
(2,1377)	1:79:A:PHE:HA	1:79:A:PHE:HB2	5	0.13	0.01	0.14
(2,1603)	1:15:A:PRO:HG3	1:16:A:SER:H	5	0.13	0.02	0.12
(2,2094)	1:63:A:ILE:HG21	1:64:A:TYR:H	5	0.13	0.02	0.12
(2,2094)	1:63:A:ILE:HG22	1:64:A:TYR:H	5	0.13	0.02	0.12
(2,2094)	1:63:A:ILE:HG23	1:64:A:TYR:H	5	0.13	0.02	0.12
(2,1968)	1:55:A:LEU:H	1:56:A:ASN:HB3	5	0.12	0.02	0.12
(2,579)	1:28:A:LYS:HB3	1:29:A:ALA:HA	5	0.12	0.02	0.12
(2,473)	1:24:A:LYS:HA	1:27:A:ARG:HD3	4	1.45	0.77	1.63
(2,553)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	4	1.3	0.6	1.23
(2,553)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	4	1.3	0.6	1.23
(2,553)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	4	1.3	0.6	1.23
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD21	4	1.28	0.29	1.16
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD22	4	1.28	0.29	1.16
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD23	4	1.28	0.29	1.16
(2,1307)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	4	1.28	0.59	1.21
(2,1307)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	4	1.28	0.59	1.21
(2,1307)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	4	1.28	0.59	1.21
(2,766)	1:69:A:LEU:HD21	1:73:A:ARG:HA	4	1.27	0.6	1.07

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,766)	1:69:A:LEU:HD22	1:73:A:ARG:HA	4	1.27	0.6	1.07
(2,766)	1:69:A:LEU:HD23	1:73:A:ARG:HA	4	1.27	0.6	1.07
(2,562)	1:28:A:LYS:HA	1:28:A:LYS:HD3	4	1.22	0.03	1.22
(2,562)	1:28:A:LYS:HA	1:28:A:LYS:HD2	4	1.22	0.03	1.22
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD21	4	0.94	0.53	0.76
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD22	4	0.94	0.53	0.76
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD23	4	0.94	0.53	0.76
(2,2413)	1:74:A:SER:HB3	1:78:A:SER:H	4	0.94	0.2	0.92
(2,2413)	1:74:A:SER:HB2	1:78:A:SER:H	4	0.94	0.2	0.92
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD21	4	0.76	0.29	0.64
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD22	4	0.76	0.29	0.64
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD23	4	0.76	0.29	0.64
(2,1084)	1:59:A:GLN:H	1:59:A:GLN:HG3	4	0.75	0.02	0.74
(2,2460)	1:33:A:TYR:HD1	1:41:A:ASP:HB3	4	0.75	0.49	0.74
(2,2460)	1:33:A:TYR:HD2	1:41:A:ASP:HB3	4	0.75	0.49	0.74
(1,275)	1:26:A:TYR:H	1:22:A:LEU:HB2	4	0.74	0.11	0.7
(1,275)	1:26:A:TYR:H	1:24:A:LYS:HG3	4	0.74	0.11	0.7
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD21	4	0.72	0.29	0.6
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD22	4	0.72	0.29	0.6
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD23	4	0.72	0.29	0.6
(2,827)	1:24:A:LYS:HE2	1:20:A:GLN:HB3	4	0.71	0.5	0.68
(2,54)	1:4:A:GLU:HG2	1:3:A:LYS:HD2	4	0.7	0.32	0.82
(1,145)	1:41:A:ASP:HB3	1:44:A:LYS:HB3	4	0.68	0.28	0.52
(1,145)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	4	0.68	0.28	0.52
(2,1083)	1:59:A:GLN:H	1:59:A:GLN:HG2	4	0.68	0.07	0.65
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD21	4	0.62	0.29	0.5
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD22	4	0.62	0.29	0.5
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD23	4	0.62	0.29	0.5
(2,825)	1:60:A:LYS:HE2	1:60:A:LYS:H	4	0.59	0.24	0.72
(2,825)	1:60:A:LYS:H	1:60:A:LYS:HE3	4	0.59	0.24	0.72
(2,241)	1:8:A:TYR:HB2	1:15:A:PRO:HA	4	0.58	0.17	0.56
(2,2170)	1:64:A:TYR:HE1	1:69:A:LEU:H	4	0.58	0.17	0.56
(2,2170)	1:64:A:TYR:HE2	1:69:A:LEU:H	4	0.58	0.17	0.56
(2,81)	1:28:A:LYS:HA	1:28:A:LYS:HD3	4	0.47	0.03	0.47
(2,81)	1:28:A:LYS:HA	1:28:A:LYS:HD2	4	0.47	0.03	0.47
(2,1123)	1:70:A:GLU:HA	1:73:A:ARG:HD2	4	0.44	0.09	0.4
(2,2448)	1:42:A:THR:HA	1:35:A:PRO:HG3	4	0.44	0.26	0.34
(1,278)	1:1:A:SER:H	1:1:A:SER:HB3	4	0.43	0.26	0.46
(1,278)	1:53:A:GLU:H	1:52:A:PHE:HA	4	0.43	0.26	0.46
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG21	4	0.38	0.18	0.4
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG22	4	0.38	0.18	0.4
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG23	4	0.38	0.18	0.4

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,789)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	4	0.37	0.26	0.27
(2,1251)	1:70:A:GLU:HA	1:70:A:GLU:HG3	4	0.34	0.24	0.22
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD21	4	0.32	0.13	0.32
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD22	4	0.32	0.13	0.32
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD23	4	0.32	0.13	0.32
(2,1075)	1:63:A:ILE:HD11	1:59:A:GLN:HG3	4	0.31	0.11	0.34
(2,1075)	1:63:A:ILE:HD12	1:59:A:GLN:HG3	4	0.31	0.11	0.34
(2,1075)	1:63:A:ILE:HD13	1:59:A:GLN:HG3	4	0.31	0.11	0.34
(2,2276)	1:79:A:PHE:HA	1:80:A:GLY:H	4	0.31	0.03	0.31
(2,1261)	1:70:A:GLU:HA	1:70:A:GLU:HG3	4	0.27	0.24	0.15
(2,444)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	4	0.27	0.07	0.28
(2,444)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	4	0.27	0.07	0.28
(2,573)	1:29:A:ALA:H	1:28:A:LYS:HG3	4	0.26	0.1	0.29
(2,1804)	1:39:A:THR:H	1:37:A:LYS:HG2	4	0.24	0.05	0.24
(2,348)	1:19:A:GLU:HA	1:19:A:GLU:HG2	4	0.23	0.01	0.23
(2,176)	1:11:A:LEU:HB2	1:10:A:LEU:HB2	4	0.22	0.08	0.23
(1,66)	1:60:A:LYS:HG2	1:60:A:LYS:HE2	4	0.22	0.03	0.22
(1,66)	1:60:A:LYS:HE3	1:60:A:LYS:HG2	4	0.22	0.03	0.22
(1,51)	1:19:A:GLU:HB2	1:19:A:GLU:HG3	4	0.22	0.0	0.22
(1,51)	1:62:A:GLU:HB2	1:62:A:GLU:HG2	4	0.22	0.0	0.22
(2,1807)	1:39:A:THR:H	1:38:A:PRO:HG2	4	0.19	0.03	0.18
(2,1300)	1:24:A:LYS:HE2	1:21:A:GLU:HA	4	0.19	0.05	0.19
(2,2133)	1:67:A:TYR:H	1:66:A:GLN:HB3	4	0.18	0.06	0.16
(1,5)	1:63:A:ILE:HD11	1:75:A:GLY:H	4	0.18	0.04	0.16
(1,5)	1:63:A:ILE:HD12	1:75:A:GLY:H	4	0.18	0.04	0.16
(1,5)	1:63:A:ILE:HD13	1:75:A:GLY:H	4	0.18	0.04	0.16
(1,5)	1:63:A:ILE:HG21	1:75:A:GLY:H	4	0.18	0.04	0.16
(1,5)	1:63:A:ILE:HG22	1:75:A:GLY:H	4	0.18	0.04	0.16
(1,5)	1:63:A:ILE:HG23	1:75:A:GLY:H	4	0.18	0.04	0.16
(2,731)	1:45:A:PHE:HB2	1:42:A:THR:HA	4	0.17	0.03	0.16
(2,967)	1:54:A:ILE:HD11	1:72:A:ALA:HA	4	0.17	0.08	0.13
(2,967)	1:54:A:ILE:HD12	1:72:A:ALA:HA	4	0.17	0.08	0.13
(2,967)	1:54:A:ILE:HD13	1:72:A:ALA:HA	4	0.17	0.08	0.13
(2,1601)	1:15:A:PRO:HB3	1:16:A:SER:H	4	0.15	0.02	0.15
(2,2464)	1:28:A:LYS:HG3	1:28:A:LYS:HE3	4	0.15	0.01	0.15
(2,2464)	1:28:A:LYS:HG3	1:28:A:LYS:HE2	4	0.15	0.01	0.15
(2,2237)	1:74:A:SER:H	1:75:A:GLY:HA2	4	0.14	0.02	0.13
(2,536)	1:29:A:ALA:H	1:27:A:ARG:HA	4	0.14	0.04	0.11
(2,2259)	1:77:A:PRO:HD2	1:78:A:SER:H	4	0.13	0.02	0.14
(2,1604)	1:16:A:SER:H	1:17:A:ALA:H	4	0.13	0.03	0.12
(1,155)	1:66:A:GLN:HA	1:66:A:GLN:HG3	4	0.13	0.01	0.13
(2,434)	1:22:A:LEU:HD11	1:11:A:LEU:H	3	1.68	0.78	2.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,434)	1:22:A:LEU:HD12	1:11:A:LEU:H	3	1.68	0.78	2.18
(2,434)	1:22:A:LEU:HD13	1:11:A:LEU:H	3	1.68	0.78	2.18
(2,1856)	1:45:A:PHE:H	1:41:A:ASP:HB3	3	1.31	0.2	1.39
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG21	3	1.21	0.3	1.39
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG22	3	1.21	0.3	1.39
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG23	3	1.21	0.3	1.39
(2,2409)	1:0:A:THR:HG21	1:7:A:LEU:HB2	3	1.21	0.3	1.39
(2,2409)	1:0:A:THR:HG22	1:7:A:LEU:HB2	3	1.21	0.3	1.39
(2,2409)	1:0:A:THR:HG23	1:7:A:LEU:HB2	3	1.21	0.3	1.39
(2,433)	1:22:A:LEU:HD11	1:52:A:PHE:HA	3	1.21	0.06	1.24
(2,433)	1:22:A:LEU:HD12	1:52:A:PHE:HA	3	1.21	0.06	1.24
(2,433)	1:22:A:LEU:HD13	1:52:A:PHE:HA	3	1.21	0.06	1.24
(2,551)	1:24:A:LYS:HA	1:27:A:ARG:HD3	3	1.18	0.37	1.23
(2,2419)	1:24:A:LYS:HB3	1:24:A:LYS:HD3	3	1.03	0.01	1.03
(2,1869)	1:46:A:LYS:H	1:41:A:ASP:HB3	3	0.98	0.1	0.98
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD21	3	0.94	0.05	0.91
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD22	3	0.94	0.05	0.91
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD23	3	0.94	0.05	0.91
(1,73)	1:51:A:ALA:H	1:54:A:ILE:HB	3	0.88	0.4	1.15
(1,73)	1:37:A:LYS:HG3	1:34:A:HIS:H	3	0.88	0.4	1.15
(2,1100)	1:60:A:LYS:HD2	1:54:A:ILE:HD11	3	0.86	0.39	1.07
(2,1100)	1:60:A:LYS:HD2	1:54:A:ILE:HD12	3	0.86	0.39	1.07
(2,1100)	1:60:A:LYS:HD2	1:54:A:ILE:HD13	3	0.86	0.39	1.07
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD11	3	0.86	0.39	1.07
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD12	3	0.86	0.39	1.07
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD13	3	0.86	0.39	1.07
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG21	3	0.75	0.36	0.93
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG22	3	0.75	0.36	0.93
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG23	3	0.75	0.36	0.93
(2,642)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	3	0.7	0.47	0.59
(2,642)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	3	0.7	0.47	0.59
(2,642)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	3	0.7	0.47	0.59
(2,771)	1:41:A:ASP:HB3	1:44:A:LYS:HB2	3	0.69	0.16	0.6
(2,530)	1:27:A:ARG:HA	1:27:A:ARG:HG2	3	0.67	0.04	0.65
(2,1505)	1:18:A:ASN:H	1:20:A:GLN:HB2	3	0.66	0.1	0.68
(2,919)	1:52:A:PHE:HB2	1:8:A:TYR:HA	3	0.64	0.3	0.66
(2,693)	1:37:A:LYS:HD3	1:38:A:PRO:HD2	3	0.63	0.33	0.71
(2,693)	1:37:A:LYS:HD2	1:38:A:PRO:HD2	3	0.63	0.33	0.71
(2,1653)	1:21:A:GLU:H	1:20:A:GLN:HB2	3	0.59	0.04	0.6
(1,406)	1:37:A:LYS:HD3	1:38:A:PRO:HD2	3	0.59	0.33	0.67
(1,406)	1:37:A:LYS:HD2	1:38:A:PRO:HD2	3	0.59	0.33	0.67
(2,1630)	1:22:A:LEU:HD21	1:19:A:GLU:H	3	0.58	0.24	0.59

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1630)	1:22:A:LEU:HD22	1:19:A:GLU:H	3	0.58	0.24	0.59
(2,1630)	1:22:A:LEU:HD23	1:19:A:GLU:H	3	0.58	0.24	0.59
(2,457)	1:23:A:LYS:H	1:23:A:LYS:HD2	3	0.53	0.3	0.71
(2,457)	1:23:A:LYS:H	1:23:A:LYS:HD3	3	0.53	0.3	0.71
(2,726)	1:33:A:TYR:HD1	1:41:A:ASP:HB2	3	0.53	0.1	0.48
(2,726)	1:33:A:TYR:HD2	1:41:A:ASP:HB2	3	0.53	0.1	0.48
(2,240)	1:8:A:TYR:HB3	1:15:A:PRO:HA	3	0.46	0.13	0.42
(2,1847)	1:41:A:ASP:HB3	1:44:A:LYS:H	3	0.45	0.04	0.45
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB1	3	0.45	0.06	0.42
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB2	3	0.45	0.06	0.42
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB3	3	0.45	0.06	0.42
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB1	3	0.45	0.06	0.42
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB2	3	0.45	0.06	0.42
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB3	3	0.45	0.06	0.42
(2,1805)	1:39:A:THR:H	1:37:A:LYS:HD2	3	0.44	0.11	0.49
(2,1805)	1:39:A:THR:H	1:37:A:LYS:HD3	3	0.44	0.11	0.49
(1,233)	1:10:A:LEU:HD11	1:10:A:LEU:HA	3	0.43	0.17	0.55
(1,233)	1:10:A:LEU:HD12	1:10:A:LEU:HA	3	0.43	0.17	0.55
(1,233)	1:10:A:LEU:HD13	1:10:A:LEU:HA	3	0.43	0.17	0.55
(1,233)	1:22:A:LEU:HD21	1:19:A:GLU:HA	3	0.43	0.17	0.55
(1,233)	1:22:A:LEU:HD22	1:19:A:GLU:HA	3	0.43	0.17	0.55
(1,233)	1:22:A:LEU:HD23	1:19:A:GLU:HA	3	0.43	0.17	0.55
(2,2261)	1:77:A:PRO:HA	1:78:A:SER:H	3	0.43	0.24	0.33
(2,1081)	1:59:A:GLN:HA	1:59:A:GLN:HG2	3	0.39	0.02	0.39
(2,1340)	1:77:A:PRO:HA	1:78:A:SER:H	3	0.38	0.24	0.28
(1,463)	1:53:A:GLU:H	1:55:A:LEU:HB2	3	0.37	0.13	0.37
(1,461)	1:8:A:TYR:HD1	1:15:A:PRO:HD3	3	0.35	0.08	0.39
(1,461)	1:8:A:TYR:HD2	1:15:A:PRO:HD3	3	0.35	0.08	0.39
(2,280)	1:14:A:SER:HB2	1:16:A:SER:H	3	0.34	0.21	0.23
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE1	3	0.31	0.12	0.23
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE2	3	0.31	0.12	0.23
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE1	3	0.31	0.12	0.23
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE2	3	0.31	0.12	0.23
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE1	3	0.31	0.12	0.23
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE2	3	0.31	0.12	0.23
(2,1820)	1:41:A:ASP:H	1:41:A:ASP:HB2	3	0.3	0.01	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD11	3	0.3	0.0	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD12	3	0.3	0.0	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD13	3	0.3	0.0	0.3
(2,1602)	1:15:A:PRO:HB2	1:16:A:SER:H	3	0.28	0.18	0.15
(2,1673)	1:22:A:LEU:HD21	1:23:A:LYS:H	3	0.28	0.08	0.31
(2,1673)	1:22:A:LEU:HD22	1:23:A:LYS:H	3	0.28	0.08	0.31

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1673)	1:22:A:LEU:HD23	1:23:A:LYS:H	3	0.28	0.08	0.31
(2,1422)	1:27:A:ARG:H	1:23:A:LYS:HB3	3	0.27	0.08	0.23
(2,1719)	1:27:A:ARG:H	1:23:A:LYS:HB3	3	0.27	0.08	0.23
(2,548)	1:27:A:ARG:HB3	1:28:A:LYS:H	3	0.26	0.01	0.25
(2,1413)	1:0:A:THR:HB	1:0:A:THR:H	3	0.25	0.06	0.23
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD11	3	0.25	0.13	0.19
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD12	3	0.25	0.13	0.19
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD13	3	0.25	0.13	0.19
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD11	3	0.24	0.09	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD12	3	0.24	0.09	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD13	3	0.24	0.09	0.31
(2,1521)	1:6:A:LYS:HA	1:10:A:LEU:H	3	0.22	0.05	0.21
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG21	3	0.22	0.13	0.14
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG22	3	0.22	0.13	0.14
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG23	3	0.22	0.13	0.14
(2,626)	1:31:A:LEU:HA	1:34:A:HIS:HB3	3	0.21	0.07	0.18
(2,472)	1:24:A:LYS:HE2	1:21:A:GLU:HA	3	0.19	0.02	0.18
(2,542)	1:27:A:ARG:HB3	1:28:A:LYS:H	3	0.18	0.01	0.18
(2,351)	1:24:A:LYS:HE2	1:21:A:GLU:HA	3	0.18	0.03	0.17
(1,454)	1:72:A:ALA:H	1:64:A:TYR:H	3	0.17	0.02	0.17
(2,331)	1:26:A:TYR:HE1	1:23:A:LYS:HA	3	0.17	0.05	0.18
(2,331)	1:26:A:TYR:HE2	1:23:A:LYS:HA	3	0.17	0.05	0.18
(2,368)	1:21:A:GLU:H	1:20:A:GLN:HG2	3	0.17	0.04	0.17
(2,368)	1:21:A:GLU:H	1:20:A:GLN:HG3	3	0.17	0.04	0.17
(2,1568)	1:8:A:TYR:HB2	1:13:A:VAL:H	3	0.17	0.03	0.15
(2,1107)	1:50:A:GLU:HA	1:54:A:ILE:HG13	3	0.17	0.03	0.18
(2,2)	1:0:A:THR:HA	1:1:A:SER:H	3	0.16	0.03	0.15
(2,2085)	1:64:A:TYR:HB3	1:63:A:ILE:H	3	0.16	0.06	0.14
(1,80)	1:28:A:LYS:HA	1:28:A:LYS:HG3	3	0.16	0.02	0.16
(1,80)	1:46:A:LYS:HA	1:46:A:LYS:HG3	3	0.16	0.02	0.16
(1,435)	1:47:A:GLU:HG3	1:47:A:GLU:HA	3	0.16	0.03	0.16
(2,277)	1:16:A:SER:HA	1:17:A:ALA:H	3	0.16	0.05	0.15
(2,2411)	1:27:A:ARG:H	1:27:A:ARG:HD3	3	0.16	0.02	0.17
(2,2411)	1:27:A:ARG:H	1:27:A:ARG:HD2	3	0.16	0.02	0.17
(2,2029)	1:60:A:LYS:HE2	1:60:A:LYS:H	3	0.16	0.02	0.16
(2,2029)	1:60:A:LYS:H	1:60:A:LYS:HE3	3	0.16	0.02	0.16
(2,2250)	1:76:A:GLY:HA2	1:76:A:GLY:H	3	0.15	0.03	0.14
(2,1829)	1:41:A:ASP:HB2	1:42:A:THR:H	3	0.14	0.01	0.15
(2,2086)	1:64:A:TYR:HB2	1:63:A:ILE:H	3	0.14	0.0	0.14
(2,2013)	1:57:A:ASP:H	1:61:A:ARG:H	3	0.14	0.03	0.13
(2,271)	1:70:A:GLU:HB3	1:71:A:ALA:H	3	0.13	0.02	0.14
(2,754)	1:70:A:GLU:HG3	1:73:A:ARG:HD2	3	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,557)	1:73:A:ARG:HG3	1:73:A:ARG:HA	3	0.12	0.01	0.12
(1,114)	1:24:A:LYS:HA	1:25:A:GLY:H	3	0.11	0.0	0.11
(1,215)	1:28:A:LYS:HA	1:28:A:LYS:H	3	0.1	0.0	0.1
(2,750)	1:43:A:GLU:HG2	1:44:A:LYS:HG2	2	1.81	0.0	1.81
(2,218)	1:22:A:LEU:HD11	1:13:A:VAL:HA	2	1.62	0.03	1.62
(2,218)	1:22:A:LEU:HD12	1:13:A:VAL:HA	2	1.62	0.03	1.62
(2,218)	1:22:A:LEU:HD13	1:13:A:VAL:HA	2	1.62	0.03	1.62
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD11	2	1.37	0.0	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD12	2	1.37	0.0	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD13	2	1.37	0.0	1.37
(2,1578)	1:22:A:LEU:HD11	1:14:A:SER:H	2	0.98	0.07	0.98
(2,1578)	1:22:A:LEU:HD12	1:14:A:SER:H	2	0.98	0.07	0.98
(2,1578)	1:22:A:LEU:HD13	1:14:A:SER:H	2	0.98	0.07	0.98
(2,1440)	1:65:A:ASP:HA	1:3:A:LYS:H	2	0.97	0.1	0.97
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD11	2	0.96	0.0	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD12	2	0.96	0.0	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD13	2	0.96	0.0	0.96
(2,1635)	1:18:A:ASN:HB3	1:19:A:GLU:H	2	0.92	0.03	0.92
(1,268)	1:51:A:ALA:HB1	1:48:A:ILE:HG21	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB1	1:48:A:ILE:HG22	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB1	1:48:A:ILE:HG23	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB2	1:48:A:ILE:HG21	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB2	1:48:A:ILE:HG22	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB2	1:48:A:ILE:HG23	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB3	1:48:A:ILE:HG21	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB3	1:48:A:ILE:HG22	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB3	1:48:A:ILE:HG23	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB1	1:11:A:LEU:HD21	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB1	1:11:A:LEU:HD22	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB1	1:11:A:LEU:HD23	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB2	1:11:A:LEU:HD21	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB2	1:11:A:LEU:HD22	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB2	1:11:A:LEU:HD23	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB3	1:11:A:LEU:HD21	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB3	1:11:A:LEU:HD22	2	0.87	0.17	0.87
(1,268)	1:51:A:ALA:HB3	1:11:A:LEU:HD23	2	0.87	0.17	0.87
(2,324)	1:22:A:LEU:HD21	1:19:A:GLU:HA	2	0.87	0.17	0.87
(2,324)	1:22:A:LEU:HD22	1:19:A:GLU:HA	2	0.87	0.17	0.87
(2,324)	1:22:A:LEU:HD23	1:19:A:GLU:HA	2	0.87	0.17	0.87
(2,1507)	1:9:A:ASP:HB3	1:9:A:ASP:H	2	0.8	0.0	0.8
(2,2027)	1:60:A:LYS:H	1:59:A:GLN:HB3	2	0.75	0.05	0.75
(2,2027)	1:60:A:LYS:H	1:59:A:GLN:HB2	2	0.75	0.05	0.75

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1846)	1:43:A:GLU:HG2	1:44:A:LYS:H	2	0.69	0.02	0.69
(2,1191)	1:65:A:ASP:HA	1:3:A:LYS:H	2	0.67	0.1	0.67
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG21	2	0.64	0.02	0.64
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG22	2	0.64	0.02	0.64
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG23	2	0.64	0.02	0.64
(2,1453)	1:4:A:GLU:H	1:6:A:LYS:HB3	2	0.64	0.2	0.64
(2,1938)	1:53:A:GLU:H	1:55:A:LEU:HB3	2	0.64	0.06	0.64
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD11	2	0.62	0.27	0.62
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD12	2	0.62	0.27	0.62
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD13	2	0.62	0.27	0.62
(2,1388)	1:0:A:THR:HB	1:-1:A:MET:HA	2	0.62	0.22	0.62
(2,901)	1:55:A:LEU:HB3	1:52:A:PHE:HA	2	0.61	0.04	0.61
(2,13)	1:2:A:VAL:HA	1:4:A:GLU:HG2	2	0.6	0.02	0.6
(1,20)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	2	0.6	0.48	0.6
(1,314)	1:60:A:LYS:HE3	1:57:A:ASP:H	2	0.6	0.02	0.6
(2,69)	1:6:A:LYS:HA	1:9:A:ASP:HB3	2	0.59	0.25	0.59
(2,2264)	1:77:A:PRO:HB2	1:79:A:PHE:H	2	0.54	0.34	0.54
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB1	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB2	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB3	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB1	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB2	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB3	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB1	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB2	2	0.49	0.1	0.49
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB3	2	0.49	0.1	0.49
(2,1262)	1:43:A:GLU:HG3	1:47:A:GLU:H	2	0.49	0.04	0.49
(2,2181)	1:70:A:GLU:H	1:70:A:GLU:HG3	2	0.48	0.3	0.48
(2,1454)	1:3:A:LYS:HB3	1:4:A:GLU:H	2	0.48	0.17	0.48
(2,2275)	1:78:A:SER:HA	1:80:A:GLY:H	2	0.45	0.13	0.45
(2,685)	1:39:A:THR:HG21	1:38:A:PRO:HA	2	0.44	0.04	0.44
(2,685)	1:39:A:THR:HG22	1:38:A:PRO:HA	2	0.44	0.04	0.44
(2,685)	1:39:A:THR:HG23	1:38:A:PRO:HA	2	0.44	0.04	0.44
(2,323)	1:18:A:ASN:HB3	1:19:A:GLU:H	2	0.44	0.03	0.44
(2,2403)	1:6:A:LYS:HB2	1:7:A:LEU:H	2	0.4	0.04	0.4
(2,2403)	1:6:A:LYS:HB3	1:7:A:LEU:H	2	0.4	0.04	0.4
(2,143)	1:9:A:ASP:HB2	1:9:A:ASP:HA	2	0.39	0.0	0.39
(2,2219)	1:73:A:ARG:H	1:69:A:LEU:HG	2	0.39	0.22	0.39
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD21	2	0.38	0.03	0.38
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD22	2	0.38	0.03	0.38
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD23	2	0.38	0.03	0.38
(2,1110)	1:55:A:LEU:HD11	1:61:A:ARG:HA	2	0.37	0.22	0.37

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1110)	1:55:A:LEU:HD12	1:61:A:ARG:HA	2	0.37	0.22	0.37
(2,1110)	1:55:A:LEU:HD13	1:61:A:ARG:HA	2	0.37	0.22	0.37
(2,1110)	1:55:A:LEU:HD21	1:61:A:ARG:HA	2	0.37	0.22	0.37
(2,1110)	1:55:A:LEU:HD22	1:61:A:ARG:HA	2	0.37	0.22	0.37
(2,1110)	1:55:A:LEU:HD23	1:61:A:ARG:HA	2	0.37	0.22	0.37
(2,1103)	1:54:A:ILE:HG12	1:60:A:LYS:HD3	2	0.36	0.06	0.36
(2,1456)	1:4:A:GLU:H	1:3:A:LYS:HG2	2	0.36	0.1	0.36
(2,571)	1:28:A:LYS:HA	1:28:A:LYS:HG3	2	0.35	0.01	0.35
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD11	2	0.33	0.2	0.33
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD12	2	0.33	0.2	0.33
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD13	2	0.33	0.2	0.33
(2,747)	1:47:A:GLU:HG2	1:48:A:ILE:HB	2	0.33	0.14	0.33
(2,501)	1:25:A:GLY:HA2	1:24:A:LYS:HD3	2	0.3	0.18	0.3
(2,1838)	1:43:A:GLU:H	1:43:A:GLU:HG2	2	0.3	0.1	0.3
(1,81)	1:60:A:LYS:HA	1:60:A:LYS:HG3	2	0.3	0.07	0.3
(2,1119)	1:73:A:ARG:HD2	1:69:A:LEU:HG	2	0.3	0.11	0.3
(2,1919)	1:34:A:HIS:H	1:36:A:ASP:HB3	2	0.3	0.07	0.3
(2,190)	1:11:A:LEU:HD11	1:11:A:LEU:HA	2	0.27	0.12	0.27
(2,190)	1:11:A:LEU:HD12	1:11:A:LEU:HA	2	0.27	0.12	0.27
(2,190)	1:11:A:LEU:HD13	1:11:A:LEU:HA	2	0.27	0.12	0.27
(1,481)	1:-1:A:MET:HA	1:0:A:THR:H	2	0.26	0.11	0.26
(2,1082)	1:59:A:GLN:HA	1:59:A:GLN:HG3	2	0.26	0.04	0.26
(2,1677)	1:23:A:LYS:H	1:23:A:LYS:HE3	2	0.26	0.15	0.26
(2,1677)	1:23:A:LYS:H	1:23:A:LYS:HE2	2	0.26	0.15	0.26
(2,2383)	1:11:A:LEU:HB2	1:52:A:PHE:HE1	2	0.26	0.12	0.26
(2,2383)	1:11:A:LEU:HB2	1:52:A:PHE:HE2	2	0.26	0.12	0.26
(2,1013)	1:61:A:ARG:HD3	1:55:A:LEU:HA	2	0.25	0.13	0.25
(2,1803)	1:39:A:THR:HG21	1:39:A:THR:H	2	0.25	0.03	0.25
(2,1803)	1:39:A:THR:HG22	1:39:A:THR:H	2	0.25	0.03	0.25
(2,1803)	1:39:A:THR:HG23	1:39:A:THR:H	2	0.25	0.03	0.25
(2,1828)	1:43:A:GLU:HG2	1:42:A:THR:H	2	0.24	0.03	0.24
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG11	2	0.23	0.1	0.23
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG12	2	0.23	0.1	0.23
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG13	2	0.23	0.1	0.23
(2,1526)	1:9:A:ASP:HB3	1:10:A:LEU:H	2	0.23	0.0	0.23
(1,11)	1:38:A:PRO:HB3	1:38:A:PRO:HG2	2	0.22	0.01	0.22
(1,11)	1:58:A:PRO:HB3	1:58:A:PRO:HG2	2	0.22	0.01	0.22
(2,1539)	1:9:A:ASP:HB3	1:11:A:LEU:H	2	0.22	0.01	0.22
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD21	2	0.2	0.02	0.2
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD22	2	0.2	0.02	0.2
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD23	2	0.2	0.02	0.2
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD21	2	0.2	0.02	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD22	2	0.2	0.02	0.2
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD23	2	0.2	0.02	0.2
(2,2039)	1:55:A:LEU:HD11	1:61:A:ARG:H	2	0.2	0.01	0.2
(2,2039)	1:55:A:LEU:HD12	1:61:A:ARG:H	2	0.2	0.01	0.2
(2,2039)	1:55:A:LEU:HD13	1:61:A:ARG:H	2	0.2	0.01	0.2
(2,2039)	1:55:A:LEU:HD21	1:61:A:ARG:H	2	0.2	0.01	0.2
(2,2039)	1:55:A:LEU:HD22	1:61:A:ARG:H	2	0.2	0.01	0.2
(2,2039)	1:55:A:LEU:HD23	1:61:A:ARG:H	2	0.2	0.01	0.2
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD11	2	0.19	0.08	0.19
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD12	2	0.19	0.08	0.19
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD13	2	0.19	0.08	0.19
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD11	2	0.19	0.08	0.19
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD12	2	0.19	0.08	0.19
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD13	2	0.19	0.08	0.19
(1,98)	1:14:A:SER:H	1:21:A:GLU:HB2	2	0.18	0.08	0.18
(2,8)	1:1:A:SER:H	1:1:A:SER:HB2	2	0.18	0.03	0.18
(2,1692)	1:25:A:GLY:H	1:24:A:LYS:HD2	2	0.18	0.04	0.18
(2,734)	1:46:A:LYS:H	1:42:A:THR:HA	2	0.17	0.06	0.17
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD11	2	0.16	0.04	0.16
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD12	2	0.16	0.04	0.16
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD13	2	0.16	0.04	0.16
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD11	2	0.16	0.04	0.16
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD12	2	0.16	0.04	0.16
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD13	2	0.16	0.04	0.16
(2,429)	1:22:A:LEU:HD11	1:22:A:LEU:HB3	2	0.16	0.01	0.16
(2,429)	1:22:A:LEU:HD12	1:22:A:LEU:HB3	2	0.16	0.01	0.16
(2,429)	1:22:A:LEU:HD13	1:22:A:LEU:HB3	2	0.16	0.01	0.16
(2,1217)	1:63:A:ILE:HG21	1:67:A:TYR:HB3	2	0.16	0.06	0.16
(2,1217)	1:63:A:ILE:HG22	1:67:A:TYR:HB3	2	0.16	0.06	0.16
(2,1217)	1:63:A:ILE:HG23	1:67:A:TYR:HB3	2	0.16	0.06	0.16
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD11	2	0.16	0.04	0.16
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD12	2	0.16	0.04	0.16
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD13	2	0.16	0.04	0.16
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD21	2	0.16	0.04	0.16
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD22	2	0.16	0.04	0.16
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD23	2	0.16	0.04	0.16
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG21	2	0.16	0.05	0.16
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG22	2	0.16	0.05	0.16
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG23	2	0.16	0.05	0.16
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG21	2	0.16	0.05	0.16
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG22	2	0.16	0.05	0.16
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG23	2	0.16	0.05	0.16

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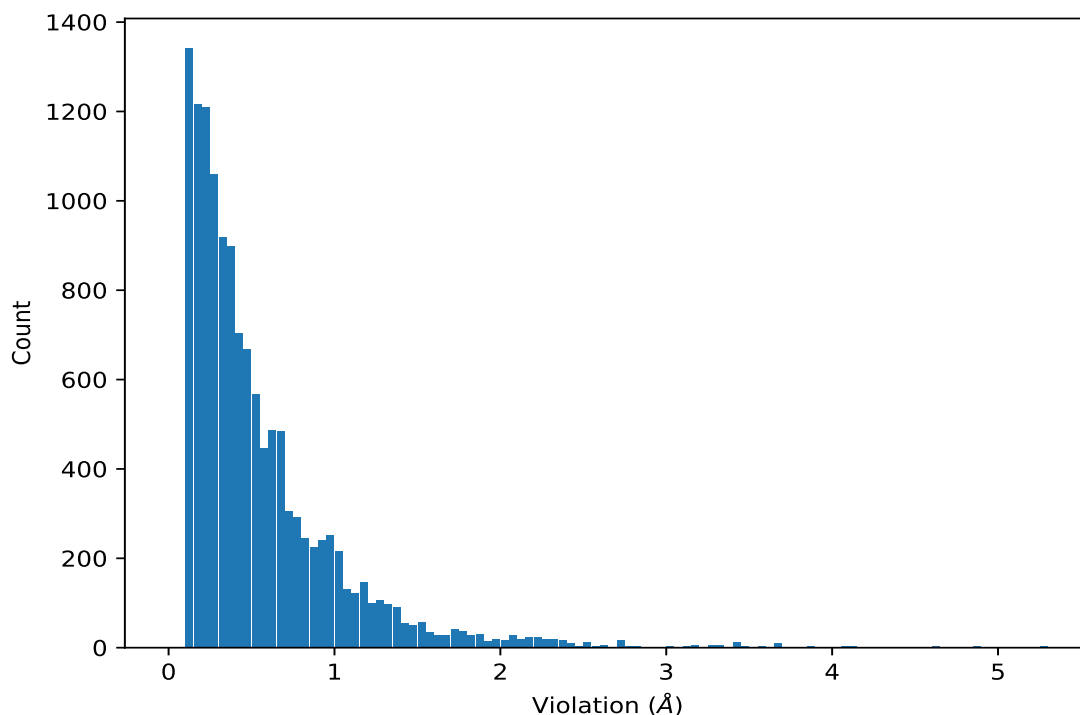
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1451)	1:4:A:GLU:HG3	1:4:A:GLU:H	2	0.16	0.02	0.16
(2,1012)	1:61:A:ARG:HB2	1:55:A:LEU:HA	2	0.16	0.05	0.16
(2,1923)	1:55:A:LEU:HD21	1:52:A:PHE:H	2	0.16	0.01	0.16
(2,1923)	1:55:A:LEU:HD22	1:52:A:PHE:H	2	0.16	0.01	0.16
(2,1923)	1:55:A:LEU:HD23	1:52:A:PHE:H	2	0.16	0.01	0.16
(2,2078)	1:72:A:ALA:HB1	1:63:A:ILE:H	2	0.15	0.02	0.15
(2,2078)	1:72:A:ALA:HB2	1:63:A:ILE:H	2	0.15	0.02	0.15
(2,2078)	1:72:A:ALA:HB3	1:63:A:ILE:H	2	0.15	0.02	0.15
(2,931)	1:53:A:GLU:HA	1:52:A:PHE:HB3	2	0.15	0.0	0.15
(2,2068)	1:65:A:ASP:HB3	1:62:A:GLU:H	2	0.15	0.02	0.15
(1,86)	1:62:A:GLU:H	1:60:A:LYS:H	2	0.14	0.02	0.14
(2,1967)	1:55:A:LEU:H	1:55:A:LEU:HB3	2	0.14	0.0	0.14
(2,1260)	1:43:A:GLU:HA	1:43:A:GLU:HG3	2	0.13	0.0	0.13
(2,2167)	1:64:A:TYR:HB2	1:69:A:LEU:H	2	0.13	0.01	0.13
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB1	2	0.12	0.02	0.12
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB2	2	0.12	0.02	0.12
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB3	2	0.12	0.02	0.12
(2,1352)	1:77:A:PRO:HB3	1:78:A:SER:H	2	0.12	0.0	0.12
(2,22)	1:2:A:VAL:HA	1:3:A:LYS:H	2	0.12	0.0	0.12
(2,1809)	1:39:A:THR:H	1:38:A:PRO:HD3	2	0.12	0.0	0.12
(2,224)	1:13:A:VAL:HA	1:14:A:SER:H	2	0.11	0.0	0.11
(2,1729)	1:28:A:LYS:HB3	1:28:A:LYS:H	2	0.11	0.0	0.11
(2,1729)	1:28:A:LYS:HB2	1:28:A:LYS:H	2	0.11	0.0	0.11

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	12	5.27
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	12	5.27
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	12	5.27
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	16	4.85
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	16	4.85
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	16	4.85
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE3	11	4.64
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE3	11	4.64
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE3	11	4.64
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	5	4.14
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	5	4.14
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	5	4.14
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD3	12	4.09
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD3	12	4.09
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD3	12	4.09
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	13	3.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	13	3.89
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	13	3.89
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	4	3.87
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	11	3.66
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	11	3.66
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	11	3.66
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	11	3.66
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	11	3.66
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	11	3.66
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	11	3.66
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	11	3.66
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	11	3.66
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	8	3.56
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	8	3.56
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	8	3.56
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	7	3.47
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD2	16	3.46
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD2	16	3.46
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD2	16	3.46
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD3	13	3.42
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD3	13	3.42
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD3	13	3.42
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	19	3.4
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	19	3.4
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	19	3.4
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	19	3.4
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	19	3.4
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	19	3.4
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	19	3.4
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	19	3.4
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	19	3.4
(2,1188)	1:2:A:VAL:HB	1:65:A:ASP:HA	19	3.34
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	7	3.33
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	7	3.33
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	7	3.33
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	14	3.31
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	1	3.29
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	1	3.29
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	1	3.29
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD3	1	3.27
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD3	1	3.27
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD3	1	3.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	7	3.18
(2,641)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	7	3.18
(2,641)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	7	3.18
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	11	3.15
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	11	3.15
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	11	3.15
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	3	3.13
(2,2348)	1:45:A:PHE:HD1	1:34:A:HIS:HD2	13	3.1
(2,2348)	1:45:A:PHE:HD2	1:34:A:HIS:HD2	13	3.1
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	14	3.01
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	10	3.01
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	10	3.01
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	10	3.01
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	6	2.97
(2,27)	1:2:A:VAL:HB	1:65:A:ASP:HA	19	2.89
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	6	2.86
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	10	2.82
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	10	2.82
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	10	2.82
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	19	2.76
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	19	2.76
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	19	2.76
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	20	2.74
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	1	2.73
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	1	2.73
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	1	2.73
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	13	2.71
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	13	2.71
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	13	2.71
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	13	2.71
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	13	2.71
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	13	2.71
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	13	2.71
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	13	2.71
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	13	2.71
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	2	2.7
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	2	2.7
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	2	2.7
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	16	2.66
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	16	2.66
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	11	2.64
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	11	2.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	11	2.64
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	7	2.62
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	12	2.62
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	12	2.56
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	10	2.55
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	10	2.55
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	12	2.54
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	12	2.54
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	1	2.53
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	1	2.53
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	1	2.53
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	1	2.53
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	1	2.53
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	1	2.53
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	1	2.53
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	1	2.53
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	1	2.53
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	4	2.51
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	19	2.49
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	19	2.49
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	19	2.49
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	3	2.47
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD2	11	2.44
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD2	11	2.44
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD2	11	2.44
(2,2348)	1:45:A:PHE:HD1	1:34:A:HIS:HD2	19	2.44
(2,2348)	1:45:A:PHE:HD2	1:34:A:HIS:HD2	19	2.44
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	3	2.44
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	8	2.43
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	12	2.43
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	17	2.4
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	17	2.4
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	17	2.4
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	15	2.39
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	15	2.39
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	15	2.39
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD1	12	2.38
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD2	12	2.38
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD1	12	2.38
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD2	12	2.38
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	5	2.38
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	5	2.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	5	2.38
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	5	2.38
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	5	2.38
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	5	2.38
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	5	2.38
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	5	2.38
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	5	2.38
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	9	2.32
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	9	2.32
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	9	2.32
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	13	2.32
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	13	2.32
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	13	2.32
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	4	2.31
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	1	2.3
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	1	2.3
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	1	2.3
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	10	2.3
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	10	2.3
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	10	2.3
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	10	2.3
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	10	2.3
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	10	2.3
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	10	2.3
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	10	2.3
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	10	2.3
(2,434)	1:22:A:LEU:HD11	1:11:A:LEU:H	8	2.29
(2,434)	1:22:A:LEU:HD12	1:11:A:LEU:H	8	2.29
(2,434)	1:22:A:LEU:HD13	1:11:A:LEU:H	8	2.29
(2,473)	1:24:A:LYS:HA	1:27:A:ARG:HD3	8	2.28
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	14	2.28
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	14	2.28
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	14	2.28
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	3	2.27
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	12	2.26
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	12	2.26
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	12	2.26
(2,766)	1:69:A:LEU:HD21	1:73:A:ARG:HA	7	2.26
(2,766)	1:69:A:LEU:HD22	1:73:A:ARG:HA	7	2.26
(2,766)	1:69:A:LEU:HD23	1:73:A:ARG:HA	7	2.26
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	10	2.25
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	10	2.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	2	2.25
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	2	2.25
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	13	2.24
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	13	2.24
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	2	2.23
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	16	2.23
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	5	2.23
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	5	2.23
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	5	2.23
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	13	2.22
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	13	2.22
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	13	2.22
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	19	2.22
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	19	2.22
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	19	2.22
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	18	2.22
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	18	2.22
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	18	2.22
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	7	2.22
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	14	2.21
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	14	2.21
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	14	2.21
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD1	16	2.2
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD2	16	2.2
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD1	16	2.2
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD2	16	2.2
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	7	2.18
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	7	2.18
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	7	2.18
(2,434)	1:22:A:LEU:HD11	1:11:A:LEU:H	9	2.18
(2,434)	1:22:A:LEU:HD12	1:11:A:LEU:H	9	2.18
(2,434)	1:22:A:LEU:HD13	1:11:A:LEU:H	9	2.18
(2,553)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	7	2.17
(2,553)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	7	2.17
(2,553)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	7	2.17
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	16	2.16
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	9	2.16
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	9	2.16
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	9	2.16
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	5	2.16
(2,1307)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	7	2.15
(2,1307)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	7	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1307)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	7	2.15
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	20	2.15
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	20	2.15
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	20	2.15
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	12	2.15
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	12	2.15
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	12	2.15
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	5	2.15
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	20	2.14
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	2	2.14
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	2	2.14
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	5	2.14
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	5	2.14
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	5	2.14
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	1	2.13
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	1	2.13
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	1	2.13
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	15	2.13
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	10	2.12
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	10	2.12
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	10	2.12
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	8	2.12
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	18	2.12
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	17	2.1
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	17	2.1
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	17	2.1
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	12	2.1
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	2	2.09
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	3	2.08
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	3	2.08
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	3	2.08
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	11	2.07
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	16	2.07
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	16	2.07
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	16	2.07
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	13	2.07
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	13	2.07
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	13	2.07
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	19	2.06
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	19	2.06
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	19	2.06
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	6	2.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	6	2.06
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	6	2.06
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	12	2.06
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	12	2.06
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	12	2.06
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	12	2.06
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	12	2.06
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	12	2.06
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	12	2.06
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	12	2.06
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	12	2.06
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	1	2.05
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	1	2.05
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	4	2.04
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	4	2.03
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	16	2.02
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	16	2.02
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	16	2.02
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	8	2.01
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	8	2.01
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	8	2.01
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	9	2.01
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	18	2.0
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	10	2.0
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	10	2.0
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	10	2.0
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	11	2.0
(2,641)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	5	2.0
(2,641)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	5	2.0
(2,641)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	5	2.0
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	7	1.99
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	7	1.99
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	7	1.99
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	9	1.99
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	19	1.98
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	19	1.98
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	2	1.98
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	2	1.98
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	2	1.98
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	17	1.97
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	14	1.96
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	2	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	2	1.96
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	2	1.96
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	14	1.96
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	6	1.95
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	6	1.95
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	5	1.95
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	8	1.93
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	5	1.93
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	5	1.93
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	5	1.93
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	17	1.93
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	17	1.93
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	17	1.93
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	5	1.92
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	6	1.91
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	19	1.9
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	2	1.9
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	2	1.9
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	2	1.9
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	12	1.9
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	1	1.89
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	1	1.89
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	1	1.89
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	12	1.89
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	12	1.89
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	12	1.89
(2,473)	1:24:A:LYS:HA	1:27:A:ARG:HD3	14	1.89
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	1	1.89
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	1	1.89
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	1	1.89
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	11	1.89
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	11	1.89
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	11	1.89
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	19	1.89
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	19	1.89
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	19	1.89
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	2	1.89
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	2	1.89
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	6	1.88
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	6	1.88
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	6	1.88
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	16	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	16	1.87
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	16	1.87
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	7	1.86
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	11	1.86
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	11	1.86
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	11	1.86
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	8	1.86
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	20	1.85
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	13	1.84
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	12	1.83
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	1	1.83
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	20	1.83
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	20	1.83
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	20	1.83
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	17	1.83
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	5	1.82
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	5	1.82
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	5	1.82
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD11	10	1.82
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD12	10	1.82
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD13	10	1.82
(2,1076)	1:63:A:ILE:HG12	1:59:A:GLN:HG3	6	1.81
(2,906)	1:8:A:TYR:HB2	1:52:A:PHE:HA	12	1.81
(2,750)	1:43:A:GLU:HG2	1:44:A:LYS:HG2	2	1.81
(2,750)	1:43:A:GLU:HG2	1:44:A:LYS:HG2	11	1.81
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	6	1.81
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	6	1.81
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD21	7	1.81
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD22	7	1.81
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD23	7	1.81
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	7	1.81
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	7	1.81
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	7	1.81
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	12	1.8
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	12	1.8
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	12	1.8
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	16	1.8
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	15	1.79
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	17	1.79
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	17	1.79
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	17	1.79
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	8	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	8	1.79
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	8	1.79
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	1	1.79
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	1	1.79
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	1	1.79
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	1	1.79
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	20	1.78
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	5	1.78
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	5	1.78
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	5	1.78
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	20	1.78
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	20	1.78
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	20	1.78
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	17	1.78
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	17	1.78
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	17	1.78
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	4	1.77
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	4	1.77
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	4	1.77
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	10	1.77
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	10	1.77
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	10	1.77
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD21	7	1.76
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD22	7	1.76
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD23	7	1.76
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	18	1.76
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	1	1.75
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	13	1.75
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	3	1.75
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	14	1.75
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	14	1.75
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	6	1.74
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	6	1.74
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	6	1.74
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	10	1.74
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	17	1.74
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	1	1.73
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	4	1.73
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	11	1.73
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	11	1.73
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	11	1.73
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	20	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	20	1.73
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	20	1.73
(2,694)	1:37:A:LYS:HD3	1:38:A:PRO:HD3	6	1.73
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	4	1.73
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	4	1.73
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	4	1.73
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	2	1.72
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	2	1.72
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	16	1.72
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	16	1.72
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	16	1.72
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	19	1.72
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	18	1.72
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	18	1.72
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	18	1.72
(2,128)	1:13:A:VAL:HG11	1:8:A:TYR:HB2	20	1.72
(2,128)	1:13:A:VAL:HG12	1:8:A:TYR:HB2	20	1.72
(2,128)	1:13:A:VAL:HG13	1:8:A:TYR:HB2	20	1.72
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	2	1.71
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	2	1.71
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	2	1.71
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	14	1.71
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	14	1.71
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	14	1.71
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	6	1.71
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	17	1.7
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	17	1.7
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	17	1.7
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	16	1.7
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	16	1.7
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	19	1.69
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	10	1.69
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	10	1.69
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	10	1.69
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	13	1.69
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	13	1.69
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	13	1.69
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	18	1.69
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	18	1.69
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	18	1.69
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	17	1.68
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	17	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	17	1.68
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	5	1.67
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	7	1.66
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	7	1.66
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	7	1.66
(2,218)	1:22:A:LEU:HD11	1:13:A:VAL:HA	8	1.66
(2,218)	1:22:A:LEU:HD12	1:13:A:VAL:HA	8	1.66
(2,218)	1:22:A:LEU:HD13	1:13:A:VAL:HA	8	1.66
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	1	1.66
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	8	1.66
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	16	1.66
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	4	1.66
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	4	1.66
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	4	1.66
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	20	1.65
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	20	1.65
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	20	1.65
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	17	1.64
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	18	1.64
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	18	1.64
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	18	1.64
(1,413)	1:4:A:GLU:HB2	1:6:A:LYS:H	7	1.64
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	3	1.63
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	3	1.63
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	3	1.63
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	13	1.62
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	13	1.62
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	13	1.62
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	10	1.61
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	8	1.61
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	1	1.61
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	1	1.61
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	1	1.61
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	10	1.61
(2,551)	1:24:A:LYS:HA	1:27:A:ARG:HD3	8	1.61
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	19	1.61
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	18	1.6
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	5	1.6
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	5	1.6
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	5	1.6
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	5	1.6
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	5	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	5	1.6
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	6	1.6
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	6	1.6
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	6	1.6
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	7	1.59
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	11	1.59
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	11	1.59
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	11	1.59
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	16	1.59
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	1	1.59
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	3	1.59
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	3	1.59
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	3	1.59
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	13	1.59
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	13	1.59
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	13	1.59
(2,218)	1:22:A:LEU:HD11	1:13:A:VAL:HA	9	1.59
(2,218)	1:22:A:LEU:HD12	1:13:A:VAL:HA	9	1.59
(2,218)	1:22:A:LEU:HD13	1:13:A:VAL:HA	9	1.59
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	19	1.59
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	9	1.58
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	9	1.58
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	9	1.58
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	12	1.57
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD1	19	1.57
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD2	19	1.57
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD1	19	1.57
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD2	19	1.57
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	2	1.57
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	14	1.56
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	9	1.56
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	9	1.56
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	9	1.56
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB2	1	1.56
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	9	1.56
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	9	1.56
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	6	1.56
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	19	1.55
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	5	1.55
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	16	1.54
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	16	1.54
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	16	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	17	1.54
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	13	1.53
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	3	1.53
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	12	1.53
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	1	1.53
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	8	1.53
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	8	1.53
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	8	1.53
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	8	1.53
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	8	1.53
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	8	1.53
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	8	1.53
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	8	1.53
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	8	1.53
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	2	1.53
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	6	1.52
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	7	1.52
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	13	1.52
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	13	1.52
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	13	1.52
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	14	1.52
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	14	1.52
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	14	1.52
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	9	1.52
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	14	1.52
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	14	1.52
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	20	1.51
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	16	1.51
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	2	1.51
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	2	1.51
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	2	1.51
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	1	1.51
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	15	1.51
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	2	1.51
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	2	1.51
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	2	1.51
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	16	1.51
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	16	1.51
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	16	1.51
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	16	1.51
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	16	1.51
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	16	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	16	1.51
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	16	1.51
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	16	1.51
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	17	1.51
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE2	18	1.5
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE2	18	1.5
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE2	18	1.5
(2,1856)	1:45:A:PHE:H	1:41:A:ASP:HB3	3	1.5
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	16	1.5
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	19	1.5
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	12	1.5
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	20	1.49
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	20	1.49
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	20	1.49
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	6	1.49
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	7	1.49
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	12	1.49
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	12	1.49
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	12	1.49
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	13	1.48
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	13	1.48
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	13	1.48
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	10	1.48
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	11	1.48
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	14	1.47
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	14	1.47
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	14	1.47
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	15	1.47
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	18	1.47
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	18	1.47
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	18	1.47
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	3	1.47
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	3	1.47
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	3	1.47
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	2	1.47
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG21	15	1.46
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG22	15	1.46
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG23	15	1.46
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	1	1.46
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	8	1.46
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	8	1.46
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	8	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	11	1.46
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	1	1.46
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	1	1.46
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	1	1.46
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	1	1.46
(2,2348)	1:45:A:PHE:HD1	1:34:A:HIS:HD2	20	1.45
(2,2348)	1:45:A:PHE:HD2	1:34:A:HIS:HD2	20	1.45
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	4	1.45
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	4	1.45
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	4	1.45
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	3	1.45
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	3	1.45
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	3	1.45
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	18	1.45
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	18	1.45
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	18	1.45
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	15	1.45
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	15	1.45
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	15	1.45
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	8	1.45
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	16	1.44
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	9	1.44
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	1	1.44
(2,553)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	5	1.44
(2,553)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	5	1.44
(2,553)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	5	1.44
(2,203)	1:11:A:LEU:HD11	1:26:A:TYR:H	20	1.44
(2,203)	1:11:A:LEU:HD12	1:26:A:TYR:H	20	1.44
(2,203)	1:11:A:LEU:HD13	1:26:A:TYR:H	20	1.44
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	17	1.44
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	5	1.43
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	1	1.43
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	2	1.43
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	12	1.43
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	12	1.43
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	12	1.43
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	16	1.43
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	16	1.43
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	16	1.43
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	8	1.43
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	13	1.43
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	13	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	13	1.43
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	8	1.42
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	5	1.42
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	14	1.42
(2,1307)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	5	1.42
(2,1307)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	5	1.42
(2,1307)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	5	1.42
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	2	1.42
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	2	1.42
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	2	1.42
(2,906)	1:8:A:TYR:HB2	1:52:A:PHE:HA	16	1.42
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	20	1.41
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	15	1.41
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	15	1.41
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	15	1.41
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	19	1.41
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	16	1.41
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	19	1.41
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	14	1.4
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	15	1.4
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	13	1.4
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	11	1.4
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	11	1.4
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	11	1.4
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	5	1.4
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	5	1.4
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	5	1.4
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	6	1.4
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	6	1.4
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	6	1.4
(1,116)	1:33:A:TYR:HD1	1:44:A:LYS:HE3	4	1.4
(1,116)	1:33:A:TYR:HD2	1:44:A:LYS:HE3	4	1.4
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG21	18	1.39
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG22	18	1.39
(2,2409)	1:7:A:LEU:HB3	1:0:A:THR:HG23	18	1.39
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD1	10	1.39
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD2	10	1.39
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD1	10	1.39
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD2	10	1.39
(2,1856)	1:45:A:PHE:H	1:41:A:ASP:HB3	15	1.39
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	12	1.39
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	12	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	12	1.39
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	2	1.39
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	2	1.39
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	2	1.39
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	2	1.39
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	8	1.39
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	8	1.39
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	8	1.39
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	14	1.39
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	14	1.39
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	2	1.39
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	2	1.39
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	2	1.39
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	2	1.39
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	9	1.39
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	9	1.39
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	9	1.39
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	7	1.39
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	8	1.38
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	8	1.38
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	8	1.38
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	11	1.38
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	11	1.38
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	11	1.38
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	12	1.38
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	8	1.38
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	7	1.38
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	7	1.38
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	7	1.38
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	20	1.38
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	20	1.38
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	20	1.38
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	1	1.38
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	10	1.38
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	4	1.38
(2,473)	1:24:A:LYS:HA	1:27:A:ARG:HD3	16	1.38
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	19	1.38
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	19	1.38
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	19	1.38
(2,2348)	1:45:A:PHE:HD1	1:34:A:HIS:HD2	1	1.37
(2,2348)	1:45:A:PHE:HD2	1:34:A:HIS:HD2	1	1.37
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	19	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,907)	1:8:A:TYR:HB3	1:52:A:PHE:HA	12	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD11	8	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD12	8	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD13	8	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD11	9	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD12	9	1.37
(2,402)	1:22:A:LEU:HA	1:22:A:LEU:HD13	9	1.37
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	6	1.36
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	18	1.36
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	9	1.36
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	9	1.36
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	9	1.36
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	14	1.36
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	14	1.36
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	14	1.36
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	8	1.36
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	5	1.36
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	5	1.36
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	5	1.36
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	10	1.36
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	10	1.36
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	10	1.36
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	12	1.36
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	8	1.36
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	8	1.36
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	15	1.36
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	15	1.36
(1,50)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	1.36
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	18	1.35
(2,629)	1:31:A:LEU:HA	1:34:A:HIS:HD2	13	1.35
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	8	1.35
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	2	1.35
(2,50)	1:4:A:GLU:H	1:6:A:LYS:HB3	2	1.35
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	2	1.35
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	2	1.35
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	2	1.35
(1,50)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	6	1.35
(1,50)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	20	1.35
(2,2348)	1:45:A:PHE:HD1	1:34:A:HIS:HD2	11	1.34
(2,2348)	1:45:A:PHE:HD2	1:34:A:HIS:HD2	11	1.34
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	16	1.34
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	16	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	16	1.34
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	16	1.34
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	4	1.34
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	17	1.34
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	10	1.34
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	7	1.34
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	7	1.34
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	7	1.34
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	14	1.34
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	14	1.34
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	14	1.34
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	9	1.34
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	9	1.34
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	9	1.34
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	5	1.34
(1,50)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	16	1.34
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	17	1.33
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	3	1.33
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	3	1.33
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	3	1.33
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	5	1.33
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	6	1.33
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	9	1.33
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	17	1.33
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	9	1.33
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	9	1.33
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	9	1.33
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	1	1.33
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	1	1.33
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	2	1.33
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	18	1.32
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	18	1.32
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	18	1.32
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	13	1.32
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	7	1.32
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	7	1.32
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	7	1.32
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	12	1.32
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	17	1.32
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	7	1.32
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	14	1.32
(2,642)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	7	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,642)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	7	1.32
(2,642)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	7	1.32
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	19	1.32
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	19	1.32
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	19	1.32
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	9	1.32
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	9	1.32
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	9	1.32
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	9	1.32
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	9	1.32
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	9	1.32
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	9	1.32
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	9	1.32
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	9	1.32
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	4	1.32
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	4	1.32
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	4	1.32
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	15	1.31
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	17	1.31
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	4	1.31
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	4	1.31
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	4	1.31
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	14	1.31
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	4	1.31
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	4	1.31
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	4	1.31
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	2	1.31
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	3	1.31
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	16	1.31
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	10	1.31
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	10	1.31
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	10	1.31
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	7	1.31
(1,50)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	12	1.31
(1,47)	1:2:A:VAL:HB	1:65:A:ASP:H	7	1.31
(2,2460)	1:33:A:TYR:HD1	1:41:A:ASP:HB3	3	1.3
(2,2460)	1:33:A:TYR:HD2	1:41:A:ASP:HB3	3	1.3
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	11	1.3
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	19	1.3
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	19	1.3
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	19	1.3
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	15	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	3	1.3
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	3	1.3
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	3	1.3
(2,3)	1:1:A:SER:HA	1:2:A:VAL:HG11	19	1.3
(2,3)	1:1:A:SER:HA	1:2:A:VAL:HG12	19	1.3
(2,3)	1:1:A:SER:HA	1:2:A:VAL:HG13	19	1.3
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	13	1.3
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	13	1.3
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	13	1.3
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	7	1.29
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	12	1.29
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	6	1.29
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	2	1.29
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	2	1.29
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	2	1.29
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	9	1.29
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	11	1.29
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	11	1.29
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	11	1.29
(2,827)	1:24:A:LYS:HE2	1:20:A:GLN:HB3	3	1.29
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	18	1.29
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	18	1.29
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	18	1.29
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	8	1.29
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	8	1.29
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	18	1.29
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	18	1.29
(1,349)	1:24:A:LYS:HE3	1:20:A:GLN:HB3	15	1.29
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	15	1.29
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	15	1.29
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	15	1.29
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	14	1.28
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	16	1.28
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	10	1.28
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	15	1.28
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	15	1.28
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	15	1.28
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	17	1.28
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	17	1.28
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	17	1.28
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	1	1.28
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	5	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	19	1.28
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD21	19	1.28
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD22	19	1.28
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD23	19	1.28
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	20	1.28
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	11	1.28
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	10	1.28
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	10	1.28
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	10	1.28
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	11	1.28
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	5	1.28
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	5	1.28
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	5	1.28
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	14	1.28
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	14	1.28
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	14	1.28
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE3	14	1.28
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE3	14	1.28
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	17	1.27
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	2	1.27
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	11	1.27
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	16	1.27
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	10	1.27
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	10	1.27
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	10	1.27
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	7	1.27
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	15	1.27
(2,433)	1:22:A:LEU:HD11	1:52:A:PHE:HA	8	1.27
(2,433)	1:22:A:LEU:HD12	1:52:A:PHE:HA	8	1.27
(2,433)	1:22:A:LEU:HD13	1:52:A:PHE:HA	8	1.27
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	12	1.27
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	12	1.27
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	12	1.27
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	19	1.27
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	19	1.27
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	19	1.27
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	20	1.27
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	6	1.27
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	6	1.27
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	6	1.27
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	6	1.26
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	6	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	6	1.26
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	1	1.26
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	17	1.26
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	2	1.26
(2,562)	1:28:A:LYS:HA	1:28:A:LYS:HD2	4	1.26
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	16	1.26
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	1	1.26
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	1	1.26
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	1	1.26
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD11	5	1.26
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD12	5	1.26
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD13	5	1.26
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	10	1.26
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	4	1.26
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	13	1.26
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	13	1.26
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	18	1.26
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	18	1.26
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	18	1.26
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	11	1.26
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	12	1.26
(2,2413)	1:74:A:SER:HB2	1:78:A:SER:H	12	1.25
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	2	1.25
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	8	1.25
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	5	1.25
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	1	1.25
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	17	1.25
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	17	1.25
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	17	1.25
(2,47)	1:6:A:LYS:HG3	1:4:A:GLU:HA	3	1.25
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	19	1.25
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	16	1.25
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	9	1.24
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	3	1.24
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	3	1.24
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	3	1.24
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	9	1.24
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	9	1.24
(2,433)	1:22:A:LEU:HD11	1:52:A:PHE:HA	3	1.24
(2,433)	1:22:A:LEU:HD12	1:52:A:PHE:HA	3	1.24
(2,433)	1:22:A:LEU:HD13	1:52:A:PHE:HA	3	1.24
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	10	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	1	1.24
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	1	1.24
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	1	1.24
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	3	1.24
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	3	1.24
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	3	1.24
(2,2354)	1:64:A:TYR:HE1	1:69:A:LEU:HD11	7	1.23
(2,2354)	1:64:A:TYR:HE1	1:69:A:LEU:HD12	7	1.23
(2,2354)	1:64:A:TYR:HE1	1:69:A:LEU:HD13	7	1.23
(2,2354)	1:64:A:TYR:HE2	1:69:A:LEU:HD11	7	1.23
(2,2354)	1:64:A:TYR:HE2	1:69:A:LEU:HD12	7	1.23
(2,2354)	1:64:A:TYR:HE2	1:69:A:LEU:HD13	7	1.23
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	12	1.23
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	12	1.23
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	12	1.23
(2,1188)	1:2:A:VAL:HB	1:65:A:ASP:HA	12	1.23
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	14	1.23
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD21	7	1.23
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD22	7	1.23
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD23	7	1.23
(2,562)	1:28:A:LYS:HA	1:28:A:LYS:HD2	5	1.23
(2,551)	1:24:A:LYS:HA	1:27:A:ARG:HD3	14	1.23
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	5	1.23
(2,502)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	15	1.23
(2,502)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	15	1.23
(2,502)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	15	1.23
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	15	1.23
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	13	1.23
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	14	1.23
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	4	1.22
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	12	1.22
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	12	1.22
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	12	1.22
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	12	1.22
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	13	1.22
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	13	1.22
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	13	1.22
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	15	1.22
(2,907)	1:8:A:TYR:HB3	1:52:A:PHE:HA	16	1.22
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	4	1.22
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	20	1.22
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	20	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	20	1.22
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	2	1.22
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	2	1.22
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	2	1.22
(2,2018)	1:59:A:GLN:H	1:59:A:GLN:HG3	16	1.21
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	9	1.21
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	9	1.21
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	9	1.21
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	9	1.21
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	10	1.21
(2,1188)	1:2:A:VAL:HB	1:65:A:ASP:HA	1	1.21
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	18	1.21
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	17	1.21
(2,562)	1:28:A:LYS:HA	1:28:A:LYS:HD3	1	1.21
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	14	1.21
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	14	1.21
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	3	1.21
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	14	1.21
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	9	1.21
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	9	1.21
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	11	1.21
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	11	1.21
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	17	1.21
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	17	1.21
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	9	1.21
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	9	1.21
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	9	1.21
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	7	1.2
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	3	1.2
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	3	1.2
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	3	1.2
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	1	1.2
(2,1494)	1:8:A:TYR:H	1:52:A:PPHE:HA	12	1.2
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	11	1.2
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE2	8	1.2
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE2	8	1.2
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE2	8	1.2
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD21	7	1.2
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD22	7	1.2
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD23	7	1.2
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	11	1.2
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	11	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	11	1.2
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	13	1.2
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	3	1.2
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	3	1.2
(1,116)	1:33:A:TYR:HD1	1:44:A:LYS:HE2	13	1.2
(1,116)	1:33:A:TYR:HD2	1:44:A:LYS:HE2	13	1.2
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	19	1.19
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	14	1.19
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	14	1.19
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	14	1.19
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	19	1.19
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	19	1.19
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	19	1.19
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	5	1.19
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	5	1.19
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	5	1.19
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	17	1.19
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	17	1.19
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	17	1.19
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD11	6	1.19
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD12	6	1.19
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD13	6	1.19
(2,562)	1:28:A:LYS:HA	1:28:A:LYS:HD3	20	1.19
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	17	1.19
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	18	1.19
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	2	1.19
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	4	1.19
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	4	1.19
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	4	1.19
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	4	1.18
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD3	10	1.18
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD3	10	1.18
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD3	10	1.18
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	6	1.18
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	17	1.18
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	20	1.18
(2,2018)	1:59:A:GLN:H	1:59:A:GLN:HG3	18	1.18
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	8	1.18
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	1	1.18
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	1	1.18
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	1	1.18
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	20	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	16	1.18
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	16	1.18
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	16	1.18
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	3	1.18
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	3	1.18
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	3	1.18
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	13	1.18
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	13	1.18
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	7	1.18
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	7	1.18
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	7	1.18
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	8	1.18
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	8	1.18
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	8	1.18
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	12	1.18
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	10	1.18
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	10	1.18
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	10	1.18
(1,73)	1:51:A:ALA:H	1:54:A:ILE:HB	1	1.18
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	6	1.17
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	19	1.17
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	9	1.17
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	15	1.17
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	15	1.17
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	15	1.17
(2,1407)	1:33:A:TYR:HD1	1:41:A:ASP:H	13	1.17
(2,1407)	1:33:A:TYR:HD2	1:41:A:ASP:H	13	1.17
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	20	1.17
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	20	1.17
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	20	1.17
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	15	1.17
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	19	1.17
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	10	1.17
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	10	1.17
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	10	1.17
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	13	1.17
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	13	1.17
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	13	1.17
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	16	1.17
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	16	1.17
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	16	1.17
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	12	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	1	1.17
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	4	1.17
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	17	1.17
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	11	1.17
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	11	1.17
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	11	1.17
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	6	1.17
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	6	1.17
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	6	1.17
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	11	1.17
(1,50)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	5	1.17
(1,50)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	15	1.17
(2,2460)	1:33:A:TYR:HD1	1:41:A:ASP:HB3	15	1.16
(2,2460)	1:33:A:TYR:HD2	1:41:A:ASP:HB3	15	1.16
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	13	1.16
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	9	1.16
(2,2018)	1:59:A:GLN:H	1:59:A:GLN:HG3	7	1.16
(2,2018)	1:59:A:GLN:H	1:59:A:GLN:HG3	10	1.16
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	1	1.16
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	4	1.16
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	11	1.16
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	8	1.16
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	8	1.16
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	8	1.16
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	5	1.16
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	5	1.16
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	5	1.16
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	20	1.16
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	6	1.16
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	7	1.16
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	9	1.16
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	16	1.16
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	16	1.16
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	15	1.16
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	15	1.16
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	15	1.16
(1,145)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	3	1.16
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	16	1.16
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	16	1.16
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	16	1.16
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	20	1.15
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	19	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1608)	1:13:A:VAL:HG11	1:17:A:ALA:H	5	1.15
(2,1608)	1:13:A:VAL:HG12	1:17:A:ALA:H	5	1.15
(2,1608)	1:13:A:VAL:HG13	1:17:A:ALA:H	5	1.15
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	11	1.15
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	10	1.15
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	10	1.15
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	10	1.15
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	15	1.15
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	11	1.15
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	11	1.15
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	11	1.15
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	1	1.15
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	1	1.15
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	1	1.15
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	6	1.15
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	6	1.15
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	6	1.15
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	16	1.15
(1,483)	1:53:A:GLU:HG2	1:53:A:GLU:H	10	1.15
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD2	17	1.15
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	5	1.15
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	5	1.15
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	5	1.15
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	14	1.15
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	14	1.15
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	14	1.15
(1,73)	1:51:A:ALA:H	1:54:A:ILE:HB	7	1.15
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	5	1.14
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	20	1.14
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	7	1.14
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	20	1.14
(2,427)	1:51:A:ALA:HA	1:10:A:LEU:HD11	10	1.14
(2,427)	1:51:A:ALA:HA	1:10:A:LEU:HD12	10	1.14
(2,427)	1:51:A:ALA:HA	1:10:A:LEU:HD13	10	1.14
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	19	1.14
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	11	1.14
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	20	1.14
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	18	1.14
(1,483)	1:53:A:GLU:HG2	1:53:A:GLU:H	20	1.14
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	7	1.14
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	19	1.14
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	19	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	19	1.14
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	18	1.13
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	16	1.13
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	2	1.13
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	6	1.13
(2,906)	1:8:A:TYR:HB2	1:52:A:PHE:HA	1	1.13
(2,827)	1:24:A:LYS:HE2	1:20:A:GLN:HB3	4	1.13
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	6	1.13
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	2	1.13
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	2	1.13
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	2	1.13
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	18	1.13
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	18	1.13
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	18	1.13
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	3	1.12
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	5	1.12
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	4	1.12
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	12	1.12
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	6	1.12
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	6	1.12
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	6	1.12
(2,906)	1:8:A:TYR:HB2	1:52:A:PHE:HA	10	1.12
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	20	1.12
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	18	1.12
(2,433)	1:22:A:LEU:HD11	1:52:A:PHE:HA	9	1.12
(2,433)	1:22:A:LEU:HD12	1:52:A:PHE:HA	9	1.12
(2,433)	1:22:A:LEU:HD13	1:52:A:PHE:HA	9	1.12
(2,238)	1:22:A:LEU:HD21	1:15:A:PRO:HA	12	1.12
(2,238)	1:22:A:LEU:HD22	1:15:A:PRO:HA	12	1.12
(2,238)	1:22:A:LEU:HD23	1:15:A:PRO:HA	12	1.12
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	1	1.12
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	17	1.12
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	7	1.12
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	12	1.12
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	12	1.12
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	12	1.12
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	19	1.12
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	2	1.11
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	2	1.11
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	2	1.11
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	2	1.11
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	2	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	2	1.11
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	2	1.11
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	2	1.11
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	2	1.11
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	3	1.11
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	3	1.11
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	3	1.11
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	3	1.11
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	3	1.11
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	3	1.11
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	5	1.11
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	13	1.11
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	18	1.11
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	18	1.11
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	18	1.11
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	8	1.11
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	8	1.11
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	8	1.11
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	2	1.11
(2,906)	1:8:A:TYR:HB2	1:52:A:PHE:HA	19	1.11
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	1	1.11
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	16	1.11
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	3	1.11
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	3	1.11
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	3	1.11
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	3	1.11
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	3	1.11
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	3	1.11
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	3	1.11
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	3	1.11
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	3	1.11
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	13	1.11
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	15	1.11
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	19	1.11
(1,483)	1:53:A:GLU:HG2	1:53:A:GLU:H	12	1.11
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	4	1.11
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	1	1.11
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	1	1.11
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	1	1.11
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	3	1.11
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	3	1.11
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	3	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	7	1.11
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	11	1.1
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	13	1.1
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	19	1.1
(2,1869)	1:46:A:LYS:H	1:41:A:ASP:HB3	3	1.1
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	14	1.1
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	17	1.1
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	4	1.1
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	19	1.1
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	15	1.1
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	6	1.1
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD21	7	1.1
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD22	7	1.1
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD23	7	1.1
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	18	1.1
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	18	1.1
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	18	1.1
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	8	1.1
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	8	1.1
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	8	1.1
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	16	1.1
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	9	1.1
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	9	1.1
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	10	1.1
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	4	1.09
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	8	1.09
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	7	1.09
(2,1690)	1:13:A:VAL:HG21	1:25:A:GLY:H	9	1.09
(2,1690)	1:13:A:VAL:HG22	1:25:A:GLY:H	9	1.09
(2,1690)	1:13:A:VAL:HG23	1:25:A:GLY:H	9	1.09
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	3	1.09
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	5	1.09
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	17	1.09
(2,1133)	1:66:A:GLN:HB3	1:63:A:ILE:HA	12	1.09
(2,766)	1:69:A:LEU:HD21	1:73:A:ARG:HA	19	1.09
(2,766)	1:69:A:LEU:HD22	1:73:A:ARG:HA	19	1.09
(2,766)	1:69:A:LEU:HD23	1:73:A:ARG:HA	19	1.09
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	9	1.09
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	9	1.09
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	1	1.09
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	10	1.09
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	10	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	10	1.09
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	20	1.09
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	6	1.09
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	6	1.09
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	1	1.09
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	20	1.09
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	20	1.09
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	20	1.09
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	10	1.08
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	2	1.08
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	10	1.08
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	19	1.08
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	18	1.08
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	13	1.08
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	12	1.08
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	12	1.08
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	12	1.08
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	6	1.08
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	5	1.08
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	5	1.08
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	5	1.08
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG21	11	1.08
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG22	11	1.08
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG23	11	1.08
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	9	1.08
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	9	1.08
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	9	1.08
(1,20)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	6	1.08
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	1	1.07
(2,2343)	1:31:A:LEU:HB2	1:34:A:HIS:HD2	18	1.07
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	7	1.07
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	14	1.07
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	10	1.07
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	7	1.07
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	16	1.07
(2,1440)	1:65:A:ASP:HA	1:3:A:LYS:H	19	1.07
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD11	12	1.07
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD12	12	1.07
(2,1100)	1:60:A:LYS:HD3	1:54:A:ILE:HD13	12	1.07
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	2	1.07
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	19	1.07
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	19	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	19	1.07
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	8	1.07
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	8	1.07
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD3	18	1.07
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	20	1.07
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	5	1.06
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	6	1.06
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	13	1.06
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	17	1.06
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	19	1.06
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	15	1.06
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	19	1.06
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	13	1.06
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	7	1.06
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	3	1.06
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	3	1.06
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	3	1.06
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	1	1.06
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	1	1.06
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	1	1.06
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	5	1.06
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	5	1.06
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	5	1.06
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	17	1.06
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	17	1.06
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	17	1.06
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	14	1.06
(1,157)	1:27:A:ARG:HD3	1:27:A:ARG:HA	11	1.06
(2,2419)	1:24:A:LYS:HB3	1:24:A:LYS:HD3	4	1.05
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	1	1.05
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	2	1.05
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	9	1.05
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	16	1.05
(2,1578)	1:22:A:LEU:HD11	1:14:A:SER:H	8	1.05
(2,1578)	1:22:A:LEU:HD12	1:14:A:SER:H	8	1.05
(2,1578)	1:22:A:LEU:HD13	1:14:A:SER:H	8	1.05
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	4	1.05
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	4	1.05
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	4	1.05
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD21	5	1.05
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD22	5	1.05
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD23	5	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD21	14	1.05
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD22	14	1.05
(2,1250)	1:70:A:GLU:HA	1:69:A:LEU:HD23	14	1.05
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	12	1.05
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	10	1.05
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	10	1.05
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	10	1.05
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	12	1.05
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	12	1.05
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	12	1.05
(2,766)	1:69:A:LEU:HD21	1:73:A:ARG:HA	5	1.05
(2,766)	1:69:A:LEU:HD22	1:73:A:ARG:HA	5	1.05
(2,766)	1:69:A:LEU:HD23	1:73:A:ARG:HA	5	1.05
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	11	1.05
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	3	1.05
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	3	1.05
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	3	1.05
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	15	1.05
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	18	1.05
(1,279)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	3	1.05
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	12	1.05
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	1	1.05
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	7	1.05
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	7	1.05
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	7	1.05
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	8	1.05
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	8	1.05
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	8	1.05
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	16	1.05
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	3	1.04
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	5	1.04
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	4	1.04
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	4	1.04
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	4	1.04
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	4	1.04
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	4	1.04
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	4	1.04
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	3	1.04
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	4	1.04
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	12	1.04
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	15	1.04
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	18	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	20	1.04
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	16	1.04
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	18	1.04
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	6	1.04
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	11	1.04
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	14	1.04
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	14	1.04
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	14	1.04
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	4	1.04
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	12	1.04
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	5	1.04
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	8	1.04
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	2	1.04
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	2	1.04
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	2	1.04
(2,324)	1:22:A:LEU:HD21	1:19:A:GLU:HA	8	1.04
(2,324)	1:22:A:LEU:HD22	1:19:A:GLU:HA	8	1.04
(2,324)	1:22:A:LEU:HD23	1:19:A:GLU:HA	8	1.04
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	6	1.04
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	13	1.04
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	13	1.04
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	13	1.04
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	7	1.04
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	17	1.04
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	17	1.04
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	13	1.04
(1,268)	1:51:A:ALA:HB1	1:48:A:ILE:HG21	20	1.04
(1,268)	1:51:A:ALA:HB1	1:48:A:ILE:HG22	20	1.04
(1,268)	1:51:A:ALA:HB1	1:48:A:ILE:HG23	20	1.04
(1,268)	1:51:A:ALA:HB2	1:48:A:ILE:HG21	20	1.04
(1,268)	1:51:A:ALA:HB2	1:48:A:ILE:HG22	20	1.04
(1,268)	1:51:A:ALA:HB2	1:48:A:ILE:HG23	20	1.04
(1,268)	1:51:A:ALA:HB3	1:48:A:ILE:HG21	20	1.04
(1,268)	1:51:A:ALA:HB3	1:48:A:ILE:HG22	20	1.04
(1,268)	1:51:A:ALA:HB3	1:48:A:ILE:HG23	20	1.04
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	8	1.04
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	11	1.04
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	11	1.04
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	11	1.04
(1,122)	1:9:A:ASP:H	1:10:A:LEU:HA	12	1.04
(2,2419)	1:24:A:LYS:HB3	1:24:A:LYS:HD3	8	1.03
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	8	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	10	1.03
(2,2179)	1:70:A:GLU:HB3	1:70:A:GLU:H	11	1.03
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	1	1.03
(2,1856)	1:45:A:PHE:H	1:41:A:ASP:HB3	12	1.03
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	12	1.03
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	3	1.03
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	8	1.03
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	6	1.03
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	6	1.03
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	6	1.03
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	6	1.03
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	17	1.03
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	17	1.03
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	17	1.03
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	4	1.03
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	4	1.03
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	4	1.03
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	9	1.03
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	16	1.03
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	17	1.03
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	8	1.03
(1,143)	1:29:A:ALA:HA	1:32:A:LYS:HA	15	1.03
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	18	1.03
(1,122)	1:9:A:ASP:H	1:10:A:LEU:HA	11	1.03
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	1	1.03
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	1	1.03
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	1	1.03
(2,2419)	1:24:A:LYS:HB3	1:24:A:LYS:HD3	3	1.02
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	7	1.02
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	13	1.02
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	9	1.02
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	16	1.02
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	16	1.02
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	11	1.02
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	9	1.02
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	18	1.02
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	20	1.02
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	5	1.02
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD21	16	1.02
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD22	16	1.02
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD23	16	1.02
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	12	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,553)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	19	1.02
(2,553)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	19	1.02
(2,553)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	19	1.02
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	8	1.02
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	16	1.02
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	16	1.02
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	16	1.02
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	8	1.02
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	8	1.02
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	8	1.02
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	18	1.02
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	18	1.02
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	18	1.02
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	20	1.02
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	20	1.02
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	20	1.02
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	16	1.02
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	19	1.02
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	3	1.02
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	3	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	2	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	3	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	4	1.02
(1,143)	1:29:A:ALA:HA	1:32:A:LYS:HA	6	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	10	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	11	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	13	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	14	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	17	1.02
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	20	1.02
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	12	1.01
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	19	1.01
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	6	1.01
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	3	1.01
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	11	1.01
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	8	1.01
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	5	1.01
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	5	1.01
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	5	1.01
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	6	1.01
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	14	1.01
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	17	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1307)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	19	1.01
(2,1307)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	19	1.01
(2,1307)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	19	1.01
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	17	1.01
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	20	1.01
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	5	1.01
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	11	1.01
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	11	1.01
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	11	1.01
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	11	1.01
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	11	1.01
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	11	1.01
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	20	1.01
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD11	17	1.01
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD12	17	1.01
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD13	17	1.01
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	6	1.01
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	6	1.01
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	6	1.01
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	7	1.01
(1,369)	1:0:A:THR:HA	1:1:A:SER:HA	13	1.01
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	17	1.01
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	18	1.01
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	1	1.01
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	9	1.01
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	12	1.01
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	16	1.01
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	19	1.01
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	8	1.01
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	8	1.01
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	8	1.01
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	9	1.01
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	9	1.01
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	9	1.01
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	19	1.0
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	11	1.0
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	8	1.0
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	13	1.0
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	16	1.0
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	15	1.0
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	6	1.0
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	6	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	7	1.0
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	4	1.0
(2,919)	1:52:A:PHE:HB2	1:8:A:TYR:HA	12	1.0
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	17	1.0
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	17	1.0
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	17	1.0
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	18	1.0
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	18	1.0
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	18	1.0
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	8	1.0
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	12	1.0
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	13	1.0
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	13	1.0
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	13	1.0
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	13	1.0
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	13	1.0
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	13	1.0
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	13	1.0
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	13	1.0
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	13	1.0
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	13	1.0
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	13	1.0
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	13	1.0
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	3	1.0
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	3	1.0
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	3	1.0
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	18	1.0
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	5	1.0
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	12	1.0
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	12	1.0
(1,143)	1:29:A:ALA:HA	1:30:A:ALA:HA	5	1.0
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	3	1.0
(1,122)	1:9:A:ASP:H	1:10:A:LEU:HA	20	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	2	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	2	1.0
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	2	1.0
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	5	0.99
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	14	0.99
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	12	0.99
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	18	0.99
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	20	0.99
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	1	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	7	0.99
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	3	0.99
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	18	0.99
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	16	0.99
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	16	0.99
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	16	0.99
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	5	0.99
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	11	0.99
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	14	0.99
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	16	0.99
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	18	0.99
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	18	0.99
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	18	0.99
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	9	0.99
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	7	0.99
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	7	0.99
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	7	0.99
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	4	0.99
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	4	0.99
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	4	0.99
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	4	0.99
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	4	0.99
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	4	0.99
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	4	0.99
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	4	0.99
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	4	0.99
(2,211)	1:26:A:TYR:HB2	1:11:A:LEU:HD11	20	0.99
(2,211)	1:26:A:TYR:HB2	1:11:A:LEU:HD12	20	0.99
(2,211)	1:26:A:TYR:HB2	1:11:A:LEU:HD13	20	0.99
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	2	0.99
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	2	0.99
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	2	0.99
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	13	0.99
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	13	0.99
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	13	0.99
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	10	0.99
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	12	0.99
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	12	0.99
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	12	0.99
(1,157)	1:27:A:ARG:HD2	1:27:A:ARG:HA	1	0.99
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	9	0.99
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	14	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:9:A:ASP:H	1:10:A:LEU:HA	15	0.99
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	19	0.99
(1,119)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	6	0.99
(1,119)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	0.99
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	6	0.98
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	7	0.98
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	7	0.98
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	7	0.98
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	20	0.98
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	20	0.98
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	20	0.98
(2,1869)	1:46:A:LYS:H	1:41:A:ASP:HB3	15	0.98
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	7	0.98
(2,693)	1:37:A:LYS:HD3	1:38:A:PRO:HD2	6	0.98
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	16	0.98
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	2	0.98
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	2	0.98
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	8	0.98
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	13	0.98
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	20	0.98
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	20	0.98
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	20	0.98
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	6	0.98
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	6	0.98
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	6	0.98
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	6	0.98
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	6	0.98
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	6	0.98
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	6	0.98
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	6	0.98
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	6	0.98
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	8	0.98
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	8	0.98
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	8	0.98
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	7	0.98
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	7	0.98
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	7	0.98
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	14	0.98
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	14	0.98
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	14	0.98
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	8	0.98
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	11	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	11	0.98
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	5	0.98
(1,119)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	16	0.98
(1,119)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	20	0.98
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	16	0.97
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	2	0.97
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	7	0.97
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE2	4	0.97
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE2	4	0.97
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE2	4	0.97
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	1	0.97
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	5	0.97
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	2	0.97
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	4	0.97
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	12	0.97
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	13	0.97
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	7	0.97
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	1	0.97
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	4	0.97
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	4	0.97
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	4	0.97
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	6	0.97
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	6	0.97
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	6	0.97
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	2	0.97
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	14	0.97
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	15	0.97
(1,135)	1:48:A:ILE:HA	1:48:A:ILE:HD11	15	0.97
(1,135)	1:48:A:ILE:HA	1:48:A:ILE:HD12	15	0.97
(1,135)	1:48:A:ILE:HA	1:48:A:ILE:HD13	15	0.97
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	7	0.97
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	10	0.97
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	13	0.97
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	7	0.97
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	7	0.97
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	7	0.97
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	16	0.97
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	16	0.97
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	16	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	1	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	1	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	1	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	7	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	7	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	7	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	12	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	12	0.97
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	12	0.97
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	14	0.96
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	9	0.96
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	9	0.96
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	9	0.96
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	11	0.96
(2,2115)	1:66:A:GLN:HB3	1:66:A:GLN:H	12	0.96
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	13	0.96
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	18	0.96
(2,1620)	1:22:A:LEU:HD21	1:18:A:ASN:H	12	0.96
(2,1620)	1:22:A:LEU:HD22	1:18:A:ASN:H	12	0.96
(2,1620)	1:22:A:LEU:HD23	1:18:A:ASN:H	12	0.96
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	1	0.96
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	3	0.96
(2,210)	1:26:A:TYR:HA	1:11:A:LEU:HD11	20	0.96
(2,210)	1:26:A:TYR:HA	1:11:A:LEU:HD12	20	0.96
(2,210)	1:26:A:TYR:HA	1:11:A:LEU:HD13	20	0.96
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	2	0.96
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	2	0.96
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	2	0.96
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	5	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD11	8	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD12	8	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD13	8	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD11	9	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD12	9	0.96
(2,86)	1:22:A:LEU:HA	1:22:A:LEU:HD13	9	0.96
(2,54)	1:4:A:GLU:HG2	1:3:A:LYS:HD2	17	0.96
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	11	0.96
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	11	0.96
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	2	0.96
(1,369)	1:0:A:THR:HA	1:1:A:SER:HA	20	0.96
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	13	0.96
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	13	0.96
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	15	0.96
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	15	0.96
(1,122)	1:9:A:ASP:H	1:10:A:LEU:HA	6	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	18	0.96
(1,116)	1:33:A:TYR:HD1	1:44:A:LYS:HE3	16	0.96
(1,116)	1:33:A:TYR:HD2	1:44:A:LYS:HE3	16	0.96
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	19	0.96
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	19	0.96
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	19	0.96
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	3	0.95
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	10	0.95
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	16	0.95
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	14	0.95
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	14	0.95
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	14	0.95
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	13	0.95
(2,2177)	1:70:A:GLU:H	1:73:A:ARG:HG2	13	0.95
(2,2115)	1:66:A:GLN:HB3	1:66:A:GLN:H	8	0.95
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	1	0.95
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	5	0.95
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	7	0.95
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	12	0.95
(2,1635)	1:18:A:ASN:HB3	1:19:A:GLU:H	3	0.95
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	20	0.95
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	19	0.95
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	12	0.95
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	14	0.95
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	15	0.95
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	17	0.95
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	19	0.95
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	20	0.95
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	2	0.95
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	9	0.95
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	10	0.95
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	15	0.95
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	4	0.95
(2,694)	1:37:A:LYS:HD3	1:38:A:PRO:HD3	13	0.95
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	10	0.95
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	18	0.95
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	12	0.95
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	5	0.95
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	17	0.95
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	17	0.95
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	17	0.95
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	5	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	5	0.95
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	5	0.95
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	8	0.95
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	8	0.95
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	8	0.95
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	9	0.95
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	9	0.95
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	9	0.95
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	15	0.95
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	15	0.95
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	15	0.95
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	7	0.95
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	7	0.95
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	7	0.95
(2,54)	1:4:A:GLU:HG2	1:3:A:LYS:HD2	20	0.95
(2,50)	1:4:A:GLU:H	1:6:A:LYS:HB3	5	0.95
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	19	0.95
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	19	0.95
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	3	0.95
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	19	0.95
(1,398)	1:63:A:ILE:HG21	1:73:A:ARG:H	5	0.95
(1,398)	1:63:A:ILE:HG22	1:73:A:ARG:H	5	0.95
(1,398)	1:63:A:ILE:HG23	1:73:A:ARG:H	5	0.95
(1,398)	1:63:A:ILE:HG21	1:73:A:ARG:H	14	0.95
(1,398)	1:63:A:ILE:HG22	1:73:A:ARG:H	14	0.95
(1,398)	1:63:A:ILE:HG23	1:73:A:ARG:H	14	0.95
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	6	0.95
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	6	0.95
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	6	0.95
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	6	0.95
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	17	0.95
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	19	0.95
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	5	0.95
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	5	0.95
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	5	0.95
(1,119)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	12	0.95
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	12	0.94
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	9	0.94
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	7	0.94
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	7	0.94
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	7	0.94
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	7	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	7	0.94
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	7	0.94
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	8	0.94
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	8	0.94
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	8	0.94
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	8	0.94
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	8	0.94
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	8	0.94
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	2	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	3	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	9	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	14	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	15	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	16	0.94
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	19	0.94
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	2	0.94
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	15	0.94
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	18	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	3	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	5	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	8	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	10	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	11	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	13	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	16	0.94
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	18	0.94
(2,1133)	1:66:A:GLN:HB3	1:63:A:ILE:HA	8	0.94
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	9	0.94
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	6	0.94
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	2	0.94
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	2	0.94
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	2	0.94
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	2	0.94
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	2	0.94
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	2	0.94
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	2	0.94
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	2	0.94
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	2	0.94
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	7	0.94
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	9	0.94
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD11	16	0.94
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD12	16	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD13	16	0.94
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	5	0.94
(1,406)	1:37:A:LYS:HD3	1:38:A:PRO:HD2	6	0.94
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	5	0.94
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	2	0.94
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	14	0.94
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD11	1	0.94
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD12	1	0.94
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD13	1	0.94
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD11	12	0.94
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD12	12	0.94
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD13	12	0.94
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	14	0.94
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	17	0.94
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	17	0.94
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	4	0.94
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	15	0.94
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	15	0.94
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	15	0.94
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	18	0.93
(2,2413)	1:74:A:SER:HB3	1:78:A:SER:H	10	0.93
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	14	0.93
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	19	0.93
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	12	0.93
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	3	0.93
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	15	0.93
(2,2115)	1:66:A:GLN:HB3	1:66:A:GLN:H	1	0.93
(2,2115)	1:66:A:GLN:HB3	1:66:A:GLN:H	2	0.93
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	2	0.93
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	14	0.93
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	14	0.93
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	3	0.93
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	5	0.93
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	5	0.93
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	5	0.93
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	4	0.93
(2,1420)	1:27:A:ARG:H	1:27:A:ARG:HB3	7	0.93
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD21	19	0.93
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD22	19	0.93
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD23	19	0.93
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	17	0.93
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	16	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	16	0.93
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	16	0.93
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	19	0.93
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	19	0.93
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	19	0.93
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	8	0.93
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	8	0.93
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	8	0.93
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	8	0.93
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	19	0.93
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	19	0.93
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	19	0.93
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	10	0.93
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	10	0.93
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	10	0.93
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG21	19	0.93
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG22	19	0.93
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG23	19	0.93
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	20	0.93
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	20	0.93
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	1	0.93
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	9	0.93
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	16	0.93
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	20	0.93
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	1	0.93
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	12	0.93
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD11	14	0.93
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD12	14	0.93
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD13	14	0.93
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	13	0.93
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	9	0.93
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	11	0.93
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	17	0.93
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	17	0.93
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	17	0.93
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	11	0.93
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	11	0.93
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	11	0.93
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	8	0.92
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	9	0.92
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	3	0.92
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	3	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	3	0.92
(2,2115)	1:66:A:GLN:HB3	1:66:A:GLN:H	4	0.92
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	3	0.92
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	12	0.92
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	16	0.92
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	18	0.92
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	17	0.92
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	13	0.92
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	13	0.92
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	13	0.92
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	20	0.92
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	20	0.92
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	20	0.92
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	8	0.92
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	9	0.92
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	9	0.92
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	9	0.92
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	6	0.92
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	7	0.92
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	15	0.92
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	11	0.92
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	5	0.92
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	5	0.92
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	20	0.92
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	20	0.92
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	20	0.92
(1,275)	1:26:A:TYR:H	1:22:A:LEU:HB2	3	0.92
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	10	0.92
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	19	0.91
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	4	0.91
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	4	0.91
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	4	0.91
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	17	0.91
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	20	0.91
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	4	0.91
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	6	0.91
(2,1642)	1:19:A:GLU:HB2	1:20:A:GLN:H	8	0.91
(2,1578)	1:22:A:LEU:HD11	1:14:A:SER:H	9	0.91
(2,1578)	1:22:A:LEU:HD12	1:14:A:SER:H	9	0.91
(2,1578)	1:22:A:LEU:HD13	1:14:A:SER:H	9	0.91
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	20	0.91
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	7	0.91
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	7	0.91
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	7	0.91
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	7	0.91
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	7	0.91
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD21	10	0.91
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD22	10	0.91
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD23	10	0.91
(2,771)	1:41:A:ASP:HB3	1:44:A:LYS:HB2	3	0.91
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	17	0.91
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	4	0.91
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	17	0.91
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	17	0.91
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	17	0.91
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	4	0.91
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	14	0.91
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	3	0.91
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	9	0.91
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	5	0.91
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	4	0.91
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	1	0.91
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	14	0.91
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	14	0.91
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	14	0.91
(2,2413)	1:74:A:SER:HB3	1:78:A:SER:H	17	0.9
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	13	0.9
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	13	0.9
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	13	0.9
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	13	0.9
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	13	0.9
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	13	0.9
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	15	0.9
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	13	0.9
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	20	0.9
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	17	0.9
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	3	0.9
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	6	0.9
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD21	12	0.9
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD22	12	0.9
(2,1026)	1:32:A:LYS:HD2	1:10:A:LEU:HD23	12	0.9
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	17	0.9
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	17	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	9	0.9
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	9	0.9
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	9	0.9
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	9	0.9
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	9	0.9
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	9	0.9
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	9	0.9
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	9	0.9
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	9	0.9
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	3	0.9
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	3	0.9
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	8	0.9
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	13	0.9
(1,398)	1:63:A:ILE:HG21	1:73:A:ARG:H	7	0.9
(1,398)	1:63:A:ILE:HG22	1:73:A:ARG:H	7	0.9
(1,398)	1:63:A:ILE:HG23	1:73:A:ARG:H	7	0.9
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	4	0.9
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	3	0.9
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	4	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	8	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	8	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	8	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	9	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	9	0.9
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	9	0.9
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	9	0.89
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	20	0.89
(2,2448)	1:42:A:THR:HA	1:35:A:PRO:HG3	19	0.89
(2,2401)	1:53:A:GLU:HG3	1:56:A:ASN:HB2	15	0.89
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	9	0.89
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	17	0.89
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	2	0.89
(2,1635)	1:18:A:ASN:HB3	1:19:A:GLU:H	19	0.89
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	2	0.89
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	18	0.89
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	1	0.89
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	1	0.89
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	1	0.89
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	15	0.89
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD11	11	0.89
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD12	11	0.89
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD13	11	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	11	0.89
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	4	0.89
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	11	0.89
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	18	0.89
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	4	0.89
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	4	0.89
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	4	0.89
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	3	0.89
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	8	0.89
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	11	0.89
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	17	0.89
(1,369)	1:0:A:THR:HA	1:1:A:SER:HA	19	0.89
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	8	0.89
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	3	0.89
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	6	0.89
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	6	0.89
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	6	0.89
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	6	0.89
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	6	0.89
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	6	0.89
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	8	0.89
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	17	0.89
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	17	0.89
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	17	0.89
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD11	15	0.89
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD12	15	0.89
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD13	15	0.89
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	17	0.89
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	17	0.89
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	17	0.89
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	8	0.88
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	11	0.88
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	14	0.88
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	17	0.88
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	17	0.88
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	17	0.88
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	17	0.88
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	17	0.88
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	17	0.88
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	19	0.88
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	19	0.88
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	19	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	19	0.88
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	19	0.88
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	19	0.88
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	2	0.88
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	11	0.88
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	10	0.88
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	9	0.88
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	4	0.88
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	12	0.88
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	10	0.88
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	7	0.88
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	9	0.88
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	6	0.88
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	6	0.88
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	2	0.88
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	4	0.88
(1,369)	1:0:A:THR:HA	1:-1:A:MET:HA	12	0.88
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	10	0.88
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	1	0.88
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	19	0.88
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	19	0.88
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	19	0.88
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	5	0.87
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	10	0.87
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	6	0.87
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	6	0.87
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	6	0.87
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	6	0.87
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	6	0.87
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	6	0.87
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	6	0.87
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	11	0.87
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	11	0.87
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	11	0.87
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	11	0.87
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	11	0.87
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	11	0.87
(2,2264)	1:77:A:PRO:HB2	1:79:A:PHE:H	20	0.87
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	18	0.87
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	9	0.87
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	13	0.87
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	18	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	13	0.87
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	2	0.87
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	5	0.87
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	18	0.87
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	6	0.87
(2,1440)	1:65:A:ASP:HA	1:3:A:LYS:H	7	0.87
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	15	0.87
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	3	0.87
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	8	0.87
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	3	0.87
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	19	0.87
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	9	0.87
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	9	0.87
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	9	0.87
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	14	0.87
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	14	0.87
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	14	0.87
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	20	0.87
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	20	0.87
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	20	0.87
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	2	0.87
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	18	0.87
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	13	0.87
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	13	0.87
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	13	0.87
(1,234)	1:32:A:LYS:H	1:30:A:ALA:HA	11	0.87
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	3	0.87
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	2	0.87
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	2	0.87
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	2	0.87
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	5	0.87
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	5	0.87
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	5	0.87
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	17	0.86
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	9	0.86
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	9	0.86
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	9	0.86
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	9	0.86
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	9	0.86
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	9	0.86
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	3	0.86
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	9	0.86
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	8	0.86
(2,1869)	1:46:A:LYS:H	1:41:A:ASP:HB3	12	0.86
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	9	0.86
(2,1676)	1:23:A:LYS:H	1:23:A:LYS:HB3	11	0.86
(2,1630)	1:22:A:LEU:HD21	1:19:A:GLU:H	8	0.86
(2,1630)	1:22:A:LEU:HD22	1:19:A:GLU:H	8	0.86
(2,1630)	1:22:A:LEU:HD23	1:19:A:GLU:H	8	0.86
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	8	0.86
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	16	0.86
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	5	0.86
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	6	0.86
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	14	0.86
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	14	0.86
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	14	0.86
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	17	0.86
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	5	0.86
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	3	0.86
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	3	0.86
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	3	0.86
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	3	0.86
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	14	0.86
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	14	0.86
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	14	0.86
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	11	0.86
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	14	0.86
(1,418)	1:62:A:GLU:H	1:62:A:GLU:HG3	10	0.86
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	3	0.86
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	3	0.86
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	3	0.86
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	15	0.86
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG21	16	0.86
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG22	16	0.86
(1,290)	1:51:A:ALA:H	1:48:A:ILE:HG23	16	0.86
(1,244)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	17	0.86
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HB3	2	0.86
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB3	14	0.86
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD11	12	0.86
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD12	12	0.86
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD13	12	0.86
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	14	0.86
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	14	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	14	0.86
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	13	0.85
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	4	0.85
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	20	0.85
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	15	0.85
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	2	0.85
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	6	0.85
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	14	0.85
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	17	0.85
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	19	0.85
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	18	0.85
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	7	0.85
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	9	0.85
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	10	0.85
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	6	0.85
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	20	0.85
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	9	0.85
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	3	0.85
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	5	0.85
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	5	0.85
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	5	0.85
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	16	0.85
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	13	0.85
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	16	0.85
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	16	0.85
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	16	0.85
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	6	0.85
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	10	0.85
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	16	0.85
(1,398)	1:63:A:ILE:HG21	1:73:A:ARG:H	19	0.85
(1,398)	1:63:A:ILE:HG22	1:73:A:ARG:H	19	0.85
(1,398)	1:63:A:ILE:HG23	1:73:A:ARG:H	19	0.85
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	7	0.85
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	8	0.85
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	5	0.85
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	8	0.85
(1,207)	1:63:A:ILE:HG12	1:72:A:ALA:HA	20	0.85
(1,181)	1:21:A:GLU:HB2	1:24:A:LYS:HE3	3	0.85
(1,143)	1:29:A:ALA:HA	1:32:A:LYS:HA	7	0.85
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	8	0.85
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	5	0.84
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	11	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	15	0.84
(2,2222)	1:73:A:ARG:HB3	1:73:A:ARG:H	18	0.84
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	11	0.84
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	1	0.84
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	4	0.84
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	14	0.84
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	16	0.84
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	9	0.84
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	13	0.84
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	4	0.84
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	13	0.84
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	19	0.84
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	14	0.84
(2,1453)	1:4:A:GLU:H	1:6:A:LYS:HB3	2	0.84
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	17	0.84
(2,1388)	1:0:A:THR:HB	1:-1:A:MET:HA	20	0.84
(2,1133)	1:66:A:GLN:HB3	1:63:A:ILE:HA	4	0.84
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	1	0.84
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	3	0.84
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	8	0.84
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	6	0.84
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	8	0.84
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	14	0.84
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	14	0.84
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	14	0.84
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	14	0.84
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	14	0.84
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	14	0.84
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	14	0.84
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	14	0.84
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	14	0.84
(2,69)	1:6:A:LYS:HA	1:9:A:ASP:HB3	16	0.84
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	12	0.84
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	12	0.84
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	12	0.84
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	19	0.84
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	19	0.84
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	19	0.84
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	1	0.84
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	3	0.84
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	5	0.84
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	5	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	5	0.84
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	4	0.83
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	6	0.83
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	13	0.83
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	17	0.83
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	20	0.83
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	20	0.83
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	20	0.83
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	20	0.83
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	20	0.83
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	20	0.83
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	12	0.83
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	18	0.83
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	12	0.83
(2,2148)	1:68:A:GLY:H	1:66:A:GLN:HB2	14	0.83
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	10	0.83
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	1	0.83
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	3	0.83
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	7	0.83
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	14	0.83
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	9	0.83
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	9	0.83
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	13	0.83
(2,1070)	1:58:A:PRO:HB3	1:59:A:GLN:HA	13	0.83
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	16	0.83
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	8	0.83
(2,1010)	1:61:A:ARG:HG2	1:55:A:LEU:HA	19	0.83
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	12	0.83
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	12	0.83
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	12	0.83
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	15	0.83
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	15	0.83
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	15	0.83
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	18	0.83
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	15	0.83
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	15	0.83
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	2	0.83
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	2	0.83
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	2	0.83
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	6	0.83
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	6	0.83
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	6	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	20	0.83
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	20	0.83
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	20	0.83
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	17	0.83
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	7	0.83
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	7	0.83
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	7	0.83
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	13	0.83
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	19	0.83
(1,234)	1:33:A:TYR:HD1	1:30:A:ALA:HA	20	0.83
(1,234)	1:33:A:TYR:HD2	1:30:A:ALA:HA	20	0.83
(1,136)	1:6:A:LYS:HG2	1:6:A:LYS:HA	10	0.83
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	6	0.83
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	12	0.83
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD21	11	0.83
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD22	11	0.83
(1,25)	1:9:A:ASP:H	1:10:A:LEU:HD23	11	0.83
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	15	0.82
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	7	0.82
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	12	0.82
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	12	0.82
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	12	0.82
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	12	0.82
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	12	0.82
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	12	0.82
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	10	0.82
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	1	0.82
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	14	0.82
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	16	0.82
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	19	0.82
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	2	0.82
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	12	0.82
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	20	0.82
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	9	0.82
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	7	0.82
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	17	0.82
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	1	0.82
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	12	0.82
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	17	0.82
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	8	0.82
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	3	0.82
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	14	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	7	0.82
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	19	0.82
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	15	0.82
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	17	0.82
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	17	0.82
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	17	0.82
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	17	0.82
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	17	0.82
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	17	0.82
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	17	0.82
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	17	0.82
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	17	0.82
(2,133)	1:13:A:VAL:HG11	1:8:A:TYR:HB3	4	0.82
(2,133)	1:13:A:VAL:HG12	1:8:A:TYR:HB3	4	0.82
(2,133)	1:13:A:VAL:HG13	1:8:A:TYR:HB3	4	0.82
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	2	0.82
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	2	0.82
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	5	0.82
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	5	0.82
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	5	0.82
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	18	0.82
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	18	0.82
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	18	0.82
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	16	0.82
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	15	0.82
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	18	0.81
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	5	0.81
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	15	0.81
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	16	0.81
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	16	0.81
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	16	0.81
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	18	0.81
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	18	0.81
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	18	0.81
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	7	0.81
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	17	0.81
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	12	0.81
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	20	0.81
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	12	0.81
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	20	0.81
(2,241)	1:8:A:TYR:HB2	1:15:A:PRO:HA	3	0.81
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD11	11	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD12	11	0.81
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD13	11	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	1	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	4	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	5	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	7	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	9	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	11	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	13	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	14	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	16	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	18	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	19	0.81
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	20	0.81
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	7	0.81
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	7	0.81
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	18	0.81
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	14	0.81
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	14	0.81
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	14	0.81
(1,119)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	15	0.81
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	1	0.8
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	3	0.8
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	12	0.8
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD1	1	0.8
(2,2336)	1:8:A:TYR:HD1	1:52:A:PHE:HD2	1	0.8
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD1	1	0.8
(2,2336)	1:8:A:TYR:HD2	1:52:A:PHE:HD2	1	0.8
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	7	0.8
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	14	0.8
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	19	0.8
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	4	0.8
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	8	0.8
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	3	0.8
(2,2027)	1:60:A:LYS:H	1:59:A:GLN:HB3	12	0.8
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	5	0.8
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	16	0.8
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	8	0.8
(2,1507)	1:9:A:ASP:HB3	1:9:A:ASP:H	8	0.8
(2,1507)	1:9:A:ASP:HB3	1:9:A:ASP:H	16	0.8
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	9	0.8
(2,1484)	1:55:A:LEU:HD21	1:8:A:TYR:H	1	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1484)	1:55:A:LEU:HD22	1:8:A:TYR:H	1	0.8
(2,1484)	1:55:A:LEU:HD23	1:8:A:TYR:H	1	0.8
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	2	0.8
(2,1457)	1:2:A:VAL:HG21	1:4:A:GLU:H	7	0.8
(2,1457)	1:2:A:VAL:HG22	1:4:A:GLU:H	7	0.8
(2,1457)	1:2:A:VAL:HG23	1:4:A:GLU:H	7	0.8
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	9	0.8
(2,789)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	3	0.8
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	16	0.8
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	4	0.8
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	4	0.8
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	12	0.8
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	18	0.8
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	14	0.8
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	18	0.8
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	18	0.8
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	18	0.8
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	18	0.8
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	18	0.8
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	18	0.8
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	18	0.8
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	18	0.8
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	18	0.8
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	9	0.8
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	2	0.8
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	3	0.8
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	6	0.8
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	8	0.8
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	15	0.8
(1,374)	1:50:A:GLU:HA	1:50:A:GLU:HB3	17	0.8
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	10	0.8
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	11	0.8
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	2	0.8
(1,119)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	5	0.8
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	2	0.79
(2,2453)	1:48:A:ILE:HG12	1:47:A:GLU:H	20	0.79
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	13	0.79
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	5	0.79
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	5	0.79
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	5	0.79
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	17	0.79
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	17	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	17	0.79
(2,2409)	1:0:A:THR:HG21	1:7:A:LEU:HB2	11	0.79
(2,2409)	1:0:A:THR:HG22	1:7:A:LEU:HB2	11	0.79
(2,2409)	1:0:A:THR:HG23	1:7:A:LEU:HB2	11	0.79
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	5	0.79
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	4	0.79
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	7	0.79
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	3	0.79
(2,2170)	1:64:A:TYR:HE1	1:69:A:LEU:H	15	0.79
(2,2170)	1:64:A:TYR:HE2	1:69:A:LEU:H	15	0.79
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	15	0.79
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	14	0.79
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	7	0.79
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	8	0.79
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	1	0.79
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	10	0.79
(2,1494)	1:8:A:TYR:H	1:52:A:PHE:HA	19	0.79
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	20	0.79
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	15	0.79
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	7	0.79
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	6	0.79
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	9	0.79
(2,1083)	1:59:A:GLN:H	1:59:A:GLN:HG2	7	0.79
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	7	0.79
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	7	0.79
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	7	0.79
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	2	0.79
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	12	0.79
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	12	0.79
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	12	0.79
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	17	0.79
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	17	0.79
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	17	0.79
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	11	0.79
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	10	0.79
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	10	0.79
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	10	0.79
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	9	0.79
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	15	0.79
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	15	0.79
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	1	0.78
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2181)	1:70:A:GLU:H	1:70:A:GLU:HG3	3	0.78
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	10	0.78
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	17	0.78
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	3	0.78
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	7	0.78
(2,1505)	1:18:A:ASN:H	1:20:A:GLN:HB2	2	0.78
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	8	0.78
(2,1084)	1:59:A:GLN:H	1:59:A:GLN:HG3	16	0.78
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	6	0.78
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	6	0.78
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	6	0.78
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	6	0.78
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	6	0.78
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	6	0.78
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	13	0.78
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	13	0.78
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	13	0.78
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	17	0.78
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	18	0.78
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	18	0.78
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	18	0.78
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	2	0.78
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	11	0.78
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	14	0.78
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	4	0.78
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	20	0.78
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	14	0.78
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	5	0.78
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	17	0.78
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	8	0.78
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	8	0.78
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	8	0.78
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	8	0.78
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	8	0.78
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	8	0.78
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	8	0.78
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	8	0.78
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	8	0.78
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	10	0.78
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	10	0.78
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	10	0.78
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	10	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	10	0.78
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	10	0.78
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	10	0.78
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	10	0.78
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	10	0.78
(2,27)	1:2:A:VAL:HB	1:65:A:ASP:HA	12	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	1	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	1	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	1	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	2	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	2	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	2	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	3	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	3	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	3	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	4	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	4	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	4	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	5	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	5	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	5	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	6	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	6	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	6	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	7	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	7	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	7	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	9	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	9	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	9	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	10	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	10	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	10	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	11	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	11	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	11	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	13	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	13	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	13	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	14	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	14	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	14	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	15	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	15	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	15	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	18	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	18	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	18	0.78
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	20	0.78
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	20	0.78
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	20	0.78
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	18	0.78
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	1	0.78
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	5	0.78
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	11	0.78
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	11	0.78
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	11	0.78
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	1	0.78
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	1	0.78
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	3	0.78
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	11	0.78
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	15	0.78
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE3	5	0.77
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE3	5	0.77
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE3	5	0.77
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	11	0.77
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	6	0.77
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	8	0.77
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	19	0.77
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	20	0.77
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	8	0.77
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	15	0.77
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	15	0.77
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	15	0.77
(2,1191)	1:65:A:ASP:HA	1:3:A:LYS:H	19	0.77
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	3	0.77
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	13	0.77
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	15	0.77
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	11	0.77
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	10	0.77
(2,457)	1:23:A:LYS:H	1:23:A:LYS:HD2	17	0.77
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	1	0.77
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	1	0.77
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	1	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	8	0.77
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	14	0.77
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	17	0.77
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	9	0.77
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	15	0.77
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	15	0.77
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	15	0.77
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	15	0.77
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	15	0.77
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	15	0.77
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	15	0.77
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	15	0.77
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	15	0.77
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	8	0.77
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	8	0.77
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	8	0.77
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	12	0.77
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	12	0.77
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	12	0.77
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	16	0.77
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	16	0.77
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	16	0.77
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	6	0.77
(1,311)	1:51:A:ALA:H	1:54:A:ILE:HB	16	0.77
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	7	0.77
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	2	0.77
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE3	19	0.77
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE3	19	0.77
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	5	0.77
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	9	0.77
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	20	0.77
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	7	0.76
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	2	0.76
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	17	0.76
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	1	0.76
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	4	0.76
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	1	0.76
(2,2261)	1:77:A:PRO:HA	1:78:A:SER:H	20	0.76
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	6	0.76
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	3	0.76
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	20	0.76
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	13	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	7	0.76
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	16	0.76
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	17	0.76
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	3	0.76
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	8	0.76
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	10	0.76
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	12	0.76
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	6	0.76
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	6	0.76
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	6	0.76
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	2	0.76
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	16	0.76
(2,1251)	1:70:A:GLU:HA	1:70:A:GLU:HG3	3	0.76
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	17	0.76
(2,1084)	1:59:A:GLN:H	1:59:A:GLN:HG3	18	0.76
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	8	0.76
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	8	0.76
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	8	0.76
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	2	0.76
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	14	0.76
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	11	0.76
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	15	0.76
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	9	0.76
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	9	0.76
(2,27)	1:2:A:VAL:HB	1:65:A:ASP:HA	1	0.76
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	14	0.76
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	2	0.76
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	2	0.76
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	2	0.76
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD2	2	0.76
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	14	0.76
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	12	0.76
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	17	0.76
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	4	0.76
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	4	0.76
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	17	0.76
(1,69)	1:30:A:ALA:H	1:32:A:LYS:HB3	5	0.76
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	5	0.75
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	5	0.75
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	5	0.75
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	5	0.75
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	5	0.75
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	17	0.75
(2,2064)	1:62:A:GLU:HB3	1:62:A:GLU:H	12	0.75
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	9	0.75
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	13	0.75
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	1	0.75
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	14	0.75
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	17	0.75
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	16	0.75
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	2	0.75
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	2	0.75
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	2	0.75
(2,1443)	1:2:A:VAL:HB	1:3:A:LYS:H	19	0.75
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	2	0.75
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	15	0.75
(2,825)	1:60:A:LYS:HE2	1:60:A:LYS:H	4	0.75
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD21	19	0.75
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD22	19	0.75
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD23	19	0.75
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	10	0.75
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	7	0.75
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	4	0.75
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	3	0.75
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	3	0.75
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	3	0.75
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	3	0.75
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	3	0.75
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	3	0.75
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	8	0.75
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	8	0.75
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	8	0.75
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB3	12	0.75
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	13	0.75
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	11	0.74
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	13	0.74
(2,2398)	1:0:A:THR:HG21	1:6:A:LYS:HD2	8	0.74
(2,2398)	1:0:A:THR:HG22	1:6:A:LYS:HD2	8	0.74
(2,2398)	1:0:A:THR:HG23	1:6:A:LYS:HD2	8	0.74
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	7	0.74
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	13	0.74
(2,2344)	1:31:A:LEU:HD21	1:34:A:HIS:HD2	13	0.74
(2,2344)	1:31:A:LEU:HD22	1:34:A:HIS:HD2	13	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2344)	1:31:A:LEU:HD23	1:34:A:HIS:HD2	13	0.74
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	14	0.74
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	14	0.74
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	14	0.74
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	14	0.74
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	14	0.74
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	14	0.74
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	2	0.74
(2,2016)	1:59:A:GLN:H	1:58:A:PRO:HB3	18	0.74
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	3	0.74
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	12	0.74
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	19	0.74
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	19	0.74
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	19	0.74
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	19	0.74
(2,1133)	1:66:A:GLN:HB3	1:63:A:ILE:HA	1	0.74
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	8	0.74
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	8	0.74
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	8	0.74
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	16	0.74
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	12	0.74
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	8	0.74
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	8	0.74
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	8	0.74
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	16	0.74
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	16	0.74
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	13	0.74
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	4	0.74
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	10	0.74
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	13	0.74
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	13	0.74
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	13	0.74
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	14	0.74
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	14	0.74
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	14	0.74
(1,275)	1:26:A:TYR:H	1:24:A:LYS:HG3	5	0.74
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	2	0.74
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB3	1	0.74
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	17	0.73
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	8	0.73
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	7	0.73
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	13	0.73
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	2	0.73
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	15	0.73
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	17	0.73
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	15	0.73
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	20	0.73
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	18	0.73
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	2	0.73
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	15	0.73
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	6	0.73
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	6	0.73
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	9	0.73
(2,1084)	1:59:A:GLN:H	1:59:A:GLN:HG3	7	0.73
(2,1084)	1:59:A:GLN:H	1:59:A:GLN:HG3	10	0.73
(2,825)	1:60:A:LYS:H	1:60:A:LYS:HE3	12	0.73
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	18	0.73
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	11	0.73
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	7	0.73
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	20	0.73
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	20	0.73
(2,530)	1:27:A:ARG:HA	1:27:A:ARG:HG2	9	0.73
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	9	0.73
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	8	0.73
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	19	0.73
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	10	0.73
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	15	0.73
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	11	0.73
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	11	0.73
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	11	0.73
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	11	0.73
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	11	0.73
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	11	0.73
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	11	0.73
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	11	0.73
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	11	0.73
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	4	0.73
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	4	0.73
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG21	16	0.73
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG22	16	0.73
(1,201)	1:51:A:ALA:H	1:48:A:ILE:HG23	16	0.73
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	3	0.73
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	9	0.72
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	11	0.72
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	8	0.72
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	17	0.72
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	18	0.72
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	3	0.72
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	9	0.72
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	2	0.72
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	7	0.72
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	19	0.72
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	19	0.72
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	17	0.72
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	20	0.72
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	19	0.72
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	2	0.72
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	3	0.72
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	6	0.72
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD21	19	0.72
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD22	19	0.72
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD23	19	0.72
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	5	0.72
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	6	0.72
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	9	0.72
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	19	0.72
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	8	0.72
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	8	0.72
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	8	0.72
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	9	0.72
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	9	0.72
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	9	0.72
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	1	0.72
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	1	0.72
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	1	0.72
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	3	0.72
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	3	0.72
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	15	0.72
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	15	0.72
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	15	0.72
(1,364)	1:62:A:GLU:HB3	1:62:A:GLU:H	12	0.72
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	9	0.72
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	9	0.72
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	9	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:23:A:LYS:H	1:23:A:LYS:HD3	16	0.72
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	1	0.72
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	1	0.72
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	1	0.72
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	18	0.72
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	18	0.72
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	18	0.72
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	6	0.72
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	14	0.72
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	8	0.72
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	14	0.72
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	10	0.71
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	17	0.71
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	18	0.71
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	2	0.71
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	4	0.71
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	6	0.71
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	10	0.71
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	11	0.71
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	9	0.71
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	18	0.71
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	4	0.71
(2,2232)	1:73:A:ARG:HG2	1:74:A:SER:H	13	0.71
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	17	0.71
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	15	0.71
(2,1933)	1:52:A:PHE:H	1:8:A:TYR:HA	16	0.71
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	12	0.71
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	19	0.71
(2,1846)	1:43:A:GLU:HG2	1:44:A:LYS:H	11	0.71
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	5	0.71
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	2	0.71
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	14	0.71
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	5	0.71
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	20	0.71
(2,1340)	1:77:A:PRO:HA	1:78:A:SER:H	20	0.71
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	6	0.71
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	5	0.71
(2,693)	1:37:A:LYS:HD2	1:38:A:PRO:HD2	7	0.71
(2,551)	1:24:A:LYS:HA	1:27:A:ARG:HD3	16	0.71
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	7	0.71
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	17	0.71
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	17	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	14	0.71
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	13	0.71
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	20	0.71
(2,457)	1:23:A:LYS:H	1:23:A:LYS:HD3	18	0.71
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	11	0.71
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	11	0.71
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	11	0.71
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	11	0.71
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	11	0.71
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	17	0.71
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	17	0.71
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	9	0.71
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	4	0.71
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	14	0.71
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	14	0.71
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	14	0.71
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	14	0.71
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	14	0.71
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	14	0.71
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	14	0.71
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	14	0.71
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	14	0.71
(2,237)	1:15:A:PRO:HA	1:15:A:PRO:HG3	14	0.71
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	1	0.71
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	16	0.71
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	4	0.71
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	4	0.71
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	4	0.71
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	13	0.71
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	4	0.71
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	17	0.71
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	17	0.71
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	17	0.71
(1,136)	1:6:A:LYS:HG2	1:6:A:LYS:HA	19	0.71
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	3	0.71
(1,122)	1:18:A:ASN:H	1:21:A:GLU:HA	5	0.71
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	6	0.71
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	18	0.71
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	15	0.7
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	4	0.7
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	7	0.7
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	17	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	6	0.7
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	11	0.7
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	10	0.7
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	10	0.7
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	10	0.7
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	10	0.7
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	10	0.7
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	10	0.7
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	15	0.7
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	15	0.7
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	15	0.7
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	15	0.7
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	15	0.7
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	15	0.7
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	14	0.7
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	3	0.7
(2,2027)	1:60:A:LYS:H	1:59:A:GLN:HB2	13	0.7
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	6	0.7
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	11	0.7
(2,1938)	1:53:A:GLU:H	1:55:A:LEU:HB3	19	0.7
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	4	0.7
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	8	0.7
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	1	0.7
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	13	0.7
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	17	0.7
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	14	0.7
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	5	0.7
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	1	0.7
(2,907)	1:8:A:TYR:HB3	1:52:A:PHE:HA	1	0.7
(2,825)	1:60:A:LYS:H	1:60:A:LYS:HE3	6	0.7
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	12	0.7
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	19	0.7
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	18	0.7
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	1	0.7
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	1	0.7
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	1	0.7
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	2	0.7
(2,324)	1:22:A:LEU:HD21	1:19:A:GLU:HA	9	0.7
(2,324)	1:22:A:LEU:HD22	1:19:A:GLU:HA	9	0.7
(2,324)	1:22:A:LEU:HD23	1:19:A:GLU:HA	9	0.7
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	2	0.7
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	1	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	16	0.7
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	1	0.7
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	1	0.7
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	1	0.7
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	1	0.7
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	1	0.7
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	1	0.7
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	1	0.7
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	1	0.7
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	1	0.7
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	11	0.7
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	11	0.7
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	11	0.7
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	6	0.7
(2,54)	1:4:A:GLU:HG2	1:3:A:LYS:HD2	14	0.7
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	4	0.7
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	11	0.7
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	13	0.7
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	18	0.7
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	19	0.7
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	10	0.7
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	10	0.7
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	10	0.7
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	6	0.7
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	6	0.7
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	6	0.7
(1,278)	1:53:A:GLU:H	1:52:A:PHE:HA	15	0.7
(1,268)	1:51:A:ALA:HB1	1:11:A:LEU:HD21	5	0.7
(1,268)	1:51:A:ALA:HB1	1:11:A:LEU:HD22	5	0.7
(1,268)	1:51:A:ALA:HB1	1:11:A:LEU:HD23	5	0.7
(1,268)	1:51:A:ALA:HB2	1:11:A:LEU:HD21	5	0.7
(1,268)	1:51:A:ALA:HB2	1:11:A:LEU:HD22	5	0.7
(1,268)	1:51:A:ALA:HB2	1:11:A:LEU:HD23	5	0.7
(1,268)	1:51:A:ALA:HB3	1:11:A:LEU:HD21	5	0.7
(1,268)	1:51:A:ALA:HB3	1:11:A:LEU:HD22	5	0.7
(1,268)	1:51:A:ALA:HB3	1:11:A:LEU:HD23	5	0.7
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	6	0.7
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	15	0.7
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	15	0.7
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	15	0.7
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	4	0.7
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	13	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	19	0.7
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	12	0.7
(1,69)	1:30:A:ALA:H	1:32:A:LYS:HB3	7	0.7
(2,2413)	1:74:A:SER:HB3	1:78:A:SER:H	18	0.69
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	15	0.69
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	20	0.69
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	1	0.69
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	1	0.69
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	1	0.69
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	1	0.69
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	1	0.69
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	1	0.69
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	10	0.69
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	14	0.69
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	3	0.69
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	4	0.69
(2,2170)	1:64:A:TYR:HE1	1:69:A:LEU:H	18	0.69
(2,2170)	1:64:A:TYR:HE2	1:69:A:LEU:H	18	0.69
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	8	0.69
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	11	0.69
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	7	0.69
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	5	0.69
(2,1261)	1:70:A:GLU:HA	1:70:A:GLU:HG3	3	0.69
(2,1233)	1:68:A:GLY:HA3	1:69:A:LEU:HB2	7	0.69
(2,1133)	1:66:A:GLN:HB3	1:63:A:ILE:HA	2	0.69
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	16	0.69
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	7	0.69
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	9	0.69
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	11	0.69
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	14	0.69
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	18	0.69
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	4	0.69
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	15	0.69
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	11	0.69
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	9	0.69
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	9	0.69
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	9	0.69
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	16	0.69
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	1	0.69
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	1	0.69
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	1	0.69
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	3	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	3	0.69
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	3	0.69
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	20	0.69
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	20	0.69
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	20	0.69
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	12	0.69
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	12	0.69
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	12	0.69
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	12	0.69
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	12	0.69
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	12	0.69
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	12	0.69
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	12	0.69
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	12	0.69
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	15	0.69
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	9	0.69
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	10	0.69
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	10	0.69
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	20	0.69
(1,244)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	8	0.69
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	18	0.69
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	20	0.69
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	17	0.69
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	17	0.69
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	17	0.69
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	2	0.69
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	2	0.69
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	2	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	1	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	2	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	5	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	6	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	7	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	8	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	9	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	10	0.69
(1,115)	1:46:A:LYS:HA	1:46:A:LYS:HB2	11	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	14	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	15	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	16	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	17	0.69
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	20	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	3	0.69
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	15	0.69
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	2	0.69
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	4	0.69
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	4	0.69
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	4	0.69
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	20	0.68
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	14	0.68
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	2	0.68
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	9	0.68
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	5	0.68
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	6	0.68
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	10	0.68
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	12	0.68
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	14	0.68
(2,2192)	1:71:A:ALA:H	1:73:A:ARG:HG2	9	0.68
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	10	0.68
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	13	0.68
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	3	0.68
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	4	0.68
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	8	0.68
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	12	0.68
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	12	0.68
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	12	0.68
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	16	0.68
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	1	0.68
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	8	0.68
(2,1505)	1:18:A:ASN:H	1:20:A:GLN:HB2	8	0.68
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	11	0.68
(2,1460)	1:5:A:THR:H	1:5:A:THR:HG21	11	0.68
(2,1460)	1:5:A:THR:H	1:5:A:THR:HG22	11	0.68
(2,1460)	1:5:A:THR:H	1:5:A:THR:HG23	11	0.68
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	3	0.68
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	3	0.68
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	3	0.68
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	5	0.68
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	15	0.68
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	12	0.68
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	12	0.68
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	12	0.68
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	1	0.68
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	6	0.68
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	9	0.68
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	16	0.68
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	19	0.68
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	20	0.68
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	19	0.68
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	13	0.68
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	13	0.68
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	13	0.68
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	18	0.68
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	19	0.68
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	2	0.68
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	18	0.68
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	11	0.68
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	10	0.68
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	10	0.68
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	10	0.68
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	2	0.68
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	18	0.68
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	10	0.68
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	20	0.68
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	11	0.68
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	17	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	2	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	2	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	2	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	4	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	4	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	4	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	5	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	5	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	5	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	6	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	6	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	6	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	7	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	7	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	7	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	8	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	8	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	8	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	9	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	9	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	10	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	10	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	10	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	11	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	11	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	11	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	12	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	12	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	12	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	13	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	13	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	13	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	14	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	14	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	14	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	15	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	15	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	15	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	16	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	16	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	16	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	17	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	17	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	17	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	18	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	18	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	18	0.68
(2,220)	1:13:A:VAL:HG21	1:13:A:VAL:HA	19	0.68
(2,220)	1:13:A:VAL:HG22	1:13:A:VAL:HA	19	0.68
(2,220)	1:13:A:VAL:HG23	1:13:A:VAL:HA	19	0.68
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	17	0.68
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	17	0.68
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	17	0.68
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	17	0.68
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	17	0.68
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	17	0.68
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	13	0.68
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	13	0.68
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	13	0.68
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	19	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	19	0.68
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	19	0.68
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	20	0.68
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	20	0.68
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	20	0.68
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	3	0.68
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	12	0.68
(1,115)	1:70:A:GLU:HB2	1:70:A:GLU:HA	18	0.68
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	7	0.68
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	1	0.68
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	17	0.68
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	8	0.67
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	1	0.67
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	20	0.67
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE3	20	0.67
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE3	20	0.67
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE3	20	0.67
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	16	0.67
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	18	0.67
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	8	0.67
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	10	0.67
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	15	0.67
(2,2117)	1:66:A:GLN:H	1:62:A:GLU:HG2	12	0.67
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	9	0.67
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	16	0.67
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	20	0.67
(2,1846)	1:43:A:GLU:HG2	1:44:A:LYS:H	2	0.67
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	20	0.67
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	4	0.67
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	7	0.67
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	2	0.67
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	7	0.67
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	8	0.67
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	10	0.67
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	15	0.67
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	17	0.67
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	16	0.67
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	16	0.67
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	16	0.67
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	15	0.67
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	19	0.67
(2,823)	1:0:A:THR:HG21	1:6:A:LYS:HE3	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,823)	1:0:A:THR:HG22	1:6:A:LYS:HE3	19	0.67
(2,823)	1:0:A:THR:HG23	1:6:A:LYS:HE3	19	0.67
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	4	0.67
(2,766)	1:69:A:LEU:HD21	1:73:A:ARG:HA	14	0.67
(2,766)	1:69:A:LEU:HD22	1:73:A:ARG:HA	14	0.67
(2,766)	1:69:A:LEU:HD23	1:73:A:ARG:HA	14	0.67
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	10	0.67
(2,726)	1:33:A:TYR:HD1	1:41:A:ASP:HB2	3	0.67
(2,726)	1:33:A:TYR:HD2	1:41:A:ASP:HB2	3	0.67
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	15	0.67
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	8	0.67
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	15	0.67
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	16	0.67
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	14	0.67
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	14	0.67
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	20	0.67
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	20	0.67
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	5	0.67
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	9	0.67
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	10	0.67
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	9	0.67
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	19	0.67
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	19	0.67
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	19	0.67
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	19	0.67
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	19	0.67
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	19	0.67
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	19	0.67
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	19	0.67
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	19	0.67
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	2	0.67
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	16	0.67
(1,406)	1:37:A:LYS:HD2	1:38:A:PRO:HD2	7	0.67
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	12	0.67
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	12	0.67
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	2	0.67
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	2	0.67
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	2	0.67
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	3	0.67
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	3	0.67
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	3	0.67
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,275)	1:26:A:TYR:H	1:22:A:LEU:HB2	8	0.67
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	13	0.67
(1,207)	1:48:A:ILE:HG12	1:30:A:ALA:HA	13	0.67
(1,91)	1:26:A:TYR:H	1:29:A:ALA:HB1	5	0.67
(1,91)	1:26:A:TYR:H	1:29:A:ALA:HB2	5	0.67
(1,91)	1:26:A:TYR:H	1:29:A:ALA:HB3	5	0.67
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	15	0.67
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	12	0.67
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	16	0.67
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	5	0.66
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	3	0.66
(2,2260)	1:78:A:SER:H	1:78:A:SER:HB3	19	0.66
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	18	0.66
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	18	0.66
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	1	0.66
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	16	0.66
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	14	0.66
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	10	0.66
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	19	0.66
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	10	0.66
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	15	0.66
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	10	0.66
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	4	0.66
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	1	0.66
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	14	0.66
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	20	0.66
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	20	0.66
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	20	0.66
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	4	0.66
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	11	0.66
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	20	0.66
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	20	0.66
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	20	0.66
(2,1083)	1:59:A:GLN:H	1:59:A:GLN:HG2	10	0.66
(2,919)	1:52:A:PHE:HB2	1:8:A:TYR:HA	16	0.66
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	1	0.66
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	1	0.66
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	1	0.66
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	6	0.66
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	14	0.66
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG21	4	0.66
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG22	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG23	4	0.66
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	3	0.66
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	8	0.66
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	15	0.66
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	17	0.66
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	17	0.66
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	17	0.66
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	14	0.66
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	19	0.66
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	12	0.66
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	16	0.66
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	20	0.66
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	6	0.66
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	8	0.66
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	8	0.66
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	8	0.66
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	8	0.66
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	8	0.66
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	8	0.66
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	8	0.66
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	8	0.66
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	8	0.66
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	15	0.66
(2,241)	1:8:A:TYR:HB2	1:15:A:PRO:HA	19	0.66
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	5	0.66
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	4	0.66
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	4	0.66
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	4	0.66
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	16	0.66
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	7	0.66
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	7	0.66
(1,278)	1:53:A:GLU:H	1:52:A:PHE:HA	18	0.66
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	3	0.66
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	14	0.66
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	14	0.66
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	14	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	2	0.66
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	4	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	5	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	6	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	9	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	10	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	12	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	14	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	15	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	17	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	18	0.66
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	19	0.66
(1,110)	1:50:A:GLU:HG2	1:54:A:ILE:HB	12	0.66
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	14	0.66
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	18	0.66
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	20	0.66
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	20	0.66
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	20	0.66
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	2	0.66
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	8	0.66
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	10	0.66
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	11	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	4	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	7	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	13	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	14	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	17	0.66
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	19	0.66
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	14	0.65
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	18	0.65
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	8	0.65
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	17	0.65
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	19	0.65
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	13	0.65
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	7	0.65
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	15	0.65
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	2	0.65
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	10	0.65
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	11	0.65
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	14	0.65
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	15	0.65
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	9	0.65
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	9	0.65
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	9	0.65
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	7	0.65
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	6	0.65
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	5	0.65
(2,1454)	1:3:A:LYS:HB3	1:4:A:GLU:H	18	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	12	0.65
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	12	0.65
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	12	0.65
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	2	0.65
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	2	0.65
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	2	0.65
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	2	0.65
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	2	0.65
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	2	0.65
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	4	0.65
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	14	0.65
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	10	0.65
(2,901)	1:55:A:LEU:HB3	1:52:A:PHE:HA	19	0.65
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	14	0.65
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	14	0.65
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	14	0.65
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	20	0.65
(2,530)	1:27:A:ARG:HA	1:27:A:ARG:HG2	2	0.65
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	14	0.65
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	11	0.65
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	11	0.65
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	4	0.65
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	7	0.65
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	7	0.65
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	7	0.65
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	7	0.65
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	7	0.65
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	7	0.65
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	7	0.65
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	7	0.65
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	7	0.65
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	14	0.65
(2,29)	1:2:A:VAL:HB	1:3:A:LYS:H	19	0.65
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD11	1	0.65
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD12	1	0.65
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD13	1	0.65
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	7	0.65
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	15	0.65
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	18	0.65
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	18	0.65
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	18	0.65
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	8	0.65
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	8	0.65
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	14	0.65
(1,244)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	20	0.65
(1,216)	1:21:A:GLU:HB2	1:21:A:GLU:HA	1	0.65
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	11	0.65
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	11	0.65
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	11	0.65
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	11	0.65
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	7	0.65
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	11	0.65
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	12	0.65
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	13	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	1	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	2	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	5	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	6	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	8	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	9	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	10	0.65
(1,19)	1:46:A:LYS:HA	1:46:A:LYS:HB2	11	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	12	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	15	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	16	0.65
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	20	0.65
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG2	13	0.65
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	8	0.64
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	14	0.64
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	6	0.64
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	20	0.64
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	2	0.64
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	8	0.64
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	5	0.64
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	14	0.64
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	17	0.64
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	4	0.64
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	5	0.64
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	12	0.64
(2,2020)	1:58:A:PRO:HD3	1:59:A:GLN:H	19	0.64
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	17	0.64
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	6	0.64
(2,1796)	1:34:A:HIS:HB2	1:34:A:HIS:H	11	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	11	0.64
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	4	0.64
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	4	0.64
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	4	0.64
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	5	0.64
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	2	0.64
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	2	0.64
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	1	0.64
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	3	0.64
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	17	0.64
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	17	0.64
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	17	0.64
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	11	0.64
(2,1193)	1:2:A:VAL:HG21	1:65:A:ASP:HB3	4	0.64
(2,1193)	1:2:A:VAL:HG22	1:65:A:ASP:HB3	4	0.64
(2,1193)	1:2:A:VAL:HG23	1:65:A:ASP:HB3	4	0.64
(2,1083)	1:59:A:GLN:H	1:59:A:GLN:HG2	18	0.64
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	15	0.64
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	15	0.64
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	15	0.64
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	5	0.64
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	19	0.64
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	1	0.64
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	1	0.64
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	1	0.64
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	12	0.64
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	16	0.64
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	19	0.64
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	19	0.64
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	19	0.64
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	18	0.64
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	10	0.64
(2,240)	1:8:A:TYR:HB3	1:15:A:PRO:HA	3	0.64
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	7	0.64
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	12	0.64
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	12	0.64
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	12	0.64
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	12	0.64
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	12	0.64
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	12	0.64
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	12	0.64
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	12	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	12	0.64
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD1	19	0.64
(1,366)	1:55:A:LEU:HB2	1:52:A:PHE:HD2	19	0.64
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	11	0.64
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	11	0.64
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	11	0.64
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	12	0.64
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	12	0.64
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	12	0.64
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	16	0.64
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	3	0.64
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	9	0.64
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	17	0.64
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	3	0.64
(1,19)	1:70:A:GLU:HB2	1:70:A:GLU:HA	18	0.64
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	7	0.63
(2,2423)	1:44:A:LYS:HD3	1:45:A:PHE:HA	15	0.63
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	18	0.63
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	18	0.63
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	2	0.63
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	2	0.63
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	18	0.63
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	5	0.63
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	16	0.63
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	6	0.63
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	3	0.63
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	9	0.63
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	11	0.63
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	9	0.63
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	18	0.63
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	9	0.63
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	14	0.63
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	20	0.63
(2,1933)	1:52:A:PHE:H	1:8:A:TYR:HA	12	0.63
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	5	0.63
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	7	0.63
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	10	0.63
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	19	0.63
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	8	0.63
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	14	0.63
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	14	0.63
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	14	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1653)	1:21:A:GLU:H	1:20:A:GLN:HB2	2	0.63
(2,1623)	1:18:A:ASN:H	1:21:A:GLU:HB3	5	0.63
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	8	0.63
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	19	0.63
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	9	0.63
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	18	0.63
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	6	0.63
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	6	0.63
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	6	0.63
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	12	0.63
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	6	0.63
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	6	0.63
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	6	0.63
(2,930)	1:53:A:GLU:HG3	1:53:A:GLU:HA	15	0.63
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	3	0.63
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	3	0.63
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	3	0.63
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	16	0.63
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	11	0.63
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	17	0.63
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	1	0.63
(2,530)	1:27:A:ARG:HA	1:27:A:ARG:HG2	6	0.63
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	4	0.63
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	10	0.63
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	8	0.63
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	13	0.63
(2,280)	1:14:A:SER:HB2	1:16:A:SER:H	8	0.63
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	7	0.63
(2,238)	1:22:A:LEU:HD21	1:15:A:PRO:HA	20	0.63
(2,238)	1:22:A:LEU:HD22	1:15:A:PRO:HA	20	0.63
(2,238)	1:22:A:LEU:HD23	1:15:A:PRO:HA	20	0.63
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD11	16	0.63
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD12	16	0.63
(2,215)	1:51:A:ALA:HB1	1:11:A:LEU:HD13	16	0.63
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD11	16	0.63
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD12	16	0.63
(2,215)	1:51:A:ALA:HB2	1:11:A:LEU:HD13	16	0.63
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD11	16	0.63
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD12	16	0.63
(2,215)	1:51:A:ALA:HB3	1:11:A:LEU:HD13	16	0.63
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	20	0.63
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	13	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	13	0.63
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	13	0.63
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	2	0.63
(1,275)	1:26:A:TYR:H	1:22:A:LEU:HB2	4	0.63
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	6	0.63
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	6	0.63
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	6	0.63
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	9	0.63
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	9	0.63
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	9	0.63
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	16	0.63
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	16	0.63
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	16	0.63
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	17	0.63
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	17	0.63
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	17	0.63
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	4	0.63
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	4	0.63
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	4	0.63
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	3	0.63
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	10	0.63
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	10	0.63
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	10	0.63
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	6	0.63
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	5	0.63
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	6	0.63
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	9	0.62
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	7	0.62
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	12	0.62
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	16	0.62
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	11	0.62
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	5	0.62
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	10	0.62
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	16	0.62
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	17	0.62
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	18	0.62
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	20	0.62
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	6	0.62
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	13	0.62
(2,1796)	1:34:A:HIS:HB2	1:34:A:HIS:H	19	0.62
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	2	0.62
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	4	0.62
(2,1566)	1:11:A:LEU:HB2	1:13:A:VAL:H	5	0.62
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	15	0.62
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG21	12	0.62
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG22	12	0.62
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG23	12	0.62
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	2	0.62
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	3	0.62
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	14	0.62
(2,907)	1:8:A:TYR:HB3	1:52:A:PHE:HA	10	0.62
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	9	0.62
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	3	0.62
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	3	0.62
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	3	0.62
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	13	0.62
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	12	0.62
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG21	11	0.62
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG22	11	0.62
(2,751)	1:47:A:GLU:HG2	1:48:A:ILE:HG23	11	0.62
(2,529)	1:27:A:ARG:HA	1:27:A:ARG:HG3	9	0.62
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	9	0.62
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	9	0.62
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	9	0.62
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	9	0.62
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	9	0.62
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	9	0.62
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	9	0.62
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	9	0.62
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	9	0.62
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	5	0.62
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	17	0.62
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	12	0.62
(2,13)	1:2:A:VAL:HA	1:4:A:GLU:HG2	8	0.62
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	6	0.62
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	6	0.62
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	12	0.62
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	5	0.62
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	19	0.62
(1,332)	1:70:A:GLU:HA	1:73:A:ARG:HG3	15	0.62
(1,314)	1:60:A:LYS:HE3	1:57:A:ASP:H	12	0.62
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	2	0.62
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	2	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	2	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	1	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	1	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	1	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	2	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	2	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	2	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	3	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	3	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	3	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	4	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	4	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	4	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	8	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	8	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	8	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	10	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	10	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	10	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	11	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	11	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	11	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	14	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	14	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	14	0.62
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	18	0.62
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	18	0.62
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	18	0.62
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	1	0.62
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	1	0.62
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	1	0.62
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	10	0.62
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	10	0.62
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	10	0.62
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	14	0.62
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	18	0.62
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	20	0.62
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	1	0.62
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	20	0.62
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	6	0.62
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	6	0.62
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	2	0.61
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	14	0.61
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	18	0.61
(2,2219)	1:73:A:ARG:H	1:69:A:LEU:HG	7	0.61
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	1	0.61
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	19	0.61
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	11	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	1	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	7	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	8	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	11	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	13	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	15	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	18	0.61
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	19	0.61
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	2	0.61
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	1	0.61
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	12	0.61
(2,1796)	1:34:A:HIS:HB2	1:34:A:HIS:H	1	0.61
(2,1796)	1:34:A:HIS:HB2	1:34:A:HIS:H	20	0.61
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	6	0.61
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	6	0.61
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	6	0.61
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	18	0.61
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	18	0.61
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	18	0.61
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	4	0.61
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	4	0.61
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	8	0.61
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	16	0.61
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	20	0.61
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	3	0.61
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	6	0.61
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	8	0.61
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	1	0.61
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	17	0.61
(2,1494)	1:8:A:TYR:H	1:52:A:PHE:HA	16	0.61
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	12	0.61
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	12	0.61
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	12	0.61
(2,1083)	1:59:A:GLN:H	1:59:A:GLN:HG2	16	0.61
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	12	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	9	0.61
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	9	0.61
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	9	0.61
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	8	0.61
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	14	0.61
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	12	0.61
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	12	0.61
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	12	0.61
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD21	19	0.61
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD22	19	0.61
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD23	19	0.61
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	7	0.61
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	7	0.61
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	7	0.61
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	17	0.61
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	17	0.61
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	17	0.61
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	3	0.61
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	12	0.61
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	13	0.61
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	20	0.61
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	1	0.61
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	16	0.61
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	18	0.61
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	18	0.61
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	18	0.61
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	10	0.61
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	17	0.61
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	6	0.61
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	6	0.61
(1,437)	1:19:A:GLU:HB3	1:19:A:GLU:HA	17	0.61
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	16	0.61
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	20	0.61
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB1	8	0.61
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB2	8	0.61
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB3	8	0.61
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	6	0.61
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	6	0.61
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	6	0.61
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	13	0.61
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	13	0.61
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	5	0.61
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	5	0.61
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	5	0.61
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	7	0.61
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	7	0.61
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	7	0.61
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	15	0.61
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	15	0.61
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	15	0.61
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	19	0.61
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	19	0.61
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	19	0.61
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	20	0.61
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	20	0.61
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	20	0.61
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	7	0.61
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	7	0.61
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	7	0.61
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	11	0.61
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	11	0.61
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	11	0.61
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	9	0.61
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	9	0.61
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	9	0.61
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	13	0.61
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	10	0.61
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	9	0.61
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	14	0.61
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	18	0.61
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	18	0.61
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	18	0.61
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG2	5	0.61
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	17	0.6
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	17	0.6
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	17	0.6
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	18	0.6
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	18	0.6
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	16	0.6
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	4	0.6
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	2	0.6
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	15	0.6
(2,2164)	1:69:A:LEU:H	1:69:A:LEU:HB2	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	13	0.6
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	16	0.6
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	2	0.6
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	3	0.6
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	12	0.6
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	13	0.6
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	1	0.6
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	3	0.6
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	1	0.6
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	17	0.6
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	18	0.6
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	19	0.6
(2,1796)	1:34:A:HIS:HB2	1:34:A:HIS:H	13	0.6
(2,1653)	1:21:A:GLU:H	1:20:A:GLN:HB2	8	0.6
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	11	0.6
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	17	0.6
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	7	0.6
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	1	0.6
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	1	0.6
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	1	0.6
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	9	0.6
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	9	0.6
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	9	0.6
(2,1123)	1:70:A:GLU:HA	1:73:A:ARG:HD2	2	0.6
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	16	0.6
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	16	0.6
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	16	0.6
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	12	0.6
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	12	0.6
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	12	0.6
(2,771)	1:41:A:ASP:HB3	1:44:A:LYS:HB2	15	0.6
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	9	0.6
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	8	0.6
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD21	5	0.6
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD22	5	0.6
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD23	5	0.6
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	10	0.6
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	13	0.6
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	13	0.6
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	13	0.6
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	17	0.6
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	19	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	16	0.6
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	16	0.6
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	16	0.6
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	10	0.6
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	2	0.6
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	2	0.6
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	2	0.6
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	2	0.6
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	2	0.6
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	2	0.6
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	5	0.6
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	5	0.6
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	5	0.6
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	5	0.6
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	5	0.6
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	5	0.6
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	15	0.6
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	15	0.6
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	15	0.6
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	14	0.6
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	1	0.6
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	9	0.6
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB1	1	0.6
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB2	1	0.6
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB3	1	0.6
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	11	0.6
(1,321)	1:51:A:ALA:HB1	1:52:A:PHE:HA	15	0.6
(1,321)	1:51:A:ALA:HB2	1:52:A:PHE:HA	15	0.6
(1,321)	1:51:A:ALA:HB3	1:52:A:PHE:HA	15	0.6
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	12	0.6
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	12	0.6
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	12	0.6
(1,251)	1:48:A:ILE:HG21	1:48:A:ILE:H	13	0.6
(1,251)	1:48:A:ILE:HG22	1:48:A:ILE:H	13	0.6
(1,251)	1:48:A:ILE:HG23	1:48:A:ILE:H	13	0.6
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	20	0.6
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	13	0.6
(1,134)	1:22:A:LEU:HA	1:22:A:LEU:HB3	11	0.6
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	9	0.6
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	17	0.6
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	17	0.6
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	17	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	9	0.6
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	18	0.6
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	4	0.6
(1,58)	1:65:A:ASP:H	1:63:A:ILE:HB	16	0.6
(1,47)	1:2:A:VAL:HB	1:65:A:ASP:H	6	0.6
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	15	0.6
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	19	0.6
(1,12)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	6	0.6
(1,12)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	0.6
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	8	0.59
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	8	0.59
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	8	0.59
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	18	0.59
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	3	0.59
(2,2275)	1:78:A:SER:HA	1:80:A:GLY:H	17	0.59
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	5	0.59
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	12	0.59
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	8	0.59
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	1	0.59
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	1	0.59
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	6	0.59
(2,2028)	1:60:A:LYS:HB3	1:60:A:LYS:H	6	0.59
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	11	0.59
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	13	0.59
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	7	0.59
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	8	0.59
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	9	0.59
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	14	0.59
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	20	0.59
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	12	0.59
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	10	0.59
(2,1695)	1:21:A:GLU:HB2	1:25:A:GLY:H	3	0.59
(2,1644)	1:18:A:ASN:HB3	1:20:A:GLN:H	3	0.59
(2,1631)	1:19:A:GLU:H	1:22:A:LEU:HB3	3	0.59
(2,1630)	1:22:A:LEU:HD21	1:19:A:GLU:H	9	0.59
(2,1630)	1:22:A:LEU:HD22	1:19:A:GLU:H	9	0.59
(2,1630)	1:22:A:LEU:HD23	1:19:A:GLU:H	9	0.59
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	13	0.59
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	9	0.59
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	8	0.59
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	4	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	1	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	3	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	5	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	6	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	7	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	8	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	9	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	11	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	12	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	15	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	16	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	19	0.59
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	20	0.59
(2,1110)	1:55:A:LEU:HD11	1:61:A:ARG:HA	16	0.59
(2,1110)	1:55:A:LEU:HD12	1:61:A:ARG:HA	16	0.59
(2,1110)	1:55:A:LEU:HD13	1:61:A:ARG:HA	16	0.59
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	3	0.59
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	16	0.59
(2,642)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	5	0.59
(2,642)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	5	0.59
(2,642)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	5	0.59
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	19	0.59
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	19	0.59
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	19	0.59
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	16	0.59
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	16	0.59
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	19	0.59
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	19	0.59
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	19	0.59
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	2	0.59
(2,367)	1:20:A:GLN:H	1:20:A:GLN:HG3	13	0.59
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	4	0.59
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB1	12	0.59
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB2	12	0.59
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB3	12	0.59
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB1	12	0.59
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB2	12	0.59
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB3	12	0.59
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB1	12	0.59
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB2	12	0.59
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB3	12	0.59
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	18	0.59
(2,140)	1:13:A:VAL:HG11	1:9:A:ASP:HA	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:13:A:VAL:HG12	1:9:A:ASP:HA	20	0.59
(2,140)	1:13:A:VAL:HG13	1:9:A:ASP:HA	20	0.59
(2,13)	1:2:A:VAL:HA	1:4:A:GLU:HG2	1	0.59
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	6	0.59
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	6	0.59
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	7	0.59
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	14	0.59
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	15	0.59
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	19	0.59
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	19	0.59
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	19	0.59
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	1	0.59
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	1	0.59
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	1	0.59
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	8	0.59
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	7	0.59
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	7	0.59
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	7	0.59
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	13	0.59
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	13	0.59
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	13	0.59
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	16	0.59
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	8	0.59
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	10	0.59
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	6	0.59
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	19	0.59
(1,12)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	16	0.59
(1,12)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	20	0.59
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	14	0.58
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	14	0.58
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	14	0.58
(2,2401)	1:53:A:GLU:HG2	1:56:A:ASN:HB2	5	0.58
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	9	0.58
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	15	0.58
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	15	0.58
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	5	0.58
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	8	0.58
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	6	0.58
(2,1938)	1:53:A:GLU:H	1:55:A:LEU:HB3	12	0.58
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	4	0.58
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	5	0.58
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	13	0.58
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	16	0.58
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	17	0.58
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	12	0.58
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	1	0.58
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	12	0.58
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	15	0.58
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	5	0.58
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	1	0.58
(2,1188)	1:2:A:VAL:HB	1:65:A:ASP:HA	10	0.58
(2,1188)	1:2:A:VAL:HB	1:65:A:ASP:HA	13	0.58
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	3	0.58
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	19	0.58
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	6	0.58
(2,606)	1:30:A:ALA:HA	1:34:A:HIS:HB3	18	0.58
(2,434)	1:22:A:LEU:HD11	1:11:A:LEU:H	3	0.58
(2,434)	1:22:A:LEU:HD12	1:11:A:LEU:H	3	0.58
(2,434)	1:22:A:LEU:HD13	1:11:A:LEU:H	3	0.58
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	12	0.58
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	12	0.58
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	12	0.58
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	6	0.58
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	17	0.58
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	20	0.58
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	12	0.58
(2,213)	1:52:A:PHE:HB3	1:11:A:LEU:HD11	5	0.58
(2,213)	1:52:A:PHE:HB3	1:11:A:LEU:HD12	5	0.58
(2,213)	1:52:A:PHE:HB3	1:11:A:LEU:HD13	5	0.58
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	18	0.58
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	18	0.58
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	18	0.58
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	18	0.58
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	18	0.58
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	18	0.58
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	4	0.58
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	13	0.58
(1,314)	1:60:A:LYS:HE3	1:57:A:ASP:H	6	0.58
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	20	0.58
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	20	0.58
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	20	0.58
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	13	0.58
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	15	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	5	0.58
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	5	0.58
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	5	0.58
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	8	0.58
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	8	0.58
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	8	0.58
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	12	0.58
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	12	0.58
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	12	0.58
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	2	0.58
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	3	0.58
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	13	0.58
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	7	0.58
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	3	0.57
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	6	0.57
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	6	0.57
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	19	0.57
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	13	0.57
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	4	0.57
(2,1870)	1:45:A:PHE:HB2	1:46:A:LYS:H	17	0.57
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	15	0.57
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	13	0.57
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	2	0.57
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	15	0.57
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	14	0.57
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	17	0.57
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	10	0.57
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	10	0.57
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	10	0.57
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	19	0.57
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	15	0.57
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	15	0.57
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	15	0.57
(2,1191)	1:65:A:ASP:HA	1:3:A:LYS:H	7	0.57
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	2	0.57
(2,901)	1:55:A:LEU:HB3	1:52:A:PHE:HA	12	0.57
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	20	0.57
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	2	0.57
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	16	0.57
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	16	0.57
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	16	0.57
(2,567)	1:24:A:LYS:HE2	1:24:A:LYS:H	12	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	20	0.57
(2,458)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	20	0.57
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	14	0.57
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	14	0.57
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	14	0.57
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	12	0.57
(2,238)	1:22:A:LEU:HD21	1:15:A:PRO:HA	1	0.57
(2,238)	1:22:A:LEU:HD22	1:15:A:PRO:HA	1	0.57
(2,238)	1:22:A:LEU:HD23	1:15:A:PRO:HA	1	0.57
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	16	0.57
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	6	0.57
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	20	0.57
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	20	0.57
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	20	0.57
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	20	0.57
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	20	0.57
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	20	0.57
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	6	0.57
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	6	0.57
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	6	0.57
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	3	0.57
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	8	0.57
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	11	0.57
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	13	0.57
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB1	5	0.57
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB2	5	0.57
(1,429)	1:7:A:LEU:H	1:51:A:ALA:HB3	5	0.57
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	2	0.57
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	8	0.57
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	13	0.57
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	13	0.57
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	13	0.57
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	1	0.57
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	19	0.57
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	19	0.57
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	19	0.57
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	17	0.57
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	17	0.57
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	10	0.57
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	18	0.57
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	20	0.57
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	2	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	5	0.57
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	5	0.57
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	5	0.57
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE2	4	0.56
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE2	4	0.56
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE2	4	0.56
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	3	0.56
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	4	0.56
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	9	0.56
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	15	0.56
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	13	0.56
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	13	0.56
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	2	0.56
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	2	0.56
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	2	0.56
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	18	0.56
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	1	0.56
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	6	0.56
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	11	0.56
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	19	0.56
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	9	0.56
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	11	0.56
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	12	0.56
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	8	0.56
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	8	0.56
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	8	0.56
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	8	0.56
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	8	0.56
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	8	0.56
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	5	0.56
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	5	0.56
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	5	0.56
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	10	0.56
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	10	0.56
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	10	0.56
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	11	0.56
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	11	0.56
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	11	0.56
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	17	0.56
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	8	0.56
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	8	0.56
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	10	0.56
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	10	0.56
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	10	0.56
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	1	0.56
(2,771)	1:41:A:ASP:HB3	1:44:A:LYS:HB2	12	0.56
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	19	0.56
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	13	0.56
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	1	0.56
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	6	0.56
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	7	0.56
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	1	0.56
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	1	0.56
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	1	0.56
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	2	0.56
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	2	0.56
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	15	0.56
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	15	0.56
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	15	0.56
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	6	0.56
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	16	0.56
(2,64)	1:5:A:THR:HG21	1:5:A:THR:HA	14	0.56
(2,64)	1:5:A:THR:HG22	1:5:A:THR:HA	14	0.56
(2,64)	1:5:A:THR:HG23	1:5:A:THR:HA	14	0.56
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	17	0.56
(2,14)	1:2:A:VAL:HA	1:4:A:GLU:HG3	16	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	3	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	3	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	3	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	3	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	3	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	3	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	9	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	9	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	9	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	9	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	9	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	9	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	15	0.56
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	15	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	15	0.56
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	15	0.56
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	15	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	15	0.56
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	2	0.56
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	17	0.56
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	10	0.56
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	12	0.56
(1,288)	1:26:A:TYR:HA	1:11:A:LEU:HD21	5	0.56
(1,288)	1:26:A:TYR:HA	1:11:A:LEU:HD22	5	0.56
(1,288)	1:26:A:TYR:HA	1:11:A:LEU:HD23	5	0.56
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	4	0.56
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	4	0.56
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	4	0.56
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HB3	11	0.56
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	15	0.56
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	4	0.56
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	4	0.56
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	4	0.56
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	10	0.56
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	11	0.56
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	7	0.56
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	11	0.56
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	5	0.56
(1,12)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	12	0.56
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	1	0.56
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	1	0.56
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	1	0.56
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	18	0.55
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	18	0.55
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	15	0.55
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	2	0.55
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	7	0.55
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	14	0.55
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	2	0.55
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	5	0.55
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	2	0.55
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	11	0.55
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	2	0.55
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	20	0.55
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	3	0.55
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	20	0.55
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	10	0.55
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	1	0.55
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	16	0.55
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	19	0.55
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	18	0.55
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	14	0.55
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	1	0.55
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	1	0.55
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	1	0.55
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	19	0.55
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	11	0.55
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	19	0.55
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	19	0.55
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	19	0.55
(2,553)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	14	0.55
(2,553)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	14	0.55
(2,553)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	14	0.55
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	1	0.55
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	1	0.55
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	4	0.55
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	4	0.55
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	10	0.55
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	10	0.55
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	10	0.55
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	11	0.55
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	11	0.55
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	11	0.55
(2,369)	1:21:A:GLU:HA	1:21:A:GLU:HG3	1	0.55
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	1	0.55
(2,304)	1:21:A:GLU:HB3	1:18:A:ASN:HA	5	0.55
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	1	0.55
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	10	0.55
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	10	0.55
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	10	0.55
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	3	0.55
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD11	20	0.55
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD12	20	0.55
(1,450)	1:53:A:GLU:H	1:11:A:LEU:HD13	20	0.55
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	18	0.55
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	2	0.55
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	2	0.55
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	2	0.55
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD11	8	0.55
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD12	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD13	8	0.55
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	3	0.55
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	3	0.55
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	3	0.55
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	18	0.55
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	6	0.55
(1,244)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	18	0.55
(1,233)	1:10:A:LEU:HD11	1:10:A:LEU:HA	8	0.55
(1,233)	1:10:A:LEU:HD12	1:10:A:LEU:HA	8	0.55
(1,233)	1:10:A:LEU:HD13	1:10:A:LEU:HA	8	0.55
(1,233)	1:10:A:LEU:HD11	1:10:A:LEU:HA	9	0.55
(1,233)	1:10:A:LEU:HD12	1:10:A:LEU:HA	9	0.55
(1,233)	1:10:A:LEU:HD13	1:10:A:LEU:HA	9	0.55
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	3	0.55
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	3	0.55
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	3	0.55
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	4	0.55
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	4	0.55
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	4	0.55
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	4	0.55
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	20	0.55
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	7	0.55
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	1	0.55
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	8	0.55
(1,44)	1:53:A:GLU:H	1:52:A:PHE:HA	16	0.55
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	18	0.55
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	2	0.55
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	2	0.55
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	2	0.55
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	14	0.55
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	14	0.55
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	14	0.55
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	16	0.55
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	16	0.55
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	16	0.55
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	19	0.54
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	19	0.54
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	19	0.54
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	10	0.54
(2,2263)	1:46:A:LYS:H	1:48:A:ILE:HG12	15	0.54
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	19	0.54
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	15	0.54
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	18	0.54
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	4	0.54
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	4	0.54
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	15	0.54
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	20	0.54
(2,1805)	1:39:A:THR:H	1:37:A:LYS:HD2	17	0.54
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	15	0.54
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	12	0.54
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	9	0.54
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	11	0.54
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	20	0.54
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	19	0.54
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	6	0.54
(2,1585)	1:14:A:SER:H	1:14:A:SER:HB3	12	0.54
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	9	0.54
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	9	0.54
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	9	0.54
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	2	0.54
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	15	0.54
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	4	0.54
(2,1447)	1:2:A:VAL:HG21	1:3:A:LYS:H	19	0.54
(2,1447)	1:2:A:VAL:HG22	1:3:A:LYS:H	19	0.54
(2,1447)	1:2:A:VAL:HG23	1:3:A:LYS:H	19	0.54
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	13	0.54
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	15	0.54
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	13	0.54
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	2	0.54
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	5	0.54
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	17	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	2	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	4	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	8	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	9	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	13	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	14	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	18	0.54
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	20	0.54
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	13	0.54
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	13	0.54
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	13	0.54
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	10	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	7	0.54
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	6	0.54
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	2	0.54
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	13	0.54
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	6	0.54
(2,541)	1:24:A:LYS:HA	1:27:A:ARG:HB3	9	0.54
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	10	0.54
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	10	0.54
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	10	0.54
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	2	0.54
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	13	0.54
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	13	0.54
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	13	0.54
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	3	0.54
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	3	0.54
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	3	0.54
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	5	0.54
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	5	0.54
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	5	0.54
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	16	0.54
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	17	0.54
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	17	0.54
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	17	0.54
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	17	0.54
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	17	0.54
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	17	0.54
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	17	0.54
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	17	0.54
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	17	0.54
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	7	0.54
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	8	0.54
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	18	0.54
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE1	12	0.54
(2,18)	1:2:A:VAL:HA	1:64:A:TYR:HE2	12	0.54
(1,434)	1:62:A:GLU:H	1:62:A:GLU:HG3	10	0.54
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	18	0.54
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	18	0.54
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	18	0.54
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	20	0.54
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	20	0.54
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	20	0.54
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	4	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	8	0.54
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	8	0.54
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	8	0.54
(1,145)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	15	0.54
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	13	0.54
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	19	0.54
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	3	0.54
(1,44)	1:2:A:VAL:H	1:1:A:SER:HB3	12	0.54
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	6	0.54
(1,27)	1:48:A:ILE:H	1:50:A:GLU:HB2	15	0.54
(2,2469)	1:62:A:GLU:H	1:61:A:ARG:HG3	12	0.53
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE2	3	0.53
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE2	3	0.53
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE2	3	0.53
(2,2401)	1:53:A:GLU:HG2	1:56:A:ASN:HB2	3	0.53
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	16	0.53
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	16	0.53
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	16	0.53
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	10	0.53
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	8	0.53
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	9	0.53
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	17	0.53
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	6	0.53
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	18	0.53
(2,1845)	1:44:A:LYS:HB3	1:44:A:LYS:H	3	0.53
(2,1831)	1:45:A:PHE:HB2	1:42:A:THR:H	13	0.53
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	13	0.53
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	13	0.53
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	13	0.53
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	10	0.53
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	8	0.53
(2,1653)	1:21:A:GLU:H	1:20:A:GLN:HB2	16	0.53
(2,1602)	1:15:A:PRO:HB2	1:16:A:SER:H	14	0.53
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	11	0.53
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	8	0.53
(2,1505)	1:18:A:ASN:H	1:20:A:GLN:HB2	16	0.53
(2,1375)	1:78:A:SER:HA	1:78:A:SER:HB3	11	0.53
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	20	0.53
(2,1307)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	14	0.53
(2,1307)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	14	0.53
(2,1307)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	14	0.53
(2,1262)	1:43:A:GLU:HG3	1:47:A:GLU:H	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	2	0.53
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	13	0.53
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	8	0.53
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	3	0.53
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	3	0.53
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	5	0.53
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	7	0.53
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	10	0.53
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	11	0.53
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	17	0.53
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	3	0.53
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	10	0.53
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	15	0.53
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	1	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	2	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	5	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	10	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	12	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	13	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	15	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	16	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	17	0.53
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	20	0.53
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	10	0.53
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	10	0.53
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	10	0.53
(2,567)	1:24:A:LYS:HE3	1:24:A:LYS:H	7	0.53
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	5	0.53
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	5	0.53
(2,507)	1:6:A:LYS:HA	1:9:A:ASP:HB3	16	0.53
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	14	0.53
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	15	0.53
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	15	0.53
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	15	0.53
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	10	0.53
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	10	0.53
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	10	0.53
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	16	0.53
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	16	0.53
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	16	0.53
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	7	0.53
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	13	0.53
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	13	0.53
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	13	0.53
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	13	0.53
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	13	0.53
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	13	0.53
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	13	0.53
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	13	0.53
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB1	3	0.53
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB2	3	0.53
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB3	3	0.53
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB1	3	0.53
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB2	3	0.53
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB3	3	0.53
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	1	0.53
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	4	0.53
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD11	5	0.53
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD12	5	0.53
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD13	5	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	5	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	6	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	7	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	9	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	10	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	14	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	16	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	17	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	18	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	19	0.53
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	20	0.53
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	1	0.53
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	7	0.53
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	11	0.53
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	8	0.53
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	8	0.53
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	8	0.53
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	8	0.53
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	8	0.53
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	8	0.53
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	7	0.53
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	7	0.53
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	8	0.53
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	16	0.53
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	9	0.53
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	6	0.53
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	16	0.53
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	16	0.53
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	16	0.53
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	19	0.53
(1,69)	1:30:A:ALA:H	1:31:A:LEU:HB2	16	0.53
(1,27)	1:46:A:LYS:HB2	1:48:A:ILE:H	4	0.53
(2,2462)	1:37:A:LYS:HE3	1:39:A:THR:HB	12	0.52
(2,2387)	1:53:A:GLU:H	1:54:A:ILE:HG12	12	0.52
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	18	0.52
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	18	0.52
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	18	0.52
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	18	0.52
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	18	0.52
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	18	0.52
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	14	0.52
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	14	0.52
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	1	0.52
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	17	0.52
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	13	0.52
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	14	0.52
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	8	0.52
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	8	0.52
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	8	0.52
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	3	0.52
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	7	0.52
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	11	0.52
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	3	0.52
(2,1655)	1:21:A:GLU:H	1:21:A:GLU:HG3	5	0.52
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	18	0.52
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	15	0.52
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	13	0.52
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	17	0.52
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	17	0.52
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	17	0.52
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	8	0.52
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	8	0.52
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	8	0.52
(2,1375)	1:78:A:SER:HA	1:78:A:SER:HB3	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1375)	1:78:A:SER:HA	1:78:A:SER:HB3	2	0.52
(2,1375)	1:78:A:SER:HA	1:78:A:SER:HB3	7	0.52
(2,1375)	1:78:A:SER:HA	1:78:A:SER:HB3	9	0.52
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	13	0.52
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	16	0.52
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	12	0.52
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	7	0.52
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	9	0.52
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	9	0.52
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	15	0.52
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	5	0.52
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	5	0.52
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	5	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	1	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	2	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	6	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	8	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	9	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	16	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	17	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	19	0.52
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	20	0.52
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	3	0.52
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	4	0.52
(2,687)	1:38:A:PRO:HA	1:38:A:PRO:HD2	8	0.52
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD21	5	0.52
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD22	5	0.52
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD23	5	0.52
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD21	14	0.52
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD22	14	0.52
(2,643)	1:70:A:GLU:HA	1:69:A:LEU:HD23	14	0.52
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	6	0.52
(2,547)	1:24:A:LYS:HA	1:27:A:ARG:HB3	9	0.52
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	6	0.52
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	6	0.52
(2,458)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	5	0.52
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	7	0.52
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	9	0.52
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	15	0.52
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	4	0.52
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	7	0.52
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	17	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	3	0.52
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	11	0.52
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	13	0.52
(2,167)	1:66:A:GLN:HB3	1:66:A:GLN:HA	15	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	2	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	3	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	5	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	6	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	8	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	9	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	12	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	14	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	15	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	17	0.52
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	20	0.52
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	14	0.52
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	14	0.52
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	14	0.52
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	14	0.52
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	14	0.52
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	14	0.52
(1,463)	1:53:A:GLU:H	1:55:A:LEU:HB2	2	0.52
(1,436)	1:21:A:GLU:HB2	1:23:A:LYS:H	17	0.52
(1,326)	1:78:A:SER:HA	1:79:A:PHE:H	18	0.52
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	9	0.52
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	14	0.52
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	14	0.52
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	14	0.52
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	16	0.52
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	16	0.52
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	16	0.52
(1,262)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	2	0.52
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	10	0.52
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	10	0.52
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	10	0.52
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	7	0.52
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	7	0.52
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	7	0.52
(1,216)	1:21:A:GLU:HA	1:21:A:GLU:HG3	7	0.52
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	17	0.52
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	1	0.52
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	1	0.52
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	14	0.52
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	14	0.52
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	14	0.52
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	18	0.52
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	18	0.52
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	18	0.52
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	19	0.52
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	2	0.51
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	13	0.51
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	20	0.51
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	4	0.51
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	16	0.51
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	10	0.51
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	3	0.51
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	15	0.51
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	18	0.51
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	16	0.51
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	19	0.51
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	19	0.51
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	19	0.51
(2,1847)	1:41:A:ASP:HB3	1:44:A:LYS:H	12	0.51
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	19	0.51
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	20	0.51
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	12	0.51
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	19	0.51
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	4	0.51
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	18	0.51
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	5	0.51
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	5	0.51
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	5	0.51
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	16	0.51
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	16	0.51
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	16	0.51
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	2	0.51
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	2	0.51
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	2	0.51
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	18	0.51
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	18	0.51
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	18	0.51
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	5	0.51
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	5	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	5	0.51
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	13	0.51
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	13	0.51
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	13	0.51
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	3	0.51
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	10	0.51
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	4	0.51
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	14	0.51
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	8	0.51
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	13	0.51
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	13	0.51
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	13	0.51
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	7	0.51
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	10	0.51
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	15	0.51
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	9	0.51
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	13	0.51
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	10	0.51
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	3	0.51
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	3	0.51
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	3	0.51
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	7	0.51
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	7	0.51
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	7	0.51
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	14	0.51
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	17	0.51
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	14	0.51
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	14	0.51
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	14	0.51
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	5	0.51
(2,81)	1:28:A:LYS:HA	1:28:A:LYS:HD2	4	0.51
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	4	0.51
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	10	0.51
(2,32)	1:3:A:LYS:HB3	1:3:A:LYS:HA	16	0.51
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	18	0.51
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	18	0.51
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	18	0.51
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	15	0.51
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	15	0.51
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	15	0.51
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	4	0.51
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	4	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	4	0.51
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	10	0.51
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	10	0.51
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	10	0.51
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	16	0.51
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	16	0.51
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	16	0.51
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	12	0.51
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	12	0.51
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	12	0.51
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	17	0.51
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	17	0.51
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	17	0.51
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	17	0.51
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	17	0.51
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	17	0.51
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	15	0.51
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	15	0.51
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	15	0.51
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	17	0.51
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	17	0.51
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	17	0.51
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	3	0.51
(1,145)	1:41:A:ASP:HB3	1:44:A:LYS:HB3	2	0.51
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	20	0.51
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	20	0.51
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	20	0.51
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	9	0.51
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	6	0.51
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	9	0.51
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	9	0.51
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	9	0.51
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	11	0.51
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	11	0.51
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	11	0.51
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	13	0.51
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	13	0.51
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	13	0.51
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	5	0.5
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	5	0.5
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	5	0.5
(2,2414)	1:10:A:LEU:HD11	1:6:A:LYS:HE3	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2414)	1:10:A:LEU:HD12	1:6:A:LYS:HE3	6	0.5
(2,2414)	1:10:A:LEU:HD13	1:6:A:LYS:HE3	6	0.5
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	3	0.5
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	4	0.5
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	4	0.5
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	19	0.5
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	4	0.5
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	6	0.5
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	17	0.5
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	10	0.5
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	12	0.5
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	13	0.5
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	17	0.5
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	17	0.5
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	17	0.5
(2,1854)	1:45:A:PHE:H	1:46:A:LYS:HG2	2	0.5
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	2	0.5
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	2	0.5
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	4	0.5
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	4	0.5
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	13	0.5
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	2	0.5
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	12	0.5
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	12	0.5
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	12	0.5
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	12	0.5
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	14	0.5
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	14	0.5
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	14	0.5
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	17	0.5
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	17	0.5
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	17	0.5
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	20	0.5
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	14	0.5
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	10	0.5
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	12	0.5
(2,1024)	1:7:A:LEU:HB2	1:55:A:LEU:HB3	8	0.5
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	13	0.5
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	11	0.5
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	16	0.5
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	9	0.5
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	10	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	11	0.5
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	13	0.5
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	14	0.5
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	14	0.5
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	14	0.5
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	18	0.5
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	18	0.5
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	18	0.5
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	15	0.5
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	15	0.5
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	1	0.5
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	1	0.5
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	1	0.5
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	1	0.5
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	1	0.5
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	1	0.5
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	1	0.5
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	1	0.5
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	1	0.5
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	5	0.5
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	5	0.5
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	5	0.5
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	5	0.5
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	5	0.5
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	5	0.5
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	5	0.5
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	5	0.5
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	5	0.5
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	12	0.5
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	12	0.5
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	12	0.5
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	18	0.5
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	18	0.5
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	18	0.5
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	4	0.5
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	4	0.5
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	4	0.5
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	6	0.5
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	6	0.5
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	6	0.5
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	15	0.5
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	18	0.5
(1,218)	1:23:A:LYS:H	1:22:A:LEU:HB2	12	0.5
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	2	0.5
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	2	0.5
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	2	0.5
(1,145)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	12	0.5
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	15	0.5
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	9	0.5
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	9	0.5
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	9	0.5
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	1	0.5
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	17	0.5
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	17	0.5
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	17	0.5
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	1	0.49
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	7	0.49
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	8	0.49
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	17	0.49
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	14	0.49
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	18	0.49
(2,2193)	1:10:A:LEU:HB3	1:10:A:LEU:H	10	0.49
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	2	0.49
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	7	0.49
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	2	0.49
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	19	0.49
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	11	0.49
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	13	0.49
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	13	0.49
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	13	0.49
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	3	0.49
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	4	0.49
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	19	0.49
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	20	0.49
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	4	0.49
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	10	0.49
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	6	0.49
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	6	0.49
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	6	0.49
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	9	0.49
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	9	0.49
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	9	0.49
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	16	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	16	0.49
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	16	0.49
(2,1805)	1:39:A:THR:H	1:37:A:LYS:HD2	5	0.49
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	17	0.49
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	14	0.49
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	14	0.49
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	5	0.49
(2,1586)	1:14:A:SER:H	1:14:A:SER:HB2	14	0.49
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	4	0.49
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	10	0.49
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	13	0.49
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	13	0.49
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	13	0.49
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	10	0.49
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	10	0.49
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	10	0.49
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	11	0.49
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	11	0.49
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	11	0.49
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	11	0.49
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	11	0.49
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	11	0.49
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	16	0.49
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	11	0.49
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	12	0.49
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	1	0.49
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	19	0.49
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	12	0.49
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	20	0.49
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	4	0.49
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	4	0.49
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	4	0.49
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	12	0.49
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	12	0.49
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	12	0.49
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	6	0.49
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	6	0.49
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	6	0.49
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	12	0.49
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD21	5	0.49
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD22	5	0.49
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD23	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD21	14	0.49
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD22	14	0.49
(2,811)	1:70:A:GLU:HA	1:69:A:LEU:HD23	14	0.49
(2,627)	1:31:A:LEU:HA	1:34:A:HIS:HB2	11	0.49
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	10	0.49
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	15	0.49
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	14	0.49
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	4	0.49
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	4	0.49
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	4	0.49
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	8	0.49
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	8	0.49
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	6	0.49
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	6	0.49
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	6	0.49
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	6	0.49
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	6	0.49
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	6	0.49
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	6	0.49
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	6	0.49
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	6	0.49
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	13	0.49
(2,15)	1:2:A:VAL:HA	1:2:A:VAL:HB	19	0.49
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	1	0.49
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	1	0.49
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	1	0.49
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	1	0.49
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	1	0.49
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	1	0.49
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD1	11	0.49
(1,475)	1:51:A:ALA:HB1	1:52:A:PHE:HD2	11	0.49
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD1	11	0.49
(1,475)	1:51:A:ALA:HB2	1:52:A:PHE:HD2	11	0.49
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD1	11	0.49
(1,475)	1:51:A:ALA:HB3	1:52:A:PHE:HD2	11	0.49
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	13	0.49
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	13	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	19	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	19	0.49
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	19	0.49
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	17	0.49
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	17	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	17	0.49
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	15	0.49
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	15	0.49
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	15	0.49
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	13	0.49
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	13	0.49
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	13	0.49
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	10	0.49
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	10	0.49
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	12	0.49
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	3	0.49
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	3	0.49
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	3	0.49
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	6	0.49
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	6	0.49
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	6	0.49
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	1	0.49
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	8	0.49
(1,58)	1:61:A:ARG:H	1:63:A:ILE:HB	19	0.49
(1,24)	1:37:A:LYS:HE3	1:34:A:HIS:H	2	0.49
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	19	0.49
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	19	0.49
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	19	0.49
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE2	13	0.48
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE2	13	0.48
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE2	13	0.48
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	13	0.48
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	13	0.48
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	13	0.48
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	13	0.48
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	20	0.48
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	11	0.48
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	12	0.48
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	13	0.48
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	13	0.48
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	20	0.48
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	3	0.48
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	6	0.48
(2,1972)	1:55:A:LEU:H	1:53:A:GLU:HB2	15	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	1	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	1	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	2	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	2	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	2	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	3	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	3	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	3	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	4	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	4	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	4	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	5	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	5	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	5	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	8	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	8	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	8	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	10	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	10	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	10	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	11	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	11	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	11	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	14	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	14	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	14	0.48
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	18	0.48
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	18	0.48
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	18	0.48
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	12	0.48
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	8	0.48
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	18	0.48
(2,1864)	1:46:A:LYS:H	1:42:A:THR:HG21	20	0.48
(2,1864)	1:46:A:LYS:H	1:42:A:THR:HG22	20	0.48
(2,1864)	1:46:A:LYS:H	1:42:A:THR:HG23	20	0.48
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	15	0.48
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	9	0.48
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	10	0.48
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	16	0.48
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	16	0.48
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	16	0.48
(2,1494)	1:8:A:TYR:H	1:52:A:PHE:HA	10	0.48
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	15	0.48
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	10	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	10	0.48
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	10	0.48
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	11	0.48
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	11	0.48
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	11	0.48
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	1	0.48
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	1	0.48
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	1	0.48
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE1	11	0.48
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE2	11	0.48
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE1	11	0.48
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE2	11	0.48
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE1	11	0.48
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE2	11	0.48
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	1	0.48
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	1	0.48
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	1	0.48
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	10	0.48
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	10	0.48
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	10	0.48
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD21	7	0.48
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD22	7	0.48
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD23	7	0.48
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	9	0.48
(2,1053)	1:58:A:PRO:HA	1:58:A:PRO:HG3	1	0.48
(2,1053)	1:58:A:PRO:HA	1:58:A:PRO:HG3	16	0.48
(2,1053)	1:58:A:PRO:HA	1:58:A:PRO:HG3	19	0.48
(2,913)	1:52:A:PHE:HB3	1:11:A:LEU:HD11	5	0.48
(2,913)	1:52:A:PHE:HB3	1:11:A:LEU:HD12	5	0.48
(2,913)	1:52:A:PHE:HB3	1:11:A:LEU:HD13	5	0.48
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	14	0.48
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	14	0.48
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	14	0.48
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	14	0.48
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	6	0.48
(2,726)	1:33:A:TYR:HD1	1:41:A:ASP:HB2	15	0.48
(2,726)	1:33:A:TYR:HD2	1:41:A:ASP:HB2	15	0.48
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	6	0.48
(2,695)	1:38:A:PRO:HD2	1:37:A:LYS:HB2	1	0.48
(2,685)	1:39:A:THR:HG21	1:38:A:PRO:HA	6	0.48
(2,685)	1:39:A:THR:HG22	1:38:A:PRO:HA	6	0.48
(2,685)	1:39:A:THR:HG23	1:38:A:PRO:HA	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	5	0.48
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	5	0.48
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	5	0.48
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	8	0.48
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	8	0.48
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	8	0.48
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	11	0.48
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	11	0.48
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	11	0.48
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	12	0.48
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	12	0.48
(2,501)	1:25:A:GLY:HA2	1:24:A:LYS:HD3	5	0.48
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	13	0.48
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE2	4	0.48
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	10	0.48
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	15	0.48
(2,274)	1:16:A:SER:HA	1:16:A:SER:HB3	18	0.48
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	12	0.48
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	15	0.48
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	9	0.48
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	9	0.48
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	9	0.48
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	9	0.48
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	9	0.48
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	9	0.48
(2,81)	1:28:A:LYS:HA	1:28:A:LYS:HD2	5	0.48
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	16	0.48
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	16	0.48
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	16	0.48
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	20	0.48
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	20	0.48
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	20	0.48
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	7	0.48
(1,429)	1:6:A:LYS:HG2	1:7:A:LEU:H	2	0.48
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	2	0.48
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	2	0.48
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	2	0.48
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	16	0.48
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	16	0.48
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	16	0.48
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	6	0.48
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	6	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	6	0.48
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	19	0.48
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	20	0.48
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	20	0.48
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	20	0.48
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	1	0.48
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	1	0.48
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	1	0.48
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	12	0.48
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	12	0.48
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	12	0.48
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	2	0.48
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	2	0.48
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	2	0.48
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	1	0.48
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	8	0.48
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	8	0.48
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	8	0.48
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	15	0.48
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	15	0.48
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	15	0.48
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	7	0.47
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	7	0.47
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	7	0.47
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	19	0.47
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	6	0.47
(2,2267)	1:79:A:PHE:HB3	1:79:A:PHE:H	12	0.47
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	2	0.47
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	1	0.47
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	18	0.47
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	18	0.47
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	3	0.47
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	17	0.47
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	18	0.47
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	20	0.47
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	20	0.47
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	20	0.47
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	12	0.47
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	12	0.47
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	20	0.47
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	18	0.47
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	16	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	1	0.47
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	1	0.47
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	1	0.47
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	7	0.47
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	7	0.47
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	7	0.47
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	15	0.47
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	15	0.47
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	15	0.47
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	19	0.47
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	19	0.47
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	19	0.47
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	20	0.47
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	20	0.47
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	20	0.47
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	12	0.47
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	20	0.47
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	20	0.47
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	8	0.47
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	18	0.47
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	11	0.47
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	10	0.47
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	4	0.47
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	8	0.47
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	6	0.47
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	3	0.47
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	3	0.47
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	3	0.47
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	11	0.47
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	11	0.47
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	11	0.47
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	11	0.47
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	18	0.47
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	18	0.47
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	18	0.47
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	5	0.47
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	8	0.47
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	4	0.47
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	18	0.47
(2,747)	1:47:A:GLU:HG2	1:48:A:ILE:HB	4	0.47
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	17	0.47
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	19	0.47
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	20	0.47
(2,403)	1:13:A:VAL:HG21	1:21:A:GLU:HA	18	0.47
(2,403)	1:13:A:VAL:HG22	1:21:A:GLU:HA	18	0.47
(2,403)	1:13:A:VAL:HG23	1:21:A:GLU:HA	18	0.47
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	6	0.47
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	6	0.47
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	6	0.47
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	12	0.47
(2,274)	1:16:A:SER:HA	1:16:A:SER:HB3	5	0.47
(2,274)	1:16:A:SER:HA	1:16:A:SER:HB3	6	0.47
(2,274)	1:16:A:SER:HA	1:16:A:SER:HB3	11	0.47
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	10	0.47
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	10	0.47
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	10	0.47
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	10	0.47
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	2	0.47
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	2	0.47
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	2	0.47
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	2	0.47
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	19	0.47
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	19	0.47
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	19	0.47
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	10	0.47
(1,366)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	10	0.47
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	18	0.47
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	18	0.47
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	18	0.47
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	15	0.47
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	20	0.47
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	20	0.47
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	20	0.47
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	9	0.47
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	1	0.47
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	1	0.47
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	1	0.47
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	15	0.47
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	15	0.47
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	15	0.47
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	16	0.47
(1,85)	1:2:A:VAL:HA	1:3:A:LYS:HA	12	0.47
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	13	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	5	0.47
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	9	0.47
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	10	0.47
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	10	0.47
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	10	0.47
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	20	0.46
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	20	0.46
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	20	0.46
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	6	0.46
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	16	0.46
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	17	0.46
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	7	0.46
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	6	0.46
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	6	0.46
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	7	0.46
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	8	0.46
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	19	0.46
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	3	0.46
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	5	0.46
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	7	0.46
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	10	0.46
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	1	0.46
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	8	0.46
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	13	0.46
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	12	0.46
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	12	0.46
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	12	0.46
(2,1886)	1:48:A:ILE:HG21	1:48:A:ILE:H	13	0.46
(2,1886)	1:48:A:ILE:HG22	1:48:A:ILE:H	13	0.46
(2,1886)	1:48:A:ILE:HG23	1:48:A:ILE:H	13	0.46
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	15	0.46
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	15	0.46
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	18	0.46
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	5	0.46
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	18	0.46
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	3	0.46
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	8	0.46
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	8	0.46
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	8	0.46
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	19	0.46
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	19	0.46
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	19	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	18	0.46
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	20	0.46
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	20	0.46
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	20	0.46
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	20	0.46
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	20	0.46
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	20	0.46
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	13	0.46
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	5	0.46
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	18	0.46
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	13	0.46
(2,1053)	1:58:A:PRO:HA	1:58:A:PRO:HG3	6	0.46
(2,1053)	1:58:A:PRO:HA	1:58:A:PRO:HG3	15	0.46
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	1	0.46
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	5	0.46
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	6	0.46
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	6	0.46
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	6	0.46
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE2	8	0.46
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	14	0.46
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	14	0.46
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	14	0.46
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	2	0.46
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	2	0.46
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	2	0.46
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	15	0.46
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	15	0.46
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	15	0.46
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	7	0.46
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	17	0.46
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	17	0.46
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	17	0.46
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	12	0.46
(2,458)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	6	0.46
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	11	0.46
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	16	0.46
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	20	0.46
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	20	0.46
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	20	0.46
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	5	0.46
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	10	0.46
(2,326)	1:70:A:GLU:HA	1:70:A:GLU:HG3	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:18:A:ASN:HB3	1:19:A:GLU:H	3	0.46
(2,274)	1:16:A:SER:HA	1:16:A:SER:HB3	10	0.46
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	1	0.46
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	1	0.46
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	1	0.46
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	17	0.46
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	17	0.46
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	17	0.46
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	13	0.46
(2,81)	1:28:A:LYS:HA	1:28:A:LYS:HD3	1	0.46
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	8	0.46
(1,326)	1:78:A:SER:H	1:78:A:SER:HA	17	0.46
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	20	0.46
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	20	0.46
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	20	0.46
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	9	0.46
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	13	0.46
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	12	0.46
(1,104)	1:63:A:ILE:HD11	1:63:A:ILE:H	11	0.46
(1,104)	1:63:A:ILE:HD12	1:63:A:ILE:H	11	0.46
(1,104)	1:63:A:ILE:HD13	1:63:A:ILE:H	11	0.46
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	11	0.46
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	11	0.46
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	11	0.46
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	20	0.46
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	7	0.46
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	7	0.46
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	7	0.46
(2,2343)	1:31:A:LEU:HB2	1:34:A:HIS:HD2	4	0.45
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	15	0.45
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	15	0.45
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	10	0.45
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	4	0.45
(2,2082)	1:62:A:GLU:HB3	1:63:A:ILE:H	12	0.45
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	11	0.45
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	11	0.45
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	11	0.45
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	17	0.45
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	17	0.45
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	17	0.45
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	6	0.45
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	10	0.45
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	14	0.45
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	8	0.45
(2,1847)	1:41:A:ASP:HB3	1:44:A:LYS:H	3	0.45
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	6	0.45
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	6	0.45
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	20	0.45
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	12	0.45
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	5	0.45
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	6	0.45
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	10	0.45
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	13	0.45
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	10	0.45
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	14	0.45
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	14	0.45
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	14	0.45
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	14	0.45
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	1	0.45
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	6	0.45
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	7	0.45
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	19	0.45
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG21	15	0.45
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG22	15	0.45
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG23	15	0.45
(2,1456)	1:4:A:GLU:H	1:3:A:LYS:HG2	17	0.45
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	9	0.45
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	9	0.45
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	9	0.45
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	8	0.45
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	8	0.45
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	8	0.45
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	19	0.45
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	19	0.45
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	19	0.45
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	7	0.45
(2,1262)	1:43:A:GLU:HG3	1:47:A:GLU:H	11	0.45
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	17	0.45
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	5	0.45
(2,1011)	1:61:A:ARG:HG3	1:55:A:LEU:HA	12	0.45
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	11	0.45
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	11	0.45
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	11	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE2	19	0.45
(2,822)	1:2:A:VAL:HG21	1:6:A:LYS:HE3	15	0.45
(2,822)	1:2:A:VAL:HG22	1:6:A:LYS:HE3	15	0.45
(2,822)	1:2:A:VAL:HG23	1:6:A:LYS:HE3	15	0.45
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	11	0.45
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	3	0.45
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	12	0.45
(2,740)	1:42:A:THR:H	1:42:A:THR:HB	20	0.45
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	10	0.45
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE2	8	0.45
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE2	8	0.45
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	19	0.45
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	19	0.45
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	19	0.45
(2,521)	1:26:A:TYR:HB2	1:11:A:LEU:HD11	20	0.45
(2,521)	1:26:A:TYR:HB2	1:11:A:LEU:HD12	20	0.45
(2,521)	1:26:A:TYR:HB2	1:11:A:LEU:HD13	20	0.45
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	6	0.45
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	7	0.45
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	12	0.45
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	16	0.45
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	20	0.45
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	4	0.45
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	8	0.45
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	8	0.45
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	8	0.45
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	8	0.45
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	7	0.45
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	7	0.45
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	7	0.45
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	12	0.45
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	12	0.45
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	12	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	1	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	3	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	4	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	6	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	7	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	11	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	17	0.45
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	20	0.45
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	19	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	19	0.45
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	19	0.45
(2,316)	1:18:A:ASN:HB2	1:20:A:GLN:H	19	0.45
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	3	0.45
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	3	0.45
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	3	0.45
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	13	0.45
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	13	0.45
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	13	0.45
(2,241)	1:8:A:TYR:HB2	1:15:A:PRO:HA	2	0.45
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	6	0.45
(2,229)	1:14:A:SER:H	1:14:A:SER:HB3	12	0.45
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	9	0.45
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	8	0.45
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	8	0.45
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	8	0.45
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	19	0.45
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	1	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	12	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	12	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	12	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	13	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	13	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	13	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	19	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	19	0.45
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	19	0.45
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	16	0.45
(1,380)	1:54:A:ILE:HD11	1:73:A:ARG:HD3	18	0.45
(1,380)	1:54:A:ILE:HD12	1:73:A:ARG:HD3	18	0.45
(1,380)	1:54:A:ILE:HD13	1:73:A:ARG:HD3	18	0.45
(1,352)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	3	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	5	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	5	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	5	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	19	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	19	0.45
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	19	0.45
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	14	0.45
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	1	0.45
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	6	0.45
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	6	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	6	0.45
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	14	0.45
(1,178)	1:26:A:TYR:HA	1:11:A:LEU:HD21	5	0.45
(1,178)	1:26:A:TYR:HA	1:11:A:LEU:HD22	5	0.45
(1,178)	1:26:A:TYR:HA	1:11:A:LEU:HD23	5	0.45
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	3	0.45
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	17	0.45
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	9	0.45
(1,47)	1:2:A:VAL:HB	1:4:A:GLU:H	17	0.45
(1,17)	1:62:A:GLU:HB3	1:62:A:GLU:H	12	0.45
(2,2403)	1:6:A:LYS:HB2	1:7:A:LEU:H	10	0.44
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	2	0.44
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	20	0.44
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	2	0.44
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	11	0.44
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	14	0.44
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	12	0.44
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	13	0.44
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	13	0.44
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	13	0.44
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	19	0.44
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	19	0.44
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	19	0.44
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	2	0.44
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	12	0.44
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	11	0.44
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	17	0.44
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	19	0.44
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	16	0.44
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	5	0.44
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	5	0.44
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	5	0.44
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	15	0.44
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	11	0.44
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	6	0.44
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	2	0.44
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	15	0.44
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	15	0.44
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	15	0.44
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	8	0.44
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	14	0.44
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	18	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	9	0.44
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	9	0.44
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	9	0.44
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	13	0.44
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	13	0.44
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	13	0.44
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	5	0.44
(2,1453)	1:4:A:GLU:H	1:6:A:LYS:HB3	5	0.44
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	18	0.44
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	4	0.44
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	4	0.44
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	4	0.44
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	15	0.44
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	18	0.44
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	1	0.44
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	2	0.44
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	11	0.44
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	14	0.44
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	10	0.44
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	10	0.44
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	10	0.44
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	19	0.44
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	19	0.44
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	19	0.44
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	17	0.44
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	6	0.44
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD21	14	0.44
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD22	14	0.44
(2,550)	1:73:A:ARG:HD3	1:69:A:LEU:HD23	14	0.44
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	17	0.44
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	5	0.44
(2,485)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	15	0.44
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	9	0.44
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	14	0.44
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	13	0.44
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	3	0.44
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	18	0.44
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	9	0.44
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	14	0.44
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	15	0.44
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	8	0.44
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	14	0.44
(2,214)	1:11:A:LEU:HB3	1:11:A:LEU:HD11	20	0.44
(2,214)	1:11:A:LEU:HB3	1:11:A:LEU:HD12	20	0.44
(2,214)	1:11:A:LEU:HB3	1:11:A:LEU:HD13	20	0.44
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	14	0.44
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	14	0.44
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	14	0.44
(2,81)	1:28:A:LYS:HA	1:28:A:LYS:HD3	20	0.44
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	3	0.44
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	8	0.44
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	9	0.44
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	9	0.44
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	9	0.44
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	1	0.44
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	4	0.44
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	4	0.44
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	4	0.44
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	9	0.44
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	9	0.44
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	9	0.44
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	14	0.44
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	14	0.44
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	14	0.44
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	5	0.44
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	9	0.44
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	9	0.44
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	9	0.44
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	19	0.44
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	19	0.44
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	19	0.44
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	4	0.44
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	1	0.44
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	7	0.44
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	16	0.44
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	20	0.44
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE2	9	0.44
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE2	9	0.44
(1,99)	1:59:A:GLN:H	1:60:A:LYS:HB2	14	0.44
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	9	0.43
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	9	0.43
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	9	0.43
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	19	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	10	0.43
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	15	0.43
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	4	0.43
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	8	0.43
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	18	0.43
(2,2170)	1:64:A:TYR:HE1	1:69:A:LEU:H	19	0.43
(2,2170)	1:64:A:TYR:HE2	1:69:A:LEU:H	19	0.43
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	10	0.43
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	17	0.43
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	9	0.43
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	9	0.43
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	9	0.43
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	9	0.43
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	19	0.43
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	19	0.43
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD11	10	0.43
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD12	10	0.43
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD13	10	0.43
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	9	0.43
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	9	0.43
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	9	0.43
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	18	0.43
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	18	0.43
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	18	0.43
(2,1831)	1:45:A:PHE:HB2	1:42:A:THR:H	14	0.43
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	8	0.43
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	4	0.43
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	2	0.43
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	2	0.43
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	2	0.43
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	4	0.43
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	16	0.43
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	14	0.43
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	6	0.43
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	9	0.43
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	19	0.43
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	20	0.43
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	14	0.43
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	2	0.43
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	4	0.43
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	15	0.43
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	13	0.43
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	20	0.43
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	7	0.43
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	1	0.43
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	1	0.43
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	1	0.43
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	15	0.43
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	17	0.43
(2,1407)	1:33:A:TYR:HD1	1:41:A:ASP:H	14	0.43
(2,1407)	1:33:A:TYR:HD2	1:41:A:ASP:H	14	0.43
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	5	0.43
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	14	0.43
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	3	0.43
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	11	0.43
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	20	0.43
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	19	0.43
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	13	0.43
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	17	0.43
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	1	0.43
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	1	0.43
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	1	0.43
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	15	0.43
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	15	0.43
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	15	0.43
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	7	0.43
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	7	0.43
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	7	0.43
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	18	0.43
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	7	0.43
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	7	0.43
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	7	0.43
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	12	0.43
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	12	0.43
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	12	0.43
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	20	0.43
(2,726)	1:33:A:TYR:HD1	1:41:A:ASP:HB2	13	0.43
(2,726)	1:33:A:TYR:HD2	1:41:A:ASP:HB2	13	0.43
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	2	0.43
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	5	0.43
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	1	0.43
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	9	0.43
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	9	0.43
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	18	0.43
(2,496)	1:25:A:GLY:HA3	1:24:A:LYS:HD3	2	0.43
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	14	0.43
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	14	0.43
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	14	0.43
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	14	0.43
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	14	0.43
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	14	0.43
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	14	0.43
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	14	0.43
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	14	0.43
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	10	0.43
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	18	0.43
(2,357)	1:20:A:GLN:H	1:20:A:GLN:HB3	19	0.43
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	19	0.43
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	11	0.43
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	11	0.43
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	11	0.43
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	11	0.43
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	11	0.43
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	11	0.43
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	11	0.43
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	11	0.43
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	11	0.43
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	19	0.43
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	19	0.43
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	19	0.43
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	19	0.43
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	19	0.43
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	19	0.43
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	19	0.43
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	19	0.43
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	19	0.43
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	2	0.43
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	8	0.43
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	1	0.43
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	3	0.43
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	8	0.43
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	12	0.43
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	19	0.43
(2,275)	1:16:A:SER:HA	1:16:A:SER:HB2	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	7	0.43
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	7	0.43
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	7	0.43
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	4	0.43
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	4	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	3	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	3	0.43
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	3	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	2	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	6	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	7	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	9	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	10	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	11	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	12	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	13	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	15	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	17	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	19	0.43
(1,390)	1:46:A:LYS:HB2	1:46:A:LYS:HG2	20	0.43
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	9	0.43
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	9	0.43
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	9	0.43
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	13	0.43
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	13	0.43
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	13	0.43
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	3	0.43
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	3	0.43
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	3	0.43
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	11	0.43
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	11	0.43
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	16	0.43
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	16	0.43
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	16	0.43
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	7	0.43
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	7	0.43
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	7	0.43
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	9	0.42
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	10	0.42
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	17	0.42
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	1	0.42
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	18	0.42
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	1	0.42
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	15	0.42
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	15	0.42
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	15	0.42
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	9	0.42
(2,2003)	1:57:A:ASP:H	1:56:A:ASN:HB2	15	0.42
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	13	0.42
(2,1785)	1:45:A:PHE:HB3	1:33:A:TYR:H	9	0.42
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	6	0.42
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	14	0.42
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	15	0.42
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	20	0.42
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	4	0.42
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	7	0.42
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	6	0.42
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	12	0.42
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	12	0.42
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	12	0.42
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	9	0.42
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	11	0.42
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	13	0.42
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	16	0.42
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	15	0.42
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	15	0.42
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	15	0.42
(2,1528)	1:10:A:LEU:HB3	1:10:A:LEU:H	10	0.42
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	17	0.42
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	2	0.42
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	12	0.42
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	12	0.42
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	12	0.42
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	10	0.42
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	16	0.42
(2,1103)	1:54:A:ILE:HG12	1:60:A:LYS:HD3	6	0.42
(2,1075)	1:63:A:ILE:HD11	1:59:A:GLN:HG3	3	0.42
(2,1075)	1:63:A:ILE:HD12	1:59:A:GLN:HG3	3	0.42
(2,1075)	1:63:A:ILE:HD13	1:59:A:GLN:HG3	3	0.42
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	7	0.42
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	10	0.42
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	15	0.42
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	18	0.42
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	18	0.42
(2,907)	1:8:A:TYR:HB3	1:52:A:PHE:HA	19	0.42
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	19	0.42
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	19	0.42
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	19	0.42
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE2	1	0.42
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	5	0.42
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	1	0.42
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	1	0.42
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	1	0.42
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	1	0.42
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	19	0.42
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	14	0.42
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	5	0.42
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	6	0.42
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	7	0.42
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	7	0.42
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	7	0.42
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	19	0.42
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	11	0.42
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	11	0.42
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	11	0.42
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	11	0.42
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	11	0.42
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	13	0.42
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	5	0.42
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	1	0.42
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	1	0.42
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	1	0.42
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	20	0.42
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	2	0.42
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	2	0.42
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	2	0.42
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	2	0.42
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	2	0.42
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	2	0.42
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	2	0.42
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	2	0.42
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	2	0.42
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	18	0.42
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	18	0.42
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB1	2	0.42
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB2	2	0.42
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB3	2	0.42
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB1	2	0.42
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB2	2	0.42
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB3	2	0.42
(2,240)	1:8:A:TYR:HB3	1:15:A:PRO:HA	7	0.42
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	6	0.42
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	13	0.42
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	13	0.42
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	13	0.42
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	16	0.42
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	16	0.42
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	16	0.42
(1,357)	1:50:A:GLU:HA	1:53:A:GLU:HB2	12	0.42
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	1	0.42
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	1	0.42
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	1	0.42
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	7	0.42
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	11	0.42
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	11	0.42
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	11	0.42
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	4	0.42
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	17	0.42
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	17	0.42
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	17	0.42
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	19	0.42
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	19	0.42
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	19	0.42
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	10	0.42
(1,116)	1:33:A:TYR:HD1	1:44:A:LYS:HE3	6	0.42
(1,116)	1:33:A:TYR:HD2	1:44:A:LYS:HE3	6	0.42
(1,76)	1:6:A:LYS:HG3	1:6:A:LYS:HE2	8	0.42
(1,12)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	15	0.42
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD3	5	0.41
(2,2439)	1:58:A:PRO:HD2	1:57:A:ASP:H	15	0.41
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	12	0.41
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG11	16	0.41
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG12	16	0.41
(2,2316)	1:8:A:TYR:HD1	1:13:A:VAL:HG13	16	0.41
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG11	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG12	16	0.41
(2,2316)	1:8:A:TYR:HD2	1:13:A:VAL:HG13	16	0.41
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	4	0.41
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	9	0.41
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	20	0.41
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	1	0.41
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	1	0.41
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	6	0.41
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	5	0.41
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	10	0.41
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	1	0.41
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	10	0.41
(2,1963)	1:55:A:LEU:HD11	1:55:A:LEU:H	16	0.41
(2,1963)	1:55:A:LEU:HD12	1:55:A:LEU:H	16	0.41
(2,1963)	1:55:A:LEU:HD13	1:55:A:LEU:H	16	0.41
(2,1833)	1:42:A:THR:H	1:42:A:THR:HB	20	0.41
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	9	0.41
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	10	0.41
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	13	0.41
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	16	0.41
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	20	0.41
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	8	0.41
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	8	0.41
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	8	0.41
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	17	0.41
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	9	0.41
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	1	0.41
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	12	0.41
(2,1677)	1:23:A:LYS:H	1:23:A:LYS:HE3	6	0.41
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	16	0.41
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	7	0.41
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	3	0.41
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	12	0.41
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	17	0.41
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	7	0.41
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	1	0.41
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	1	0.41
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	1	0.41
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	6	0.41
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	9	0.41
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	9	0.41
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	9	0.41
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD21	19	0.41
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD22	19	0.41
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD23	19	0.41
(2,1123)	1:70:A:GLU:HA	1:73:A:ARG:HD2	12	0.41
(2,1119)	1:73:A:ARG:HD2	1:69:A:LEU:HG	12	0.41
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	17	0.41
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	15	0.41
(2,1081)	1:59:A:GLN:HA	1:59:A:GLN:HG2	12	0.41
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	6	0.41
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	18	0.41
(2,1065)	1:59:A:GLN:H	1:58:A:PRO:HB3	18	0.41
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	9	0.41
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	16	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	4	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	4	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	6	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	6	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	7	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	7	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	11	0.41
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	11	0.41
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	14	0.41
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	14	0.41
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	14	0.41
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	1	0.41
(2,782)	1:47:A:GLU:HB2	1:44:A:LYS:HD3	12	0.41
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	14	0.41
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	4	0.41
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	16	0.41
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	20	0.41
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	8	0.41
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	8	0.41
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	19	0.41
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	19	0.41
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	11	0.41
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	17	0.41
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD21	12	0.41
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD22	12	0.41
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD23	12	0.41
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	18	0.41
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	18	0.41
(2,323)	1:18:A:ASN:HB3	1:19:A:GLU:H	19	0.41
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	3	0.41
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	20	0.41
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD11	18	0.41
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD12	18	0.41
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD13	18	0.41
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	15	0.41
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	3	0.41
(2,47)	1:6:A:LYS:HG3	1:4:A:GLU:HA	8	0.41
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	1	0.41
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	1	0.41
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	1	0.41
(1,470)	1:44:A:LYS:HE2	1:44:A:LYS:HB3	3	0.41
(1,461)	1:8:A:TYR:HD1	1:15:A:PRO:HD3	12	0.41
(1,461)	1:8:A:TYR:HD2	1:15:A:PRO:HD3	12	0.41
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	3	0.41
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD21	10	0.41
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD22	10	0.41
(1,341)	1:32:A:LYS:H	1:31:A:LEU:HD23	10	0.41
(1,304)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	10	0.41
(1,304)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	20	0.41
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	10	0.41
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	10	0.41
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	10	0.41
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	5	0.41
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	10	0.41
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	14	0.41
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	14	0.41
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	14	0.41
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	4	0.41
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	8	0.41
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	8	0.41
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	8	0.41
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	4	0.41
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	5	0.41
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	6	0.41
(1,134)	1:22:A:LEU:HA	1:22:A:LEU:HB3	9	0.41
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	19	0.41
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	5	0.41
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	2	0.41
(1,47)	1:2:A:VAL:HB	1:65:A:ASP:H	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:48:A:ILE:H	1:50:A:GLU:HB2	13	0.41
(1,12)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	5	0.41
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE2	16	0.4
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE2	16	0.4
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE2	16	0.4
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD3	8	0.4
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD3	14	0.4
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD2	17	0.4
(2,2405)	1:6:A:LYS:HG2	1:9:A:ASP:H	10	0.4
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	15	0.4
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	5	0.4
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	12	0.4
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	6	0.4
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	7	0.4
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	16	0.4
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	2	0.4
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	15	0.4
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	15	0.4
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	17	0.4
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	19	0.4
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	13	0.4
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	11	0.4
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	20	0.4
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	10	0.4
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	10	0.4
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	3	0.4
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	3	0.4
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	3	0.4
(2,1963)	1:55:A:LEU:HD11	1:55:A:LEU:H	11	0.4
(2,1963)	1:55:A:LEU:HD12	1:55:A:LEU:H	11	0.4
(2,1963)	1:55:A:LEU:HD13	1:55:A:LEU:H	11	0.4
(2,1847)	1:41:A:ASP:HB3	1:44:A:LYS:H	15	0.4
(2,1838)	1:43:A:GLU:H	1:43:A:GLU:HG2	11	0.4
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	8	0.4
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	11	0.4
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	7	0.4
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	7	0.4
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	5	0.4
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	7	0.4
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	20	0.4
(2,1675)	1:23:A:LYS:H	1:23:A:LYS:HG2	17	0.4
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	13	0.4
(2,1494)	1:8:A:TYR:H	1:52:A:PHE:HA	1	0.4
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	16	0.4
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	15	0.4
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	11	0.4
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	4	0.4
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	4	0.4
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	4	0.4
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	4	0.4
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	4	0.4
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	4	0.4
(2,1388)	1:0:A:THR:HB	1:-1:A:MET:HA	4	0.4
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	8	0.4
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	17	0.4
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	17	0.4
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	17	0.4
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	6	0.4
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	19	0.4
(2,1106)	1:60:A:LYS:HD2	1:54:A:ILE:HA	4	0.4
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	10	0.4
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	10	0.4
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	10	0.4
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	3	0.4
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	6	0.4
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	12	0.4
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	13	0.4
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	19	0.4
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	2	0.4
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	2	0.4
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	2	0.4
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	2	0.4
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	16	0.4
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	16	0.4
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	16	0.4
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	15	0.4
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	19	0.4
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	5	0.4
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	20	0.4
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	20	0.4
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	20	0.4
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	13	0.4
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	18	0.4
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	20	0.4
(2,694)	1:37:A:LYS:HD2	1:38:A:PRO:HD3	4	0.4
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	17	0.4
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	20	0.4
(2,685)	1:39:A:THR:HG21	1:38:A:PRO:HA	9	0.4
(2,685)	1:39:A:THR:HG22	1:38:A:PRO:HA	9	0.4
(2,685)	1:39:A:THR:HG23	1:38:A:PRO:HA	9	0.4
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	17	0.4
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	17	0.4
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	17	0.4
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	8	0.4
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	8	0.4
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	9	0.4
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	16	0.4
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	5	0.4
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	15	0.4
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	12	0.4
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	12	0.4
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	12	0.4
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	17	0.4
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	17	0.4
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	11	0.4
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	11	0.4
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB1	19	0.4
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB2	19	0.4
(2,293)	1:8:A:TYR:HD1	1:17:A:ALA:HB3	19	0.4
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB1	19	0.4
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB2	19	0.4
(2,293)	1:8:A:TYR:HD2	1:17:A:ALA:HB3	19	0.4
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	19	0.4
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	19	0.4
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	19	0.4
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	19	0.4
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	6	0.4
(2,41)	1:3:A:LYS:HG2	1:3:A:LYS:HE3	20	0.4
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	13	0.4
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	14	0.4
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	14	0.4
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	14	0.4
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	17	0.4
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	17	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	17	0.4
(1,429)	1:6:A:LYS:HG2	1:7:A:LEU:H	18	0.4
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG21	2	0.4
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG22	2	0.4
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG23	2	0.4
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	2	0.4
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	2	0.4
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	2	0.4
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	20	0.4
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	20	0.4
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	20	0.4
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	15	0.4
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	15	0.4
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	15	0.4
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	5	0.4
(1,304)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	17	0.4
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	11	0.4
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	1	0.4
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	6	0.4
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	8	0.4
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	12	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	16	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	16	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	16	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	17	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	17	0.4
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	17	0.4
(1,159)	1:51:A:ALA:H	1:48:A:ILE:HG21	20	0.4
(1,159)	1:51:A:ALA:H	1:48:A:ILE:HG22	20	0.4
(1,159)	1:51:A:ALA:H	1:48:A:ILE:HG23	20	0.4
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	14	0.4
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	18	0.4
(1,128)	1:-1:A:MET:HB3	1:-1:A:MET:H	4	0.4
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE3	11	0.4
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE3	11	0.4
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	3	0.4
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	3	0.4
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	3	0.4
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	20	0.4
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	20	0.4
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	20	0.4
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	15	0.39
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	15	0.39
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	9	0.39
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	4	0.39
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	4	0.39
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	4	0.39
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	8	0.39
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	8	0.39
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	2	0.39
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	9	0.39
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	6	0.39
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	5	0.39
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	6	0.39
(2,2170)	1:64:A:TYR:HE1	1:69:A:LEU:H	1	0.39
(2,2170)	1:64:A:TYR:HE2	1:69:A:LEU:H	1	0.39
(2,2118)	1:65:A:ASP:HB2	1:66:A:GLN:H	8	0.39
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	15	0.39
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	15	0.39
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	1	0.39
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	14	0.39
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	7	0.39
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	7	0.39
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	7	0.39
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	10	0.39
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	10	0.39
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	10	0.39
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	17	0.39
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	17	0.39
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	17	0.39
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	2	0.39
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	8	0.39
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	9	0.39
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	13	0.39
(2,1823)	1:33:A:TYR:HB3	1:41:A:ASP:H	13	0.39
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	16	0.39
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	7	0.39
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	17	0.39
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	17	0.39
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	17	0.39
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	17	0.39
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	17	0.39
(2,1719)	1:27:A:ARG:H	1:23:A:LYS:HB3	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	18	0.39
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	16	0.39
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	3	0.39
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	8	0.39
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	3	0.39
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	9	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	1	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	3	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	8	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	10	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	11	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	19	0.39
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	20	0.39
(2,1536)	1:11:A:LEU:HB3	1:11:A:LEU:H	20	0.39
(2,1484)	1:55:A:LEU:HD21	1:8:A:TYR:H	10	0.39
(2,1484)	1:55:A:LEU:HD22	1:8:A:TYR:H	10	0.39
(2,1484)	1:55:A:LEU:HD23	1:8:A:TYR:H	10	0.39
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	9	0.39
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	11	0.39
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	11	0.39
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	11	0.39
(2,1422)	1:27:A:ARG:H	1:23:A:LYS:HB3	8	0.39
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	3	0.39
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	17	0.39
(2,1125)	1:62:A:GLU:HB2	1:62:A:GLU:HA	12	0.39
(2,1123)	1:70:A:GLU:HA	1:73:A:ARG:HD2	15	0.39
(2,1081)	1:59:A:GLN:HA	1:59:A:GLN:HG2	7	0.39
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	7	0.39
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	15	0.39
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	12	0.39
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	7	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	1	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	2	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	4	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	5	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	7	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	8	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	10	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	12	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	13	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	16	0.39
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	18	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	2	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	2	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	13	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	13	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	17	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	17	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	20	0.39
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	20	0.39
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	7	0.39
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	7	0.39
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	7	0.39
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	18	0.39
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	18	0.39
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	18	0.39
(2,832)	1:60:A:LYS:HE2	1:54:A:ILE:H	14	0.39
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	5	0.39
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	5	0.39
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	5	0.39
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	1	0.39
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	7	0.39
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	11	0.39
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	20	0.39
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	5	0.39
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	18	0.39
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	14	0.39
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	13	0.39
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	13	0.39
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	13	0.39
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	18	0.39
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD21	5	0.39
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD22	5	0.39
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD23	5	0.39
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD21	14	0.39
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD22	14	0.39
(2,561)	1:70:A:GLU:HA	1:69:A:LEU:HD23	14	0.39
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	1	0.39
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	1	0.39
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	1	0.39
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	8	0.39
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	8	0.39
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	15	0.39
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	15	0.39
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	15	0.39
(2,308)	1:18:A:ASN:HB3	1:18:A:ASN:HA	19	0.39
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB1	3	0.39
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB2	3	0.39
(2,303)	1:22:A:LEU:HD21	1:17:A:ALA:HB3	3	0.39
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB1	3	0.39
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB2	3	0.39
(2,303)	1:22:A:LEU:HD22	1:17:A:ALA:HB3	3	0.39
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB1	3	0.39
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB2	3	0.39
(2,303)	1:22:A:LEU:HD23	1:17:A:ALA:HB3	3	0.39
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	11	0.39
(2,217)	1:13:A:VAL:HG21	1:25:A:GLY:HA2	15	0.39
(2,217)	1:13:A:VAL:HG22	1:25:A:GLY:HA2	15	0.39
(2,217)	1:13:A:VAL:HG23	1:25:A:GLY:HA2	15	0.39
(2,190)	1:11:A:LEU:HD11	1:11:A:LEU:HA	5	0.39
(2,190)	1:11:A:LEU:HD12	1:11:A:LEU:HA	5	0.39
(2,190)	1:11:A:LEU:HD13	1:11:A:LEU:HA	5	0.39
(2,143)	1:9:A:ASP:HB2	1:9:A:ASP:HA	8	0.39
(2,143)	1:9:A:ASP:HB2	1:9:A:ASP:HA	16	0.39
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	12	0.39
(2,47)	1:6:A:LYS:HG3	1:4:A:GLU:HA	18	0.39
(1,461)	1:8:A:TYR:HD1	1:15:A:PRO:HD3	10	0.39
(1,461)	1:8:A:TYR:HD2	1:15:A:PRO:HD3	10	0.39
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	10	0.39
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	11	0.39
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG21	7	0.39
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG22	7	0.39
(1,450)	1:27:A:ARG:H	1:48:A:ILE:HG23	7	0.39
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	1	0.39
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	1	0.39
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	1	0.39
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	7	0.39
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	7	0.39
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	7	0.39
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	11	0.39
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	11	0.39
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	11	0.39
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	20	0.39
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	20	0.39
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	12	0.39
(1,304)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	2	0.39
(1,304)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	3	0.39
(1,304)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	5	0.39
(1,304)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	12	0.39
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	3	0.39
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	18	0.39
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	19	0.39
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	20	0.39
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	13	0.39
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	13	0.39
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	13	0.39
(1,134)	1:20:A:GLN:HA	1:20:A:GLN:HB2	8	0.39
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	13	0.39
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	20	0.39
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE2	14	0.38
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE2	14	0.38
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE2	14	0.38
(2,2424)	1:5:A:THR:HA	1:6:A:LYS:HD2	5	0.38
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	19	0.38
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	20	0.38
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	3	0.38
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	9	0.38
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	6	0.38
(2,2084)	1:62:A:GLU:HG2	1:63:A:ILE:H	12	0.38
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	7	0.38
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	4	0.38
(2,1963)	1:55:A:LEU:HD11	1:55:A:LEU:H	2	0.38
(2,1963)	1:55:A:LEU:HD12	1:55:A:LEU:H	2	0.38
(2,1963)	1:55:A:LEU:HD13	1:55:A:LEU:H	2	0.38
(2,1963)	1:55:A:LEU:HD11	1:55:A:LEU:H	13	0.38
(2,1963)	1:55:A:LEU:HD12	1:55:A:LEU:H	13	0.38
(2,1963)	1:55:A:LEU:HD13	1:55:A:LEU:H	13	0.38
(2,1961)	1:7:A:LEU:HG	1:55:A:LEU:H	19	0.38
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	1	0.38
(2,1831)	1:45:A:PHE:HB2	1:42:A:THR:H	4	0.38
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	2	0.38
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	12	0.38
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	6	0.38
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	15	0.38
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	20	0.38
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	2	0.38
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	4	0.38
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	17	0.38
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	13	0.38
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	13	0.38
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	13	0.38
(2,1458)	1:2:A:VAL:HG11	1:4:A:GLU:H	13	0.38
(2,1458)	1:2:A:VAL:HG12	1:4:A:GLU:H	13	0.38
(2,1458)	1:2:A:VAL:HG13	1:4:A:GLU:H	13	0.38
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	20	0.38
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	20	0.38
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	20	0.38
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	12	0.38
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	3	0.38
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	3	0.38
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	3	0.38
(2,1123)	1:70:A:GLU:HA	1:73:A:ARG:HD2	17	0.38
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	2	0.38
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	13	0.38
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	1	0.38
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	8	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	3	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	6	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	11	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	14	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	15	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	17	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	18	0.38
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	19	0.38
(2,1013)	1:61:A:ARG:HD3	1:55:A:LEU:HA	1	0.38
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	4	0.38
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	20	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	1	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	1	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	3	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	3	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	5	0.38
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	5	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	6	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	6	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	18	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	18	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	18	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	20	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	20	0.38
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	20	0.38
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	3	0.38
(2,826)	1:13:A:VAL:HG21	1:24:A:LYS:HE3	4	0.38
(2,826)	1:13:A:VAL:HG22	1:24:A:LYS:HE3	4	0.38
(2,826)	1:13:A:VAL:HG23	1:24:A:LYS:HE3	4	0.38
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	11	0.38
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	20	0.38
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	10	0.38
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	10	0.38
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	10	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	2	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	3	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	5	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	6	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	8	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	9	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	12	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	14	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	15	0.38
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	17	0.38
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	8	0.38
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	8	0.38
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	9	0.38
(2,627)	1:31:A:LEU:HA	1:34:A:HIS:HB2	19	0.38
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	6	0.38
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	8	0.38
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	8	0.38
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	8	0.38
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	8	0.38
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	8	0.38
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	8	0.38
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	8	0.38
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	8	0.38
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	8	0.38
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	9	0.38
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	17	0.38
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	17	0.38
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	10	0.38
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	10	0.38
(2,305)	1:18:A:ASN:HA	1:19:A:GLU:HB3	10	0.38
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	13	0.38
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	18	0.38
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	16	0.38
(2,241)	1:8:A:TYR:HB2	1:15:A:PRO:HA	7	0.38
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	12	0.38
(2,191)	1:11:A:LEU:HB3	1:11:A:LEU:HA	5	0.38
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	8	0.38
(2,116)	1:7:A:LEU:HG	1:55:A:LEU:H	19	0.38
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	4	0.38
(2,78)	1:4:A:GLU:HA	1:6:A:LYS:HB2	2	0.38
(2,50)	1:4:A:GLU:H	1:6:A:LYS:HB3	1	0.38
(2,48)	1:4:A:GLU:HA	1:6:A:LYS:HB2	2	0.38
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	11	0.38
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	11	0.38
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	11	0.38
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	11	0.38
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	8	0.38
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	1	0.38
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	1	0.38
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	1	0.38
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD11	8	0.38
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD12	8	0.38
(1,341)	1:32:A:LYS:H	1:48:A:ILE:HD13	8	0.38
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	18	0.38
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	18	0.38
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	18	0.38
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	4	0.38
(1,304)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	13	0.38
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	7	0.38
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	8	0.38
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	9	0.38
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	2	0.38
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	10	0.38
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	13	0.38
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	14	0.38
(1,242)	1:46:A:LYS:HA	1:47:A:GLU:H	17	0.38
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	6	0.38
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	10	0.38
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	10	0.38
(1,188)	1:38:A:PRO:HB2	1:38:A:PRO:HD3	16	0.38
(1,188)	1:58:A:PRO:HD3	1:58:A:PRO:HB2	19	0.38
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	4	0.38
(1,134)	1:43:A:GLU:HA	1:43:A:GLU:HB2	14	0.38
(1,110)	1:50:A:GLU:HG2	1:54:A:ILE:HB	16	0.38
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	20	0.38
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD3	16	0.37
(2,2383)	1:11:A:LEU:HB2	1:52:A:PHE:HE1	12	0.37
(2,2383)	1:11:A:LEU:HB2	1:52:A:PHE:HE2	12	0.37
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	5	0.37
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	3	0.37
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	16	0.37
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	10	0.37
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	19	0.37
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	5	0.37
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	16	0.37
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	3	0.37
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	3	0.37
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	3	0.37
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	5	0.37
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	5	0.37
(2,2033)	1:58:A:PRO:HD3	1:60:A:LYS:H	12	0.37
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	8	0.37
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	10	0.37
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	10	0.37
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	10	0.37
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	1	0.37
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	1	0.37
(2,1919)	1:34:A:HIS:H	1:36:A:ASP:HB3	4	0.37
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	4	0.37
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	4	0.37
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	4	0.37
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	11	0.37
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	18	0.37
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	3	0.37
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	3	0.37
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	10	0.37
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	10	0.37
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	15	0.37
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	19	0.37
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	19	0.37
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	10	0.37
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	10	0.37
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	10	0.37
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	12	0.37
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	18	0.37
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	14	0.37
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	5	0.37
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	16	0.37
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	2	0.37
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	2	0.37
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	2	0.37
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	7	0.37
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	7	0.37
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	7	0.37
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	18	0.37
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	2	0.37
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	2	0.37
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	2	0.37
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	2	0.37
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	1	0.37
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	1	0.37
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	1	0.37
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	1	0.37
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	1	0.37
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	1	0.37
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	14	0.37
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	11	0.37
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	2	0.37
(2,1301)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	15	0.37
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	8	0.37
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	8	0.37
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	8	0.37
(2,1075)	1:63:A:ILE:HD11	1:59:A:GLN:HG3	8	0.37
(2,1075)	1:63:A:ILE:HD12	1:59:A:GLN:HG3	8	0.37
(2,1075)	1:63:A:ILE:HD13	1:59:A:GLN:HG3	8	0.37
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	4	0.37
(2,1034)	1:56:A:ASN:HB3	1:56:A:ASN:HA	9	0.37
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	8	0.37
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB2	15	0.37
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	8	0.37
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	20	0.37
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	2	0.37
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	2	0.37
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	2	0.37
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	4	0.37
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	4	0.37
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	4	0.37
(2,801)	1:33:A:TYR:HD1	1:45:A:PHE:HA	16	0.37
(2,801)	1:33:A:TYR:HD2	1:45:A:PHE:HA	16	0.37
(2,789)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	2	0.37
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	4	0.37
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	10	0.37
(2,765)	1:3:A:LYS:HB3	1:3:A:LYS:HA	16	0.37
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	7	0.37
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	11	0.37
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	13	0.37
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	1	0.37
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	4	0.37
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	4	0.37
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	15	0.37
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	15	0.37
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	20	0.37
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	20	0.37
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	20	0.37
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	14	0.37
(2,573)	1:29:A:ALA:H	1:28:A:LYS:HG3	10	0.37
(2,567)	1:24:A:LYS:HE2	1:24:A:LYS:H	20	0.37
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	8	0.37
(2,458)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	11	0.37
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	16	0.37
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	16	0.37
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	16	0.37
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	16	0.37
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	9	0.37
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	9	0.37
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	2	0.37
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	2	0.37
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	13	0.37
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	2	0.37
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	7	0.37
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	17	0.37
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	18	0.37
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	16	0.37
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	16	0.37
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	16	0.37
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	16	0.37
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	16	0.37
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	16	0.37
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	16	0.37
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	16	0.37
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	16	0.37
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	16	0.37
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	13	0.37
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	8	0.37
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	9	0.37
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	18	0.37
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	16	0.37
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	16	0.37
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	16	0.37
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	12	0.37
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	12	0.37
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	12	0.37
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	18	0.37
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	19	0.37
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	1	0.37
(2,14)	1:2:A:VAL:HA	1:4:A:GLU:HG3	7	0.37
(1,481)	1:-1:A:MET:HA	1:0:A:THR:H	20	0.37
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	8	0.37
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	8	0.37
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	8	0.37
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	15	0.37
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	15	0.37
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	15	0.37
(1,463)	1:53:A:GLU:H	1:55:A:LEU:HB2	11	0.37
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	9	0.37
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	18	0.37
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	18	0.37
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	18	0.37
(1,370)	1:72:A:ALA:HA	1:76:A:GLY:H	13	0.37
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	3	0.37
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	11	0.37
(1,304)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	8	0.37
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	2	0.37
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	7	0.37
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	11	0.37
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	4	0.37
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	3	0.37
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	14	0.37
(1,242)	1:31:A:LEU:HA	1:34:A:HIS:H	15	0.37
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	3	0.37
(1,188)	1:38:A:PRO:HB2	1:38:A:PRO:HD3	1	0.37
(1,188)	1:38:A:PRO:HB2	1:38:A:PRO:HD3	6	0.37
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	5	0.37
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	9	0.37
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	9	0.37
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	9	0.37
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	9	0.37
(1,134)	1:20:A:GLN:HA	1:20:A:GLN:HB2	2	0.37
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	4	0.37
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	5	0.37
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	17	0.37
(1,81)	1:60:A:LYS:HA	1:60:A:LYS:HG3	8	0.37
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	6	0.36
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	6	0.36
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	6	0.36
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	12	0.36
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	15	0.36
(2,2403)	1:6:A:LYS:HB3	1:7:A:LEU:H	19	0.36
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	6	0.36
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	10	0.36
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	10	0.36
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	11	0.36
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	18	0.36
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	5	0.36
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	6	0.36
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	14	0.36
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	9	0.36
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	17	0.36
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	16	0.36
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	16	0.36
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	16	0.36
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	2	0.36
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	7	0.36
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	20	0.36
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	11	0.36
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	11	0.36
(2,1933)	1:52:A:PHE:H	1:8:A:TYR:HA	10	0.36
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	12	0.36
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	12	0.36
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	12	0.36
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	3	0.36
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	14	0.36
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	3	0.36
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	5	0.36
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	11	0.36
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	11	0.36
(2,1673)	1:22:A:LEU:HD21	1:23:A:LYS:H	8	0.36
(2,1673)	1:22:A:LEU:HD22	1:23:A:LYS:H	8	0.36
(2,1673)	1:22:A:LEU:HD23	1:23:A:LYS:H	8	0.36
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	12	0.36
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	11	0.36
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	13	0.36
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	9	0.36
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	12	0.36
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	14	0.36
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	15	0.36
(2,1576)	1:13:A:VAL:H	1:14:A:SER:H	18	0.36
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	4	0.36
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	4	0.36
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	4	0.36
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	15	0.36
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	3	0.36
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	3	0.36
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	3	0.36
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	18	0.36
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	13	0.36
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	13	0.36
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	13	0.36
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	17	0.36
(2,1081)	1:59:A:GLN:HA	1:59:A:GLN:HG2	13	0.36
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	17	0.36
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	10	0.36
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	10	0.36
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	11	0.36
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	20	0.36
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	20	0.36
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	20	0.36
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	5	0.36
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	5	0.36
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	5	0.36
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	17	0.36
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	17	0.36
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	17	0.36
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	17	0.36
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	2	0.36
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	7	0.36
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	20	0.36
(2,757)	1:70:A:GLU:HA	1:70:A:GLU:HG3	3	0.36
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	18	0.36
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	3	0.36
(2,688)	1:40:A:GLY:H	1:38:A:PRO:HA	5	0.36
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	6	0.36
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	6	0.36
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	17	0.36
(2,571)	1:28:A:LYS:HA	1:28:A:LYS:HG3	10	0.36
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	1	0.36
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	18	0.36
(2,444)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	20	0.36
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	7	0.36
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	7	0.36
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	7	0.36
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	14	0.36
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	14	0.36
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	14	0.36
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	1	0.36
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	12	0.36
(2,394)	1:22:A:LEU:H	1:21:A:GLU:HG2	14	0.36
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	4	0.36
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	4	0.36
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	4	0.36
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	6	0.36
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	6	0.36
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	13	0.36
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	13	0.36
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE2	14	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	1	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	4	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	5	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	6	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	8	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	10	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	11	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	14	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	15	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	16	0.36
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	20	0.36
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	2	0.36
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	5	0.36
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	3	0.36
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	4	0.36
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	19	0.36
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	5	0.36
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	5	0.36
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	5	0.36
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	5	0.36
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	12	0.36
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	14	0.36
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	14	0.36
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	14	0.36
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	15	0.36
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	15	0.36
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	15	0.36
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	12	0.36
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	12	0.36
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	12	0.36
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	19	0.36
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	19	0.36
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	19	0.36
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	1	0.36
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	3	0.36
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	16	0.36
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	19	0.36
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	16	0.36
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	16	0.36
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	16	0.36
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,188)	1:38:A:PRO:HB2	1:38:A:PRO:HD3	15	0.36
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	19	0.36
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	6	0.36
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	1	0.35
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	1	0.35
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	1	0.35
(2,2450)	1:58:A:PRO:HD3	1:57:A:ASP:H	1	0.35
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	5	0.35
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	7	0.35
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	15	0.35
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	7	0.35
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	15	0.35
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	3	0.35
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	3	0.35
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	11	0.35
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	11	0.35
(2,2276)	1:79:A:PHE:HA	1:80:A:GLY:H	9	0.35
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	14	0.35
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	8	0.35
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	5	0.35
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	4	0.35
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	4	0.35
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	18	0.35
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	18	0.35
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	18	0.35
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	1	0.35
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	7	0.35
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	15	0.35
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	10	0.35
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	10	0.35
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	10	0.35
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	17	0.35
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	14	0.35
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	14	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	1	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	1	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	5	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	5	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	11	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	11	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	12	0.35
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	17	0.35
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	15	0.35
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	20	0.35
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	8	0.35
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	8	0.35
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	8	0.35
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	1	0.35
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	17	0.35
(2,1764)	1:32:A:LYS:H	1:32:A:LYS:HG2	19	0.35
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	2	0.35
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	3	0.35
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	9	0.35
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	17	0.35
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	4	0.35
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	10	0.35
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	15	0.35
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	3	0.35
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	3	0.35
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	3	0.35
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	1	0.35
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	14	0.35
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	14	0.35
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	14	0.35
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	3	0.35
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	2	0.35
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	6	0.35
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	8	0.35
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	8	0.35
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	8	0.35
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG21	12	0.35
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG22	12	0.35
(2,1418)	1:1:A:SER:H	1:2:A:VAL:HG23	12	0.35
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	13	0.35
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	6	0.35
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	6	0.35
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	6	0.35
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	6	0.35
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	6	0.35
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	6	0.35
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	11	0.35
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	8	0.35
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	7	0.35
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	3	0.35
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	12	0.35
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	12	0.35
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	12	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	9	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	9	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	14	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	14	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	16	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	16	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	19	0.35
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	19	0.35
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	3	0.35
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	3	0.35
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	3	0.35
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD11	4	0.35
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD12	4	0.35
(2,872)	1:47:A:GLU:HG3	1:10:A:LEU:HD13	4	0.35
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	7	0.35
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	19	0.35
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	5	0.35
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	5	0.35
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	5	0.35
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	2	0.35
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	7	0.35
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	16	0.35
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	9	0.35
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	9	0.35
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	9	0.35
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	11	0.35
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	11	0.35
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	11	0.35
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	4	0.35
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	18	0.35
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	7	0.35
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	10	0.35
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	16	0.35
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	4	0.35
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	4	0.35
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	4	0.35
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	15	0.35
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	15	0.35
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	4	0.35
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	8	0.35
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	8	0.35
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	8	0.35
(2,567)	1:24:A:LYS:HE2	1:24:A:LYS:H	6	0.35
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	4	0.35
(2,559)	1:26:A:TYR:HE1	1:27:A:ARG:HG3	16	0.35
(2,559)	1:26:A:TYR:HE2	1:27:A:ARG:HG3	16	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	8	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	12	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	13	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	14	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	15	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	17	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	19	0.35
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	20	0.35
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	3	0.35
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	16	0.35
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD21	3	0.35
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD22	3	0.35
(2,401)	1:22:A:LEU:HA	1:22:A:LEU:HD23	3	0.35
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	12	0.35
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	12	0.35
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	12	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	1	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	2	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	3	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	4	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	5	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	6	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	7	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	8	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	9	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	11	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	12	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	13	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	14	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	15	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	16	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	18	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	19	0.35
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	20	0.35
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	9	0.35
(2,307)	1:18:A:ASN:HB2	1:18:A:ASN:HA	13	0.35
(2,281)	1:14:A:SER:H	1:14:A:SER:HB2	14	0.35
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	18	0.35
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	7	0.35
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	15	0.35
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	2	0.35
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	16	0.35
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	17	0.35
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	17	0.35
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	17	0.35
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD11	13	0.35
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD12	13	0.35
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD13	13	0.35
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	10	0.35
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD11	5	0.35
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD12	5	0.35
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD13	5	0.35
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	18	0.35
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	18	0.35
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	18	0.35
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	20	0.35
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	8	0.35
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	8	0.35
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	8	0.35
(1,374)	1:28:A:LYS:HA	1:28:A:LYS:HB3	12	0.35
(1,326)	1:78:A:SER:HA	1:79:A:PHE:H	5	0.35
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	16	0.35
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	13	0.35
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	4	0.35
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	5	0.35
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	10	0.35
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	12	0.35
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	20	0.35
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	2	0.35
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	10	0.35
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	17	0.35
(1,249)	1:60:A:LYS:HG3	1:57:A:ASP:HB3	6	0.35
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	2	0.35
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	8	0.35
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	12	0.35
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	18	0.35
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	20	0.35
(1,173)	1:21:A:GLU:HB3	1:21:A:GLU:HG3	8	0.35
(1,173)	1:70:A:GLU:HB2	1:70:A:GLU:HG2	9	0.35
(1,173)	1:70:A:GLU:HB2	1:70:A:GLU:HG2	15	0.35
(1,173)	1:21:A:GLU:HB3	1:21:A:GLU:HG3	16	0.35
(1,173)	1:21:A:GLU:HB3	1:21:A:GLU:HG3	20	0.35
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	14	0.35
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	2	0.35
(1,44)	1:2:A:VAL:H	1:1:A:SER:HB3	14	0.35
(1,24)	1:37:A:LYS:HE2	1:34:A:HIS:H	19	0.35
(1,23)	1:62:A:GLU:HA	1:62:A:GLU:HG3	12	0.35
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG2	18	0.35
(2,2448)	1:42:A:THR:HA	1:35:A:PRO:HG3	2	0.34
(2,2448)	1:42:A:THR:HA	1:35:A:PRO:HG3	15	0.34
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	1	0.34
(2,2347)	1:31:A:LEU:HA	1:34:A:HIS:HD2	13	0.34
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	20	0.34
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	2	0.34
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	16	0.34
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	19	0.34
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	19	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	4	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	4	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	4	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	9	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	9	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	9	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	19	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	19	0.34
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	19	0.34
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	19	0.34
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	4	0.34
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	11	0.34
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	18	0.34
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	18	0.34
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	18	0.34
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	7	0.34
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	8	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	8	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	10	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	10	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	14	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	14	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	16	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	16	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	19	0.34
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	19	0.34
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	8	0.34
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	8	0.34
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	8	0.34
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	8	0.34
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	10	0.34
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	10	0.34
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	10	0.34
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	20	0.34
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	20	0.34
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	20	0.34
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	17	0.34
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	8	0.34
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	11	0.34
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	13	0.34
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	6	0.34
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	13	0.34
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	20	0.34
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	15	0.34
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	3	0.34
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	3	0.34
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	3	0.34
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	7	0.34
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	14	0.34
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	11	0.34
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	17	0.34
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	6	0.34
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	17	0.34
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	17	0.34
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	17	0.34
(2,1531)	1:7:A:LEU:HD21	1:10:A:LEU:H	8	0.34
(2,1531)	1:7:A:LEU:HD22	1:10:A:LEU:H	8	0.34
(2,1531)	1:7:A:LEU:HD23	1:10:A:LEU:H	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	13	0.34
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	8	0.34
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	8	0.34
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG21	11	0.34
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG22	11	0.34
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG23	11	0.34
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	4	0.34
(2,1413)	1:0:A:THR:HB	1:0:A:THR:H	14	0.34
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	16	0.34
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	9	0.34
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	9	0.34
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	9	0.34
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	9	0.34
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	9	0.34
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	9	0.34
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	7	0.34
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	20	0.34
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	20	0.34
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	20	0.34
(2,1236)	1:68:A:GLY:HA2	1:69:A:LEU:HB2	7	0.34
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	7	0.34
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	16	0.34
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	6	0.34
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	7	0.34
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	12	0.34
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	16	0.34
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	20	0.34
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	19	0.34
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	18	0.34
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	2	0.34
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	13	0.34
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	14	0.34
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE1	12	0.34
(2,920)	1:52:A:PHE:HB2	1:52:A:PHE:HE2	12	0.34
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	15	0.34
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	15	0.34
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	15	0.34
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	9	0.34
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	14	0.34
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	1	0.34
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	1	0.34
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,741)	1:43:A:GLU:H	1:42:A:THR:HB	20	0.34
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	9	0.34
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	7	0.34
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	1	0.34
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	12	0.34
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	8	0.34
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	13	0.34
(2,571)	1:28:A:LYS:HA	1:28:A:LYS:HG3	12	0.34
(2,567)	1:24:A:LYS:HE2	1:24:A:LYS:H	16	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	3	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	5	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	7	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	10	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	11	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	16	0.34
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	18	0.34
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	4	0.34
(2,325)	1:19:A:GLU:HB3	1:19:A:GLU:HA	10	0.34
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	20	0.34
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	20	0.34
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	20	0.34
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	20	0.34
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	20	0.34
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	20	0.34
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	20	0.34
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	20	0.34
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	20	0.34
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	19	0.34
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	20	0.34
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	13	0.34
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	15	0.34
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	15	0.34
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	15	0.34
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	6	0.34
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	6	0.34
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	6	0.34
(2,189)	1:11:A:LEU:HD21	1:11:A:LEU:HA	20	0.34
(2,189)	1:11:A:LEU:HD22	1:11:A:LEU:HA	20	0.34
(2,189)	1:11:A:LEU:HD23	1:11:A:LEU:HA	20	0.34
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	8	0.34
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	8	0.34
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:6:A:LYS:HA	1:9:A:ASP:HB3	8	0.34
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	10	0.34
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	6	0.34
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	10	0.34
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	16	0.34
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	7	0.34
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	20	0.34
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	10	0.34
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	8	0.34
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	13	0.34
(1,286)	1:46:A:LYS:H	1:45:A:PHE:HA	15	0.34
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	6	0.34
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	18	0.34
(1,242)	1:31:A:LEU:HA	1:34:A:HIS:H	7	0.34
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	9	0.34
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	15	0.34
(1,191)	1:47:A:GLU:HA	1:48:A:ILE:H	19	0.34
(1,173)	1:70:A:GLU:HB2	1:70:A:GLU:HG2	7	0.34
(1,173)	1:70:A:GLU:HB2	1:70:A:GLU:HG2	10	0.34
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	8	0.34
(1,128)	1:-1:A:MET:HB3	1:-1:A:MET:H	18	0.34
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE2	12	0.34
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE2	12	0.34
(1,99)	1:59:A:GLN:H	1:60:A:LYS:HB2	19	0.34
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	17	0.34
(2,2460)	1:33:A:TYR:HD1	1:41:A:ASP:HB3	12	0.33
(2,2460)	1:33:A:TYR:HD2	1:41:A:ASP:HB3	12	0.33
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	7	0.33
(2,2276)	1:79:A:PHE:HA	1:80:A:GLY:H	11	0.33
(2,2261)	1:77:A:PRO:HA	1:78:A:SER:H	7	0.33
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	15	0.33
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	18	0.33
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	15	0.33
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	2	0.33
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	3	0.33
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	7	0.33
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	18	0.33
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	12	0.33
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	8	0.33
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	1	0.33
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	1	0.33
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	1	0.33
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	6	0.33
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	6	0.33
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	6	0.33
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	5	0.33
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	5	0.33
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	12	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	2	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	2	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	9	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	9	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	15	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	15	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	18	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	18	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	20	0.33
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	20	0.33
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	19	0.33
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	4	0.33
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	7	0.33
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	9	0.33
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	6	0.33
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	11	0.33
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	7	0.33
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	13	0.33
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	13	0.33
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	15	0.33
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	15	0.33
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	15	0.33
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	4	0.33
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	15	0.33
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	20	0.33
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	13	0.33
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	10	0.33
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	8	0.33
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	8	0.33
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	8	0.33
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	9	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	5	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	5	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	5	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	6	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	6	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	11	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	11	0.33
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	11	0.33
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG11	19	0.33
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG12	19	0.33
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG13	19	0.33
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	13	0.33
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	13	0.33
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	13	0.33
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	1	0.33
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	17	0.33
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	11	0.33
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	11	0.33
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	11	0.33
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	5	0.33
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	5	0.33
(2,1104)	1:24:A:LYS:HD3	1:24:A:LYS:HG3	15	0.33
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	8	0.33
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	14	0.33
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	14	0.33
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	14	0.33
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	16	0.33
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	16	0.33
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	16	0.33
(2,932)	1:53:A:GLU:HA	1:52:A:PHE:HA	15	0.33
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	9	0.33
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	9	0.33
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	9	0.33
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	7	0.33
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	7	0.33
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	7	0.33
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	6	0.33
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	18	0.33
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	18	0.33
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	18	0.33
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	20	0.33
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	15	0.33
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	15	0.33
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	5	0.33
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,573)	1:29:A:ALA:H	1:28:A:LYS:HG3	12	0.33
(2,543)	1:27:A:ARG:H	1:27:A:ARG:HB3	4	0.33
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	10	0.33
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	10	0.33
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	6	0.33
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	7	0.33
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	6	0.33
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	6	0.33
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	6	0.33
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	20	0.33
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	3	0.33
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	10	0.33
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	12	0.33
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	13	0.33
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	18	0.33
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	6	0.33
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	10	0.33
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	10	0.33
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	10	0.33
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	16	0.33
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	16	0.33
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	2	0.33
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	5	0.33
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	6	0.33
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	17	0.33
(2,240)	1:8:A:TYR:HB3	1:15:A:PRO:HA	2	0.33
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	4	0.33
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	4	0.33
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	4	0.33
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	7	0.33
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	7	0.33
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	7	0.33
(2,82)	1:60:A:LYS:HE2	1:54:A:ILE:HG12	9	0.33
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	15	0.33
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	10	0.33
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	17	0.33
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	1	0.33
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	9	0.33
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	5	0.33
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	16	0.33
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	19	0.33
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	1	0.33
(1,173)	1:70:A:GLU:HB2	1:70:A:GLU:HG2	11	0.33
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	2	0.33
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	3	0.33
(1,121)	1:64:A:TYR:HD1	1:65:A:ASP:H	4	0.33
(1,121)	1:64:A:TYR:HD2	1:65:A:ASP:H	4	0.33
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	6	0.33
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	14	0.33
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	14	0.33
(1,75)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	14	0.33
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	4	0.32
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	20	0.32
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	6	0.32
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	6	0.32
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	6	0.32
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	19	0.32
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	19	0.32
(2,2275)	1:78:A:SER:HA	1:80:A:GLY:H	12	0.32
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	8	0.32
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	1	0.32
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	14	0.32
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	11	0.32
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	8	0.32
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	17	0.32
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	12	0.32
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	2	0.32
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	2	0.32
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	2	0.32
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	6	0.32
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	6	0.32
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	6	0.32
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	14	0.32
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	14	0.32
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	14	0.32
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	15	0.32
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	6	0.32
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	17	0.32
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	20	0.32
(2,2005)	1:57:A:ASP:H	1:60:A:LYS:HB3	6	0.32
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	3	0.32
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	3	0.32
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	13	0.32
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	15	0.32
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	15	0.32
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	15	0.32
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	20	0.32
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	1	0.32
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	16	0.32
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	18	0.32
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	19	0.32
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	20	0.32
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	10	0.32
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	16	0.32
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	1	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	7	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	7	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	7	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	16	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	16	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	16	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	19	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	19	0.32
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	19	0.32
(2,1704)	1:26:A:TYR:H	1:27:A:ARG:HG2	1	0.32
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	3	0.32
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	7	0.32
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	14	0.32
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	17	0.32
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	1	0.32
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	20	0.32
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	15	0.32
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	15	0.32
(2,1384)	1:79:A:PHE:HB3	1:79:A:PHE:H	9	0.32
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	13	0.32
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	8	0.32
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	8	0.32
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	13	0.32
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	10	0.32
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	10	0.32
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	10	0.32
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	20	0.32
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	20	0.32
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	5	0.32
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	8	0.32
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	8	0.32
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	8	0.32
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	13	0.32
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	5	0.32
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	5	0.32
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	5	0.32
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	10	0.32
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	3	0.32
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	7	0.32
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	18	0.32
(2,627)	1:31:A:LEU:HA	1:34:A:HIS:HB2	1	0.32
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	1	0.32
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	1	0.32
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	1	0.32
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	17	0.32
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	17	0.32
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	17	0.32
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	15	0.32
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	15	0.32
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	2	0.32
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	2	0.32
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	2	0.32
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	17	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	1	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	3	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	5	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	7	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	9	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	14	0.32
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	19	0.32
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	2	0.32
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	20	0.32
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	20	0.32
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	20	0.32
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	4	0.32
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	4	0.32
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	4	0.32
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	4	0.32
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	4	0.32
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	4	0.32
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	4	0.32
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	4	0.32
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	4	0.32
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	4	0.32
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	2	0.32
(2,238)	1:22:A:LEU:HD21	1:15:A:PRO:HA	10	0.32
(2,238)	1:22:A:LEU:HD22	1:15:A:PRO:HA	10	0.32
(2,238)	1:22:A:LEU:HD23	1:15:A:PRO:HA	10	0.32
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	3	0.32
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	10	0.32
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	18	0.32
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	18	0.32
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	18	0.32
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	7	0.32
(2,176)	1:11:A:LEU:HB2	1:10:A:LEU:HB2	6	0.32
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	20	0.32
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	20	0.32
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	20	0.32
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	16	0.32
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	2	0.32
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	4	0.32
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	8	0.32
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	13	0.32
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	16	0.32
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	19	0.32
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	1	0.32
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	9	0.32
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	12	0.32
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	12	0.32
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	12	0.32
(1,374)	1:28:A:LYS:HA	1:28:A:LYS:HB3	10	0.32
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	17	0.32
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	14	0.32
(1,244)	1:4:A:GLU:HG2	1:3:A:LYS:HD3	12	0.32
(1,242)	1:31:A:LEU:HA	1:34:A:HIS:H	9	0.32
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	18	0.32
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	18	0.32
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	18	0.32
(1,205)	1:72:A:ALA:H	1:63:A:ILE:HB	19	0.32
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	10	0.32
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	11	0.32
(1,62)	1:46:A:LYS:HG3	1:42:A:THR:HA	7	0.32
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	3	0.32
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	3	0.32
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	3	0.32
(1,9)	1:48:A:ILE:HD11	1:49:A:SER:H	12	0.32
(1,9)	1:48:A:ILE:HD12	1:49:A:SER:H	12	0.32
(1,9)	1:48:A:ILE:HD13	1:49:A:SER:H	12	0.32
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	15	0.31
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	18	0.31
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	18	0.31
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	18	0.31
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	4	0.31
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	4	0.31
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	4	0.31
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	4	0.31
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	4	0.31
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	4	0.31
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	6	0.31
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	12	0.31
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	16	0.31
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	20	0.31
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	12	0.31
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	12	0.31
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	12	0.31
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	9	0.31
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	13	0.31
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	16	0.31
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	17	0.31
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	1	0.31
(2,1991)	1:52:A:PHE:HA	1:56:A:ASN:H	12	0.31
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	17	0.31
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	17	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD11	15	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD12	15	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD13	15	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD11	18	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD12	18	0.31
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD13	18	0.31
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	2	0.31
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	2	0.31
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	5	0.31
(2,1820)	1:41:A:ASP:H	1:41:A:ASP:HB2	12	0.31
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	2	0.31
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	4	0.31
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	3	0.31
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	3	0.31
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	3	0.31
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	9	0.31
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	9	0.31
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	14	0.31
(2,1673)	1:22:A:LEU:HD21	1:23:A:LYS:H	9	0.31
(2,1673)	1:22:A:LEU:HD22	1:23:A:LYS:H	9	0.31
(2,1673)	1:22:A:LEU:HD23	1:23:A:LYS:H	9	0.31
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	1	0.31
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	11	0.31
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	12	0.31
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	1	0.31
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	7	0.31
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	16	0.31
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	16	0.31
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	16	0.31
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	16	0.31
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	18	0.31
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	18	0.31
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	18	0.31
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	19	0.31
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	19	0.31
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	19	0.31
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	9	0.31
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	9	0.31
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	13	0.31
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	13	0.31
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	8	0.31
(2,1454)	1:3:A:LYS:HB3	1:4:A:GLU:H	19	0.31
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	7	0.31
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	7	0.31
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	7	0.31
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	7	0.31
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	13	0.31
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	13	0.31
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	13	0.31
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	12	0.31
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	16	0.31
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	16	0.31
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	16	0.31
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	4	0.31
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	13	0.31
(2,1100)	1:60:A:LYS:HD2	1:54:A:ILE:HD11	4	0.31
(2,1100)	1:60:A:LYS:HD2	1:54:A:ILE:HD12	4	0.31
(2,1100)	1:60:A:LYS:HD2	1:54:A:ILE:HD13	4	0.31
(2,1075)	1:63:A:ILE:HD11	1:59:A:GLN:HG3	20	0.31
(2,1075)	1:63:A:ILE:HD12	1:59:A:GLN:HG3	20	0.31
(2,1075)	1:63:A:ILE:HD13	1:59:A:GLN:HG3	20	0.31
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	6	0.31
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	15	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	1	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	1	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	1	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	5	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	5	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	5	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	7	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	7	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	7	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	8	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	8	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	8	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	13	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	13	0.31
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	13	0.31
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	20	0.31
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB1	9	0.31
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB2	9	0.31
(2,888)	1:7:A:LEU:HG	1:51:A:ALA:HB3	9	0.31
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	13	0.31
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	1	0.31
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	1	0.31
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	1	0.31
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	3	0.31
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	8	0.31
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	14	0.31
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	19	0.31
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	14	0.31
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	14	0.31
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	13	0.31
(2,721)	1:41:A:ASP:HB3	1:44:A:LYS:HB2	3	0.31
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	4	0.31
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	9	0.31
(2,626)	1:31:A:LEU:HA	1:34:A:HIS:HB3	4	0.31
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	15	0.31
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	11	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	4	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	5	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	6	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	7	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	8	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	9	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	10	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	11	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	12	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	13	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	14	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	16	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	17	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	18	0.31
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	20	0.31
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	19	0.31
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	7	0.31
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	15	0.31
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	16	0.31
(2,452)	1:20:A:GLN:HA	1:23:A:LYS:HB3	6	0.31
(2,444)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	5	0.31
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	15	0.31
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	15	0.31
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	15	0.31
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	1	0.31
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	1	0.31
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	1	0.31
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	9	0.31
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	9	0.31
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	13	0.31
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	14	0.31
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	7	0.31
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	14	0.31
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	14	0.31
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	14	0.31
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	1	0.31
(2,50)	1:4:A:GLU:H	1:6:A:LYS:HB3	19	0.31
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	17	0.31
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	8	0.31
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	10	0.31
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	12	0.31
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	3	0.31
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	6	0.31
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	12	0.31
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	9	0.31
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	17	0.31
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	15	0.31
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	15	0.31
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	15	0.31
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	8	0.31
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	8	0.31
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	8	0.31
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	10	0.31
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	16	0.31
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	18	0.31
(1,249)	1:60:A:LYS:HG3	1:57:A:ASP:HB3	12	0.31
(1,242)	1:31:A:LEU:HA	1:34:A:HIS:H	16	0.31
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	11	0.31
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	7	0.31
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	1	0.31
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	19	0.31
(1,136)	1:6:A:LYS:HG2	1:6:A:LYS:HA	2	0.31
(1,75)	1:5:A:THR:HG21	1:15:A:PRO:HG2	6	0.31
(1,75)	1:5:A:THR:HG22	1:15:A:PRO:HG2	6	0.31
(1,75)	1:5:A:THR:HG23	1:15:A:PRO:HG2	6	0.31
(1,73)	1:37:A:LYS:HG3	1:34:A:HIS:H	13	0.31
(1,68)	1:72:A:ALA:HB1	1:76:A:GLY:H	14	0.31
(1,68)	1:72:A:ALA:HB2	1:76:A:GLY:H	14	0.31
(1,68)	1:72:A:ALA:HB3	1:76:A:GLY:H	14	0.31
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	12	0.3
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	18	0.3
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	20	0.3
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	15	0.3
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	2	0.3
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	7	0.3
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	7	0.3
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	7	0.3
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	7	0.3
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	7	0.3
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	7	0.3
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE2	8	0.3
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE2	8	0.3
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	8	0.3
(2,2249)	1:77:A:PRO:HD2	1:76:A:GLY:H	19	0.3
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	1	0.3
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	9	0.3
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	6	0.3
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	12	0.3
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	13	0.3
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	15	0.3
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	16	0.3
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	2	0.3
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	15	0.3
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	12	0.3
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	12	0.3
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	14	0.3
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	14	0.3
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	14	0.3
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	4	0.3
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	1	0.3
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	1	0.3
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	1	0.3
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	8	0.3
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	8	0.3
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	6	0.3
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	6	0.3
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	11	0.3
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	14	0.3
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	13	0.3
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	13	0.3
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	13	0.3
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	2	0.3
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	10	0.3
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	14	0.3
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1820)	1:41:A:ASP:H	1:41:A:ASP:HB2	3	0.3
(2,1804)	1:39:A:THR:H	1:37:A:LYS:HG2	17	0.3
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	16	0.3
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	18	0.3
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	13	0.3
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	9	0.3
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	9	0.3
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	9	0.3
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	19	0.3
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	5	0.3
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	2	0.3
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	3	0.3
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	16	0.3
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	1	0.3
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	3	0.3
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	3	0.3
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	3	0.3
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	11	0.3
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	11	0.3
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	11	0.3
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	10	0.3
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	10	0.3
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	8	0.3
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	3	0.3
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	3	0.3
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	17	0.3
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	5	0.3
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	1	0.3
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	17	0.3
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	17	0.3
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	17	0.3
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	17	0.3
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	17	0.3
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	17	0.3
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	20	0.3
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	15	0.3
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	10	0.3
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	10	0.3
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	10	0.3
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	19	0.3
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	13	0.3
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1103)	1:54:A:ILE:HG12	1:60:A:LYS:HD3	12	0.3
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	4	0.3
(2,1082)	1:59:A:GLN:HA	1:59:A:GLN:HG3	13	0.3
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	19	0.3
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	1	0.3
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	1	0.3
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	16	0.3
(2,1054)	1:58:A:PRO:HB2	1:58:A:PRO:HA	19	0.3
(2,967)	1:54:A:ILE:HD11	1:72:A:ALA:HA	17	0.3
(2,967)	1:54:A:ILE:HD12	1:72:A:ALA:HA	17	0.3
(2,967)	1:54:A:ILE:HD13	1:72:A:ALA:HA	17	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	4	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	4	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	4	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	9	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	9	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	9	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	17	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	17	0.3
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	17	0.3
(2,902)	1:11:A:LEU:HD21	1:52:A:PHE:HA	5	0.3
(2,902)	1:11:A:LEU:HD22	1:52:A:PHE:HA	5	0.3
(2,902)	1:11:A:LEU:HD23	1:52:A:PHE:HA	5	0.3
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	16	0.3
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	16	0.3
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	16	0.3
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	16	0.3
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	16	0.3
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	16	0.3
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	11	0.3
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	11	0.3
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	11	0.3
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	11	0.3
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	11	0.3
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	11	0.3
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	12	0.3
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	5	0.3
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	13	0.3
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	13	0.3
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	16	0.3
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	16	0.3
(2,641)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,641)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	19	0.3
(2,641)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	19	0.3
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	11	0.3
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	11	0.3
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	11	0.3
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	20	0.3
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	20	0.3
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	20	0.3
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	16	0.3
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	16	0.3
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	1	0.3
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	2	0.3
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	3	0.3
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	15	0.3
(2,469)	1:60:A:LYS:HA	1:60:A:LYS:HB2	19	0.3
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	16	0.3
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	11	0.3
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	11	0.3
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	11	0.3
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	13	0.3
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	13	0.3
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	2	0.3
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	2	0.3
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	1	0.3
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	10	0.3
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	4	0.3
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	18	0.3
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	13	0.3
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	13	0.3
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	13	0.3
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	13	0.3
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	13	0.3
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	13	0.3
(2,115)	1:7:A:LEU:HG	1:64:A:TYR:HD1	19	0.3
(2,115)	1:7:A:LEU:HG	1:64:A:TYR:HD2	19	0.3
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	15	0.3
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	15	0.3
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	15	0.3
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	15	0.3
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	15	0.3
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	15	0.3
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	15	0.3
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	15	0.3
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	13	0.3
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	5	0.3
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	12	0.3
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	17	0.3
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HG3	20	0.3
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	2	0.3
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	6	0.3
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	11	0.3
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	15	0.3
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	20	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD11	1	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD12	1	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD13	1	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD11	12	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD12	12	0.3
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD13	12	0.3
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	7	0.3
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	7	0.3
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	7	0.3
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	3	0.3
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	3	0.3
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	3	0.3
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	1	0.3
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	1	0.3
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	1	0.3
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	15	0.3
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	15	0.3
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	11	0.3
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	2	0.3
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	2	0.3
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	2	0.3
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	3	0.3
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	3	0.3
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	3	0.3
(1,294)	1:28:A:LYS:HD3	1:28:A:LYS:HG2	17	0.3
(1,266)	1:33:A:TYR:H	1:32:A:LYS:HA	15	0.3
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	2	0.3
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	2	0.3
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	2	0.3
(1,205)	1:72:A:ALA:H	1:63:A:ILE:HB	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	11	0.3
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	11	0.3
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	11	0.3
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HB3	6	0.3
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	7	0.3
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	18	0.3
(1,121)	1:64:A:TYR:HD1	1:65:A:ASP:H	6	0.3
(1,121)	1:64:A:TYR:HD2	1:65:A:ASP:H	6	0.3
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	14	0.3
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	8	0.3
(1,47)	1:2:A:VAL:HB	1:65:A:ASP:H	15	0.3
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	2	0.29
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	16	0.29
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	6	0.29
(2,2343)	1:31:A:LEU:HB2	1:34:A:HIS:HD2	10	0.29
(2,2339)	1:34:A:HIS:HD2	1:34:A:HIS:HA	19	0.29
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	7	0.29
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	7	0.29
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	12	0.29
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	17	0.29
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	19	0.29
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	6	0.29
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	12	0.29
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	12	0.29
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	12	0.29
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	19	0.29
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	19	0.29
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	5	0.29
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	18	0.29
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	7	0.29
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	7	0.29
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	7	0.29
(2,1821)	1:41:A:ASP:H	1:41:A:ASP:HB3	6	0.29
(2,1805)	1:39:A:THR:H	1:37:A:LYS:HD3	7	0.29
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	4	0.29
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	3	0.29
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	5	0.29
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	8	0.29
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	9	0.29
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	14	0.29
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	17	0.29
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	14	0.29
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	14	0.29
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	1	0.29
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	1	0.29
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	4	0.29
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	10	0.29
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	13	0.29
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	17	0.29
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	13	0.29
(2,1650)	1:21:A:GLU:H	1:23:A:LYS:HD2	16	0.29
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	12	0.29
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	15	0.29
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	7	0.29
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	7	0.29
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	7	0.29
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	1	0.29
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	1	0.29
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	1	0.29
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	2	0.29
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	2	0.29
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	2	0.29
(2,1521)	1:6:A:LYS:HA	1:10:A:LEU:H	7	0.29
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	19	0.29
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	13	0.29
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	10	0.29
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	12	0.29
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	8	0.29
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	15	0.29
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	15	0.29
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	15	0.29
(2,1407)	1:33:A:TYR:HD1	1:41:A:ASP:H	18	0.29
(2,1407)	1:33:A:TYR:HD2	1:41:A:ASP:H	18	0.29
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	2	0.29
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	17	0.29
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	17	0.29
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	17	0.29
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	9	0.29
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	9	0.29
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	9	0.29
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	16	0.29
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	16	0.29
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	3	0.29
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	3	0.29
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	3	0.29
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	6	0.29
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	6	0.29
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	6	0.29
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	10	0.29
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	6	0.29
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE2	16	0.29
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	8	0.29
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	8	0.29
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	8	0.29
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	2	0.29
(2,688)	1:40:A:GLY:H	1:38:A:PRO:HA	20	0.29
(2,614)	1:30:A:ALA:HB1	1:27:A:ARG:HB2	18	0.29
(2,614)	1:30:A:ALA:HB2	1:27:A:ARG:HB2	18	0.29
(2,614)	1:30:A:ALA:HB3	1:27:A:ARG:HB2	18	0.29
(2,458)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	3	0.29
(2,458)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	9	0.29
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	8	0.29
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	8	0.29
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	8	0.29
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	19	0.29
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	19	0.29
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	19	0.29
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	7	0.29
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	7	0.29
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	7	0.29
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	7	0.29
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	7	0.29
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	13	0.29
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	13	0.29
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	14	0.29
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	14	0.29
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	2	0.29
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	2	0.29
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	2	0.29
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	2	0.29
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	11	0.29
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	11	0.29
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	11	0.29
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	11	0.29
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	15	0.29
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD11	4	0.29
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD12	4	0.29
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD13	4	0.29
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	9	0.29
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	9	0.29
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	9	0.29
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	9	0.29
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	1	0.29
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	7	0.29
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	11	0.29
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	15	0.29
(2,23)	1:2:A:VAL:HA	1:4:A:GLU:H	7	0.29
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	4	0.29
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	17	0.29
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	18	0.29
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	18	0.29
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	14	0.29
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD11	14	0.29
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD12	14	0.29
(1,426)	1:31:A:LEU:H	1:31:A:LEU:HD13	14	0.29
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	6	0.29
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	5	0.29
(1,357)	1:50:A:GLU:HA	1:53:A:GLU:HB2	10	0.29
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	5	0.29
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	4	0.29
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	9	0.29
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	4	0.29
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	11	0.29
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	11	0.29
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	11	0.29
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD21	3	0.29
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD22	3	0.29
(1,219)	1:10:A:LEU:HA	1:10:A:LEU:HD23	3	0.29
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	14	0.29
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	17	0.29
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	10	0.29
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	10	0.29
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	10	0.29
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE3	10	0.29
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE3	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:4:A:GLU:HG3	1:3:A:LYS:HD2	14	0.29
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	15	0.29
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	1	0.29
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	3	0.29
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	17	0.29
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	18	0.29
(1,78)	1:19:A:GLU:HA	1:22:A:LEU:HB2	12	0.29
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	16	0.28
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	16	0.28
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	16	0.28
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE2	19	0.28
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE2	19	0.28
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE2	19	0.28
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	2	0.28
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	14	0.28
(2,2276)	1:79:A:PHE:HA	1:80:A:GLY:H	7	0.28
(2,2276)	1:79:A:PHE:HA	1:80:A:GLY:H	13	0.28
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	2	0.28
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	17	0.28
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	4	0.28
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	19	0.28
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	4	0.28
(2,2133)	1:67:A:TYR:H	1:66:A:GLN:HB3	8	0.28
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	15	0.28
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	11	0.28
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	12	0.28
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	3	0.28
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	14	0.28
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	8	0.28
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	4	0.28
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	4	0.28
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	4	0.28
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	17	0.28
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	7	0.28
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	7	0.28
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	7	0.28
(2,1820)	1:41:A:ASP:H	1:41:A:ASP:HB2	15	0.28
(2,1803)	1:39:A:THR:HG21	1:39:A:THR:H	6	0.28
(2,1803)	1:39:A:THR:HG22	1:39:A:THR:H	6	0.28
(2,1803)	1:39:A:THR:HG23	1:39:A:THR:H	6	0.28
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	5	0.28
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	17	0.28
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	17	0.28
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	18	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	2	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	2	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	2	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	5	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	5	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	5	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	12	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	12	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	12	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	16	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	16	0.28
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	16	0.28
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	18	0.28
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	9	0.28
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	19	0.28
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	3	0.28
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	11	0.28
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	6	0.28
(2,1630)	1:22:A:LEU:HD21	1:19:A:GLU:H	12	0.28
(2,1630)	1:22:A:LEU:HD22	1:19:A:GLU:H	12	0.28
(2,1630)	1:22:A:LEU:HD23	1:19:A:GLU:H	12	0.28
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	8	0.28
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	8	0.28
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	8	0.28
(2,1428)	1:2:A:VAL:HG11	1:2:A:VAL:H	16	0.28
(2,1428)	1:2:A:VAL:HG12	1:2:A:VAL:H	16	0.28
(2,1428)	1:2:A:VAL:HG13	1:2:A:VAL:H	16	0.28
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	8	0.28
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	11	0.28
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	19	0.28
(2,1340)	1:77:A:PRO:HA	1:78:A:SER:H	7	0.28
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	1	0.28
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	4	0.28
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	18	0.28
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	4	0.28
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	11	0.28
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	11	0.28
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	11	0.28
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	17	0.28
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	17	0.28
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	17	0.28
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	14	0.28
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	18	0.28
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	3	0.28
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	11	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	11	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	11	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	11	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	18	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	18	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	18	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	19	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	19	0.28
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	19	0.28
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	12	0.28
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	12	0.28
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	12	0.28
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	12	0.28
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	12	0.28
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	12	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	1	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	1	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	1	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	2	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	2	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	2	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	4	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	4	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	4	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	5	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	5	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	5	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	6	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	6	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	6	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	8	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	8	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	8	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	10	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	10	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	13	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	13	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	13	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	14	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	14	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	14	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	15	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	15	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	15	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	18	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	18	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	18	0.28
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	19	0.28
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	19	0.28
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	19	0.28
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	3	0.28
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	3	0.28
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	3	0.28
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	13	0.28
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	13	0.28
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	13	0.28
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	12	0.28
(2,759)	1:43:A:GLU:HG2	1:42:A:THR:HB	20	0.28
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	5	0.28
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	19	0.28
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	19	0.28
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	19	0.28
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	19	0.28
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	5	0.28
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	5	0.28
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	5	0.28
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB2	12	0.28
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	18	0.28
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	14	0.28
(2,458)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	1	0.28
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	6	0.28
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	20	0.28
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	16	0.28
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	16	0.28
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	16	0.28
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	17	0.28
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	17	0.28
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	20	0.28
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	20	0.28
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	8	0.28
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	8	0.28
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	8	0.28
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	8	0.28
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	8	0.28
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	10	0.28
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	10	0.28
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	11	0.28
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	11	0.28
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	16	0.28
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	16	0.28
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	7	0.28
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	14	0.28
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	10	0.28
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	14	0.28
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	5	0.28
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	20	0.28
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	2	0.28
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	1	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	1	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	3	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	7	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	8	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	11	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	12	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	13	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	14	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	15	0.28
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	19	0.28
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	13	0.28
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	11	0.28
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	19	0.28
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	18	0.28
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	7	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	11	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	11	0.28
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	11	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	6	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	7	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	9	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	11	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	12	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	13	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	16	0.28
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	18	0.28
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	12	0.28
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	1	0.28
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	2	0.28
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	19	0.28
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	4	0.28
(1,231)	1:24:A:LYS:HD3	1:24:A:LYS:HE2	6	0.28
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	7	0.28
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	11	0.28
(1,142)	1:22:A:LEU:HA	1:23:A:LYS:H	15	0.28
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	16	0.28
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	15	0.28
(1,110)	1:50:A:GLU:HG2	1:54:A:ILE:HB	6	0.28
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	7	0.28
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	2	0.28
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	8	0.28
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	10	0.28
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	11	0.28
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	13	0.28
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	1	0.27
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	1	0.27
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	1	0.27
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	5	0.27
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	5	0.27
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	5	0.27
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	3	0.27
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	10	0.27
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	2	0.27
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	14	0.27
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	20	0.27
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	14	0.27
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	6	0.27
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	6	0.27
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	18	0.27
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	16	0.27
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	3	0.27
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	6	0.27
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	7	0.27
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	8	0.27
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	8	0.27
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	8	0.27
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	7	0.27
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	11	0.27
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	11	0.27
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	11	0.27
(2,1828)	1:43:A:GLU:HG2	1:42:A:THR:H	11	0.27
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	1	0.27
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	12	0.27
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	19	0.27
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	2	0.27
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	11	0.27
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	11	0.27
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	11	0.27
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	5	0.27
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	18	0.27
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	15	0.27
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	1	0.27
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	18	0.27
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	8	0.27
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	19	0.27
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	4	0.27
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	4	0.27
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	4	0.27
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	7	0.27
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	15	0.27
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	12	0.27
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	3	0.27
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	4	0.27
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	5	0.27
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	9	0.27
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	14	0.27
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	20	0.27
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	16	0.27
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	6	0.27
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	6	0.27
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	18	0.27
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	18	0.27
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	18	0.27
(2,1263)	1:47:A:GLU:HG2	1:50:A:GLU:H	2	0.27
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	6	0.27
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	9	0.27
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	16	0.27
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	10	0.27
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	4	0.27
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	8	0.27
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	13	0.27
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	2	0.27
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	2	0.27
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	2	0.27
(2,919)	1:52:A:PHE:HB2	1:8:A:TYR:HA	19	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	3	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	3	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	3	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	7	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	7	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	7	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	9	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	9	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	9	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	11	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	11	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	11	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	12	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	12	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	12	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	16	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	16	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	16	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	17	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	17	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	17	0.27
(2,858)	1:48:A:ILE:HG21	1:48:A:ILE:HG13	20	0.27
(2,858)	1:48:A:ILE:HG22	1:48:A:ILE:HG13	20	0.27
(2,858)	1:48:A:ILE:HG23	1:48:A:ILE:HG13	20	0.27
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	1	0.27
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD11	9	0.27
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD12	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,821)	1:60:A:LYS:HE2	1:54:A:ILE:HD13	9	0.27
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	16	0.27
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	16	0.27
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	16	0.27
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	12	0.27
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	14	0.27
(2,641)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	11	0.27
(2,641)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	11	0.27
(2,641)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	11	0.27
(2,548)	1:27:A:ARG:HB3	1:28:A:LYS:H	9	0.27
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	1	0.27
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	16	0.27
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	16	0.27
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	16	0.27
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	19	0.27
(2,458)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	19	0.27
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	4	0.27
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	4	0.27
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	4	0.27
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	4	0.27
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	5	0.27
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	5	0.27
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	5	0.27
(2,319)	1:18:A:ASN:HB2	1:19:A:GLU:H	19	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	1	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	1	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	3	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	3	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	4	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	4	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	5	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	5	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	6	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	6	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	15	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	15	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	19	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	19	0.27
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	20	0.27
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	20	0.27
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	5	0.27
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	6	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	13	0.27
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	17	0.27
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	19	0.27
(2,245)	1:15:A:PRO:HA	1:14:A:SER:HA	12	0.27
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	8	0.27
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	17	0.27
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	8	0.27
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	8	0.27
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	8	0.27
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	11	0.27
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	12	0.27
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	18	0.27
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	20	0.27
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	9	0.27
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	12	0.27
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD21	2	0.27
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD22	2	0.27
(1,479)	1:69:A:LEU:H	1:69:A:LEU:HD23	2	0.27
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	5	0.27
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	10	0.27
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	17	0.27
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	2	0.27
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	19	0.27
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	17	0.27
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	17	0.27
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	17	0.27
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	3	0.27
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	9	0.27
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	10	0.27
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	12	0.27
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	13	0.27
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	20	0.27
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	12	0.27
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	4	0.27
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	10	0.27
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	12	0.27
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	3	0.27
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	3	0.27
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	3	0.27
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	1	0.27
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	2	0.27
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	14	0.27
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	15	0.27
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	17	0.27
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	20	0.27
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	5	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	5	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	7	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	9	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	10	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	13	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	17	0.27
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	19	0.27
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	16	0.27
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD11	7	0.27
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD12	7	0.27
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD13	7	0.27
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD11	7	0.27
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD12	7	0.27
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD13	7	0.27
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	9	0.27
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	17	0.27
(1,128)	1:23:A:LYS:HB3	1:24:A:LYS:H	11	0.27
(1,98)	1:14:A:SER:H	1:21:A:GLU:HB2	13	0.27
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	4	0.27
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	16	0.27
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	19	0.27
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	20	0.27
(1,24)	1:37:A:LYS:HE2	1:34:A:HIS:H	17	0.27
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	12	0.26
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	12	0.26
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	12	0.26
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	1	0.26
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	7	0.26
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	17	0.26
(2,2450)	1:58:A:PRO:HD3	1:57:A:ASP:H	6	0.26
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	9	0.26
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	1	0.26
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	1	0.26
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	12	0.26
(2,2247)	1:63:A:ILE:HG13	1:76:A:GLY:H	11	0.26
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	3	0.26
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	5	0.26
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	10	0.26
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	9	0.26
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	7	0.26
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	17	0.26
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	6	0.26
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	6	0.26
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	20	0.26
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	15	0.26
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	18	0.26
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	11	0.26
(2,2051)	1:64:A:TYR:HB2	1:65:A:ASP:H	18	0.26
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	9	0.26
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	17	0.26
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	14	0.26
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	14	0.26
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	14	0.26
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	14	0.26
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	6	0.26
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	19	0.26
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD1	4	0.26
(2,1935)	1:52:A:PHE:H	1:52:A:PHE:HD2	4	0.26
(2,1933)	1:52:A:PHE:H	1:8:A:TYR:HA	1	0.26
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	1	0.26
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	4	0.26
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	5	0.26
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	13	0.26
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	13	0.26
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	13	0.26
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	3	0.26
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	3	0.26
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	3	0.26
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	17	0.26
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	17	0.26
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	17	0.26
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	6	0.26
(2,1831)	1:45:A:PHE:HB2	1:42:A:THR:H	11	0.26
(2,1804)	1:39:A:THR:H	1:37:A:LYS:HG2	5	0.26
(2,1786)	1:33:A:TYR:HB3	1:33:A:TYR:H	7	0.26
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	3	0.26
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	9	0.26
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	10	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	1	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	1	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	1	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	17	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	17	0.26
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	17	0.26
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	2	0.26
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	7	0.26
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	4	0.26
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	18	0.26
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	20	0.26
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	12	0.26
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	16	0.26
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	7	0.26
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	13	0.26
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	20	0.26
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	20	0.26
(2,1469)	1:3:A:LYS:HB2	1:6:A:LYS:H	11	0.26
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	11	0.26
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	19	0.26
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	20	0.26
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	4	0.26
(2,1456)	1:4:A:GLU:H	1:3:A:LYS:HG2	14	0.26
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	12	0.26
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	16	0.26
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	2	0.26
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	6	0.26
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	8	0.26
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	19	0.26
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	9	0.26
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	4	0.26
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	4	0.26
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	4	0.26
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	14	0.26
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	5	0.26
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	6	0.26
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	6	0.26
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	18	0.26
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	18	0.26
(2,1198)	1:65:A:ASP:HB2	1:62:A:GLU:HA	15	0.26
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	2	0.26
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	7	0.26
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	15	0.26
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	15	0.26
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	7	0.26
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	5	0.26
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	20	0.26
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	9	0.26
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	18	0.26
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	4	0.26
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	9	0.26
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	9	0.26
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	9	0.26
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	1	0.26
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	1	0.26
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	1	0.26
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	15	0.26
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	4	0.26
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	6	0.26
(2,717)	1:40:A:GLY:HA3	1:41:A:ASP:HA	12	0.26
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	8	0.26
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	13	0.26
(2,627)	1:31:A:LEU:HA	1:34:A:HIS:HB2	13	0.26
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	11	0.26
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	11	0.26
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	11	0.26
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	20	0.26
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	20	0.26
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	20	0.26
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	7	0.26
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	17	0.26
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	17	0.26
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	17	0.26
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	17	0.26
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	17	0.26
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	17	0.26
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	17	0.26
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	17	0.26
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	17	0.26
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	9	0.26
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	9	0.26
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	12	0.26
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	12	0.26
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	12	0.26
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	17	0.26
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	17	0.26
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	17	0.26
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	17	0.26
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	12	0.26
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	12	0.26
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	17	0.26
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	17	0.26
(2,314)	1:45:A:PHE:HE1	1:45:A:PHE:HB2	18	0.26
(2,314)	1:45:A:PHE:HE2	1:45:A:PHE:HB2	18	0.26
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	20	0.26
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	1	0.26
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	2	0.26
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	9	0.26
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	16	0.26
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	1	0.26
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	6	0.26
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	11	0.26
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	13	0.26
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	13	0.26
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	13	0.26
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	19	0.26
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	19	0.26
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	19	0.26
(2,176)	1:11:A:LEU:HB2	1:10:A:LEU:HB2	18	0.26
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	1	0.26
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	5	0.26
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	7	0.26
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	4	0.26
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	4	0.26
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	8	0.26
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	14	0.26
(1,456)	1:26:A:TYR:HA	1:27:A:ARG:H	16	0.26
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	3	0.26
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	12	0.26
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	12	0.26
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	12	0.26
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	2	0.26
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	11	0.26
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	17	0.26
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	18	0.26
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	16	0.26
(1,334)	1:72:A:ALA:HB1	1:74:A:SER:H	17	0.26
(1,334)	1:72:A:ALA:HB2	1:74:A:SER:H	17	0.26
(1,334)	1:72:A:ALA:HB3	1:74:A:SER:H	17	0.26
(1,332)	1:70:A:GLU:HA	1:73:A:ARG:HG3	6	0.26
(1,294)	1:6:A:LYS:HG2	1:6:A:LYS:HD2	2	0.26
(1,294)	1:24:A:LYS:HD3	1:24:A:LYS:HG2	8	0.26
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	15	0.26
(1,294)	1:28:A:LYS:HD3	1:28:A:LYS:HG2	19	0.26
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	19	0.26
(1,241)	1:6:A:LYS:HG3	1:10:A:LEU:HD11	2	0.26
(1,241)	1:6:A:LYS:HG3	1:10:A:LEU:HD12	2	0.26
(1,241)	1:6:A:LYS:HG3	1:10:A:LEU:HD13	2	0.26
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	15	0.26
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	19	0.26
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	5	0.26
(1,231)	1:24:A:LYS:HD3	1:24:A:LYS:HE2	12	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	1	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	3	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	6	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	12	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	14	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	16	0.26
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	18	0.26
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	19	0.26
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	18	0.26
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	3	0.26
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	13	0.26
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	17	0.26
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	18	0.26
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	20	0.26
(1,79)	1:6:A:LYS:H	1:9:A:ASP:H	14	0.26
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	15	0.26
(1,68)	1:72:A:ALA:HB1	1:76:A:GLY:H	4	0.26
(1,68)	1:72:A:ALA:HB2	1:76:A:GLY:H	4	0.26
(1,68)	1:72:A:ALA:HB3	1:76:A:GLY:H	4	0.26
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	13	0.26
(1,24)	1:37:A:LYS:HE2	1:34:A:HIS:H	9	0.26
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	14	0.25
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	5	0.25
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	2	0.25
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	2	0.25
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	2	0.25
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	14	0.25
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	14	0.25
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	14	0.25
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	16	0.25
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	16	0.25
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	16	0.25
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	5	0.25
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	5	0.25
(2,2278)	1:-1:A:MET:HB2	1:-1:A:MET:H	10	0.25
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	2	0.25
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	13	0.25
(2,2182)	1:70:A:GLU:H	1:73:A:ARG:HD2	8	0.25
(2,2132)	1:67:A:TYR:H	1:66:A:GLN:HB2	3	0.25
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	6	0.25
(2,2085)	1:64:A:TYR:HB3	1:63:A:ILE:H	1	0.25
(2,2018)	1:59:A:GLN:H	1:59:A:GLN:HG3	12	0.25
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	20	0.25
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	5	0.25
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	4	0.25
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	2	0.25
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	19	0.25
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	18	0.25
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	3	0.25
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	12	0.25
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	19	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	10	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	10	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	10	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	18	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	18	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	18	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	20	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	20	0.25
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	20	0.25
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	8	0.25
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	8	0.25
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	5	0.25
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	20	0.25
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	12	0.25
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	7	0.25
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	11	0.25
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	6	0.25
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	6	0.25
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	6	0.25
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	19	0.25
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	19	0.25
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	19	0.25
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	5	0.25
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	6	0.25
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	6	0.25
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	6	0.25
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	3	0.25
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	20	0.25
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	1	0.25
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	19	0.25
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	11	0.25
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	14	0.25
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	10	0.25
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	18	0.25
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	18	0.25
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	18	0.25
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	12	0.25
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	12	0.25
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	12	0.25
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	12	0.25
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	12	0.25
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	12	0.25
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	10	0.25
(2,1300)	1:24:A:LYS:HE2	1:21:A:GLU:HA	10	0.25
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	20	0.25
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	20	0.25
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	20	0.25
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	2	0.25
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	2	0.25
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	2	0.25
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	3	0.25
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	3	0.25
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	6	0.25
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	12	0.25
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	13	0.25
(2,1251)	1:70:A:GLU:HA	1:70:A:GLU:HG3	7	0.25
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	2	0.25
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	10	0.25
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	3	0.25
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	1	0.25
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	3	0.25
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	12	0.25
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	6	0.25
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	8	0.25
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	15	0.25
(2,641)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	1	0.25
(2,641)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	1	0.25
(2,641)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	1	0.25
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	6	0.25
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	6	0.25
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	6	0.25
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	4	0.25
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	4	0.25
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	4	0.25
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	18	0.25
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	18	0.25
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	18	0.25
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	1	0.25
(2,548)	1:27:A:ARG:HB3	1:28:A:LYS:H	2	0.25
(2,548)	1:27:A:ARG:HB3	1:28:A:LYS:H	6	0.25
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	9	0.25
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	9	0.25
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	10	0.25
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	3	0.25
(2,444)	1:23:A:LYS:HE3	1:23:A:LYS:HB2	6	0.25
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	2	0.25
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	2	0.25
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	2	0.25
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	11	0.25
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	11	0.25
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	11	0.25
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	16	0.25
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	16	0.25
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	14	0.25
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	14	0.25
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	14	0.25
(2,329)	1:26:A:TYR:HB2	1:23:A:LYS:HA	20	0.25
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	14	0.25
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	7	0.25
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	7	0.25
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	7	0.25
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	7	0.25
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	7	0.25
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	7	0.25
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	7	0.25
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	7	0.25
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	7	0.25
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	18	0.25
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	18	0.25
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	18	0.25
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	18	0.25
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	18	0.25
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	18	0.25
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	18	0.25
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	18	0.25
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	18	0.25
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	3	0.25
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	4	0.25
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	12	0.25
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	15	0.25
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	18	0.25
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	20	0.25
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	9	0.25
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	20	0.25
(2,233)	1:15:A:PRO:HA	1:15:A:PRO:HG2	14	0.25
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	9	0.25
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	9	0.25
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	9	0.25
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	15	0.25
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	15	0.25
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	15	0.25
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	18	0.25
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG21	13	0.25
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG22	13	0.25
(2,109)	1:7:A:LEU:HG	1:0:A:THR:HG23	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	16	0.25
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	13	0.25
(1,453)	1:45:A:PHE:HE1	1:48:A:ILE:HD11	7	0.25
(1,453)	1:45:A:PHE:HE1	1:48:A:ILE:HD12	7	0.25
(1,453)	1:45:A:PHE:HE1	1:48:A:ILE:HD13	7	0.25
(1,453)	1:45:A:PHE:HE2	1:48:A:ILE:HD11	7	0.25
(1,453)	1:45:A:PHE:HE2	1:48:A:ILE:HD12	7	0.25
(1,453)	1:45:A:PHE:HE2	1:48:A:ILE:HD13	7	0.25
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	7	0.25
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	20	0.25
(1,429)	1:6:A:LYS:HG3	1:7:A:LEU:H	20	0.25
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	7	0.25
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	8	0.25
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	20	0.25
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	8	0.25
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	11	0.25
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	16	0.25
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	5	0.25
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	13	0.25
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	6	0.25
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	6	0.25
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	6	0.25
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	6	0.25
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	8	0.25
(1,282)	1:29:A:ALA:H	1:28:A:LYS:HA	10	0.25
(1,278)	1:1:A:SER:H	1:1:A:SER:HB3	6	0.25
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	1	0.25
(1,242)	1:31:A:LEU:HA	1:34:A:HIS:H	20	0.25
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	16	0.25
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	9	0.25
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	9	0.25
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	9	0.25
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	2	0.25
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	4	0.25
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	8	0.25
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	11	0.25
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	15	0.25
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	3	0.25
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	19	0.25
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	19	0.25
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	19	0.25
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	2	0.25
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	8	0.25
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	10	0.25
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	1	0.25
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	15	0.25
(1,75)	1:5:A:THR:HG21	1:15:A:PRO:HG2	1	0.25
(1,75)	1:5:A:THR:HG22	1:15:A:PRO:HG2	1	0.25
(1,75)	1:5:A:THR:HG23	1:15:A:PRO:HG2	1	0.25
(1,66)	1:60:A:LYS:HG2	1:60:A:LYS:HE2	3	0.25
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	1	0.25
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	5	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	2	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	2	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	2	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	8	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	8	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	8	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	16	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	16	0.25
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	16	0.25
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	18	0.24
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	18	0.24
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	18	0.24
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	3	0.24
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	11	0.24
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	13	0.24
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	16	0.24
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	19	0.24
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	13	0.24
(2,2393)	1:19:A:GLU:HG2	1:23:A:LYS:HD2	8	0.24
(2,2343)	1:31:A:LEU:HB3	1:34:A:HIS:HD2	1	0.24
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	15	0.24
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	3	0.24
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	4	0.24
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	11	0.24
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	13	0.24
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	15	0.24
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	18	0.24
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	3	0.24
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	14	0.24
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	18	0.24
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	13	0.24
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	13	0.24
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	11	0.24
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	2	0.24
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	13	0.24
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	5	0.24
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	14	0.24
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	1	0.24
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	1	0.24
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	1	0.24
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	8	0.24
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	8	0.24
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	8	0.24
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	19	0.24
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	5	0.24
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	9	0.24
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	9	0.24
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	9	0.24
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	2	0.24
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	7	0.24
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	11	0.24
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	17	0.24
(2,1865)	1:46:A:LYS:H	1:44:A:LYS:HD3	12	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	6	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	6	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	6	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	15	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	15	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	15	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	19	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	19	0.24
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	19	0.24
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	13	0.24
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	18	0.24
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	3	0.24
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	11	0.24
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	2	0.24
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	2	0.24
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	2	0.24
(2,1579)	1:13:A:VAL:HG21	1:14:A:SER:H	3	0.24
(2,1579)	1:13:A:VAL:HG22	1:14:A:SER:H	3	0.24
(2,1579)	1:13:A:VAL:HG23	1:14:A:SER:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	6	0.24
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	6	0.24
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	6	0.24
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	14	0.24
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	19	0.24
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	18	0.24
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	18	0.24
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	14	0.24
(2,1471)	1:4:A:GLU:HA	1:6:A:LYS:H	18	0.24
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	2	0.24
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	13	0.24
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB1	4	0.24
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB2	4	0.24
(2,1419)	1:27:A:ARG:H	1:30:A:ALA:HB3	4	0.24
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	18	0.24
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	4	0.24
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	4	0.24
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	4	0.24
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	19	0.24
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	19	0.24
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	19	0.24
(2,1211)	1:66:A:GLN:HB3	1:66:A:GLN:H	12	0.24
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	10	0.24
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	7	0.24
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	16	0.24
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	19	0.24
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	3	0.24
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	5	0.24
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	20	0.24
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	4	0.24
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	11	0.24
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD11	15	0.24
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD12	15	0.24
(2,940)	1:54:A:ILE:HA	1:54:A:ILE:HD13	15	0.24
(2,918)	1:52:A:PHE:HB3	1:8:A:TYR:HA	7	0.24
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	10	0.24
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	2	0.24
(2,827)	1:24:A:LYS:HE2	1:20:A:GLN:HB3	7	0.24
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	13	0.24
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	14	0.24
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	17	0.24
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	17	0.24
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	9	0.24
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	17	0.24
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	7	0.24
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	18	0.24
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	19	0.24
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	14	0.24
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	14	0.24
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	14	0.24
(2,573)	1:29:A:ALA:H	1:28:A:LYS:HG3	20	0.24
(2,558)	1:26:A:TYR:HE1	1:27:A:ARG:HG2	8	0.24
(2,558)	1:26:A:TYR:HE2	1:27:A:ARG:HG2	8	0.24
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	12	0.24
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	14	0.24
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	15	0.24
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	17	0.24
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	19	0.24
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	20	0.24
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	5	0.24
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	5	0.24
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	5	0.24
(2,473)	1:24:A:LYS:HA	1:27:A:ARG:HD3	1	0.24
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	10	0.24
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	13	0.24
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	13	0.24
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	13	0.24
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	13	0.24
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	13	0.24
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	13	0.24
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	13	0.24
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	13	0.24
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	13	0.24
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	19	0.24
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	7	0.24
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	7	0.24
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	7	0.24
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	3	0.24
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	3	0.24
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	2	0.24
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	2	0.24
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	2	0.24
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	9	0.24
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	9	0.24
(2,348)	1:19:A:GLU:HA	1:19:A:GLU:HG2	8	0.24
(2,348)	1:19:A:GLU:HA	1:19:A:GLU:HG2	13	0.24
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	10	0.24
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	12	0.24
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	8	0.24
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	10	0.24
(2,272)	1:70:A:GLU:HB3	1:70:A:GLU:H	11	0.24
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	14	0.24
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	14	0.24
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	14	0.24
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	7	0.24
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	16	0.24
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	18	0.24
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	18	0.24
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	18	0.24
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	7	0.24
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	7	0.24
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	4	0.24
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	1	0.24
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	3	0.24
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	5	0.24
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	20	0.24
(2,14)	1:2:A:VAL:HA	1:4:A:GLU:HG3	13	0.24
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	16	0.24
(1,461)	1:8:A:TYR:HD1	1:15:A:PRO:HD3	16	0.24
(1,461)	1:8:A:TYR:HD2	1:15:A:PRO:HD3	16	0.24
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	10	0.24
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	9	0.24
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	9	0.24
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	9	0.24
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	1	0.24
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	5	0.24
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	14	0.24
(1,383)	1:53:A:GLU:H	1:52:A:PHE:HA	16	0.24
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	15	0.24
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	2	0.24
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	14	0.24
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	15	0.24
(1,294)	1:28:A:LYS:HD3	1:28:A:LYS:HG2	11	0.24
(1,294)	1:6:A:LYS:HG2	1:6:A:LYS:HD2	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:6:A:LYS:HG2	1:6:A:LYS:HD2	18	0.24
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	15	0.24
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	4	0.24
(1,231)	1:24:A:LYS:HD3	1:24:A:LYS:HE2	1	0.24
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	9	0.24
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	18	0.24
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	8	0.24
(1,182)	1:62:A:GLU:H	1:62:A:GLU:HA	20	0.24
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	12	0.24
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	12	0.24
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	12	0.24
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	13	0.24
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	11	0.24
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	16	0.24
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	11	0.24
(1,75)	1:5:A:THR:HG21	1:15:A:PRO:HG2	4	0.24
(1,75)	1:5:A:THR:HG22	1:15:A:PRO:HG2	4	0.24
(1,75)	1:5:A:THR:HG23	1:15:A:PRO:HG2	4	0.24
(1,66)	1:60:A:LYS:HE3	1:60:A:LYS:HG2	4	0.24
(1,5)	1:63:A:ILE:HD11	1:75:A:GLY:H	15	0.24
(1,5)	1:63:A:ILE:HD12	1:75:A:GLY:H	15	0.24
(1,5)	1:63:A:ILE:HD13	1:75:A:GLY:H	15	0.24
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	6	0.23
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG21	6	0.23
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG22	6	0.23
(2,2418)	1:1:A:SER:H	1:2:A:VAL:HG23	6	0.23
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	2	0.23
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	2	0.23
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	2	0.23
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	2	0.23
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	2	0.23
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	2	0.23
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	2	0.23
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	2	0.23
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	2	0.23
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	2	0.23
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	2	0.23
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	2	0.23
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	16	0.23
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	18	0.23
(2,2235)	1:73:A:ARG:HD2	1:74:A:SER:H	9	0.23
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	15	0.23
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	2	0.23
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	8	0.23
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	15	0.23
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	7	0.23
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	10	0.23
(2,2030)	1:60:A:LYS:H	1:54:A:ILE:HA	7	0.23
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	17	0.23
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	1	0.23
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	5	0.23
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	5	0.23
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	5	0.23
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	3	0.23
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	8	0.23
(2,1919)	1:34:A:HIS:H	1:36:A:ASP:HB3	6	0.23
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	6	0.23
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	6	0.23
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	6	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	1	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	3	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	9	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	10	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	16	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	19	0.23
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	20	0.23
(2,1866)	1:46:A:LYS:H	1:46:A:LYS:HG2	10	0.23
(2,1807)	1:39:A:THR:H	1:38:A:PRO:HG2	12	0.23
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	16	0.23
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	1	0.23
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	12	0.23
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	12	0.23
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	18	0.23
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	18	0.23
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	15	0.23
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	18	0.23
(2,1719)	1:27:A:ARG:H	1:23:A:LYS:HB3	2	0.23
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	1	0.23
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	17	0.23
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	18	0.23
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	5	0.23
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	8	0.23
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	1	0.23
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	1	0.23
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	1	0.23
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	10	0.23
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	10	0.23
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	10	0.23
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	19	0.23
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	19	0.23
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	19	0.23
(2,1539)	1:9:A:ASP:HB3	1:11:A:LEU:H	16	0.23
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	11	0.23
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	4	0.23
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	17	0.23
(2,1526)	1:9:A:ASP:HB3	1:10:A:LEU:H	8	0.23
(2,1526)	1:9:A:ASP:HB3	1:10:A:LEU:H	16	0.23
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	14	0.23
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	2	0.23
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	5	0.23
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	5	0.23
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	3	0.23
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	5	0.23
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	7	0.23
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	9	0.23
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	20	0.23
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	1	0.23
(2,1422)	1:27:A:ARG:H	1:23:A:LYS:HB3	2	0.23
(2,1413)	1:0:A:THR:HB	1:0:A:THR:H	20	0.23
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	17	0.23
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	2	0.23
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE1	12	0.23
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE2	12	0.23
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE1	12	0.23
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE2	12	0.23
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE1	12	0.23
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE2	12	0.23
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE1	16	0.23
(2,1295)	1:51:A:ALA:HB1	1:33:A:TYR:HE2	16	0.23
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE1	16	0.23
(2,1295)	1:51:A:ALA:HB2	1:33:A:TYR:HE2	16	0.23
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE1	16	0.23
(2,1295)	1:51:A:ALA:HB3	1:33:A:TYR:HE2	16	0.23
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	14	0.23
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	14	0.23
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	20	0.23
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	7	0.23
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	7	0.23
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	7	0.23
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	3	0.23
(2,1217)	1:63:A:ILE:HG21	1:67:A:TYR:HB3	2	0.23
(2,1217)	1:63:A:ILE:HG22	1:67:A:TYR:HB3	2	0.23
(2,1217)	1:63:A:ILE:HG23	1:67:A:TYR:HB3	2	0.23
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	1	0.23
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	1	0.23
(2,1211)	1:66:A:GLN:HB3	1:66:A:GLN:H	8	0.23
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	11	0.23
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	20	0.23
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	19	0.23
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE3	10	0.23
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	19	0.23
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	10	0.23
(2,734)	1:46:A:LYS:H	1:42:A:THR:HA	11	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	1	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	2	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	3	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	4	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	5	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	6	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	7	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	8	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	9	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	10	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	11	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	12	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	13	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	14	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	15	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	16	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	17	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	18	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	19	0.23
(2,646)	1:32:A:LYS:HB3	1:32:A:LYS:HA	20	0.23
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	12	0.23
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	12	0.23
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	17	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	3	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	5	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	8	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	10	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	11	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	13	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	16	0.23
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	18	0.23
(2,533)	1:26:A:TYR:HE1	1:27:A:ARG:HA	3	0.23
(2,533)	1:26:A:TYR:HE2	1:27:A:ARG:HA	3	0.23
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	5	0.23
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	2	0.23
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	15	0.23
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	4	0.23
(2,453)	1:23:A:LYS:H	1:23:A:LYS:HB3	11	0.23
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	7	0.23
(2,368)	1:21:A:GLU:H	1:20:A:GLN:HG3	12	0.23
(2,331)	1:26:A:TYR:HE1	1:23:A:LYS:HA	6	0.23
(2,331)	1:26:A:TYR:HE2	1:23:A:LYS:HA	6	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	2	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	2	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	2	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	2	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	2	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	2	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	2	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	2	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	2	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	11	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	11	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	11	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	11	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	11	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	11	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	11	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	11	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	11	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	12	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	12	0.23
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	12	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	12	0.23
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	12	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	12	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	12	0.23
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	12	0.23
(2,280)	1:14:A:SER:HB2	1:16:A:SER:H	9	0.23
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	20	0.23
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	20	0.23
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	20	0.23
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	17	0.23
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	1	0.23
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	3	0.23
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	6	0.23
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	2	0.23
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	6	0.23
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	8	0.23
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	18	0.23
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	4	0.23
(1,483)	1:53:A:GLU:HG2	1:53:A:GLU:H	19	0.23
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	5	0.23
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	6	0.23
(1,429)	1:6:A:LYS:HG3	1:7:A:LEU:H	7	0.23
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	9	0.23
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	9	0.23
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	9	0.23
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB3	14	0.23
(1,320)	1:77:A:PRO:HD3	1:78:A:SER:H	7	0.23
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	5	0.23
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	5	0.23
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	5	0.23
(1,294)	1:28:A:LYS:HD3	1:28:A:LYS:HG2	10	0.23
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD2	1	0.23
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD2	5	0.23
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	13	0.23
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	3	0.23
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	10	0.23
(1,231)	1:24:A:LYS:HD3	1:24:A:LYS:HE2	17	0.23
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	20	0.23
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	2	0.23
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	2	0.23
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	5	0.23
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	1	0.23
(1,135)	1:10:A:LEU:HD11	1:48:A:ILE:HA	13	0.23
(1,135)	1:10:A:LEU:HD12	1:48:A:ILE:HA	13	0.23
(1,135)	1:10:A:LEU:HD13	1:48:A:ILE:HA	13	0.23
(1,103)	1:59:A:GLN:HA	1:59:A:GLN:HG3	19	0.23
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	15	0.23
(1,81)	1:60:A:LYS:HA	1:60:A:LYS:HG3	2	0.23
(1,79)	1:6:A:LYS:H	1:9:A:ASP:H	9	0.23
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	9	0.23
(1,44)	1:2:A:VAL:H	1:1:A:SER:HB3	3	0.23
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	3	0.23
(1,11)	1:58:A:PRO:HB3	1:58:A:PRO:HG2	19	0.23
(2,2458)	1:10:A:LEU:HD11	1:44:A:LYS:HE3	11	0.22
(2,2458)	1:10:A:LEU:HD12	1:44:A:LYS:HE3	11	0.22
(2,2458)	1:10:A:LEU:HD13	1:44:A:LYS:HE3	11	0.22
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	8	0.22
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	9	0.22
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	15	0.22
(2,2450)	1:58:A:PRO:HD3	1:57:A:ASP:H	16	0.22
(2,2444)	1:3:A:LYS:HB3	1:3:A:LYS:HD2	12	0.22
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	20	0.22
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	9	0.22
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	9	0.22
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	9	0.22
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	4	0.22
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	4	0.22
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	15	0.22
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	15	0.22
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	5	0.22
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	5	0.22
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	13	0.22
(2,2211)	1:64:A:TYR:HE1	1:72:A:ALA:H	11	0.22
(2,2211)	1:64:A:TYR:HE2	1:72:A:ALA:H	11	0.22
(2,2211)	1:64:A:TYR:HE1	1:72:A:ALA:H	16	0.22
(2,2211)	1:64:A:TYR:HE2	1:72:A:ALA:H	16	0.22
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	3	0.22
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	19	0.22
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	14	0.22
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	14	0.22
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	14	0.22
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	5	0.22
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	8	0.22
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	5	0.22
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	10	0.22
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	10	0.22
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	3	0.22
(2,2046)	1:61:A:ARG:HG3	1:61:A:ARG:H	8	0.22
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	11	0.22
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	11	0.22
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	11	0.22
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	5	0.22
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	4	0.22
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	5	0.22
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	4	0.22
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	6	0.22
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	12	0.22
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	14	0.22
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	18	0.22
(2,1842)	1:43:A:GLU:H	1:42:A:THR:HB	20	0.22
(2,1828)	1:43:A:GLU:HG2	1:42:A:THR:H	2	0.22
(2,1803)	1:39:A:THR:HG21	1:39:A:THR:H	9	0.22
(2,1803)	1:39:A:THR:HG22	1:39:A:THR:H	9	0.22
(2,1803)	1:39:A:THR:HG23	1:39:A:THR:H	9	0.22
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	10	0.22
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	10	0.22
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	12	0.22
(2,1692)	1:25:A:GLY:H	1:24:A:LYS:HD2	16	0.22
(2,1685)	1:43:A:GLU:HG3	1:44:A:LYS:H	3	0.22
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	13	0.22
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	4	0.22
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	17	0.22
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	1	0.22
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	16	0.22
(2,1625)	1:18:A:ASN:H	1:18:A:ASN:HB2	3	0.22
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	10	0.22
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	18	0.22
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	20	0.22
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	20	0.22
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	20	0.22
(2,1568)	1:8:A:TYR:HB2	1:13:A:VAL:H	15	0.22
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	4	0.22
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	4	0.22
(2,1539)	1:9:A:ASP:HB3	1:11:A:LEU:H	8	0.22
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	5	0.22
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	11	0.22
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	11	0.22
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	18	0.22
(2,1438)	1:3:A:LYS:H	1:4:A:GLU:H	16	0.22
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	15	0.22
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	17	0.22
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	19	0.22
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	4	0.22
(2,1332)	1:77:A:PRO:HA	1:77:A:PRO:HB2	16	0.22
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	12	0.22
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	14	0.22
(2,1291)	1:72:A:ALA:HB1	1:73:A:ARG:HD2	12	0.22
(2,1291)	1:72:A:ALA:HB2	1:73:A:ARG:HD2	12	0.22
(2,1291)	1:72:A:ALA:HB3	1:73:A:ARG:HD2	12	0.22
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD21	14	0.22
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD22	14	0.22
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD23	14	0.22
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	10	0.22
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	10	0.22
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	19	0.22
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	19	0.22
(2,1173)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	15	0.22
(2,1173)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	15	0.22
(2,1173)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	15	0.22
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	7	0.22
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	18	0.22
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	11	0.22
(2,1082)	1:59:A:GLN:HA	1:59:A:GLN:HG3	12	0.22
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	3	0.22
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	9	0.22
(2,956)	1:7:A:LEU:HG	1:54:A:ILE:HB	19	0.22
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	12	0.22
(2,869)	1:50:A:GLU:HA	1:50:A:GLU:HG3	5	0.22
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	11	0.22
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	11	0.22
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	11	0.22
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	11	0.22
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	11	0.22
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	5	0.22
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	14	0.22
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	15	0.22
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	13	0.22
(2,814)	1:72:A:ALA:H	1:70:A:GLU:HA	17	0.22
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	5	0.22
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	6	0.22
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	6	0.22
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	6	0.22
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD21	14	0.22
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD22	14	0.22
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD23	14	0.22
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD21	14	0.22
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD22	14	0.22
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD23	14	0.22
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	8	0.22
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	12	0.22
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	15	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	1	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	6	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	7	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	8	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	9	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	10	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	11	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	14	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	16	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	17	0.22
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	18	0.22
(2,731)	1:45:A:PHE:HB2	1:42:A:THR:HA	4	0.22
(2,688)	1:40:A:GLY:H	1:38:A:PRO:HA	12	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	3	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	3	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	3	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	4	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	4	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	4	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	10	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	10	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	10	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	13	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	13	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	16	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	16	0.22
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	16	0.22
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	7	0.22
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	16	0.22
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	15	0.22
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	15	0.22
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	15	0.22
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	11	0.22
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	4	0.22
(2,549)	1:27:A:ARG:H	1:27:A:ARG:HB3	7	0.22
(2,472)	1:24:A:LYS:HE2	1:21:A:GLU:HA	10	0.22
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	1	0.22
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	1	0.22
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	9	0.22
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	12	0.22
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	13	0.22
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	18	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	1	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	1	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	1	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	1	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	1	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	1	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	1	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	1	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	1	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	5	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	5	0.22
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	5	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	5	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	5	0.22
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	5	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	5	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	5	0.22
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	5	0.22
(2,352)	1:64:A:TYR:HE1	1:69:A:LEU:HA	4	0.22
(2,352)	1:64:A:TYR:HE2	1:69:A:LEU:HA	4	0.22
(2,351)	1:24:A:LYS:HE2	1:21:A:GLU:HA	10	0.22
(2,348)	1:19:A:GLU:HA	1:19:A:GLU:HG2	9	0.22
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	8	0.22
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	8	0.22
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	8	0.22
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	8	0.22
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	8	0.22
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	8	0.22
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	8	0.22
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	8	0.22
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	8	0.22
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	16	0.22
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	16	0.22
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	16	0.22
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	16	0.22
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	16	0.22
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	16	0.22
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	16	0.22
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	16	0.22
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	16	0.22
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	9	0.22
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	9	0.22
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	9	0.22
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	16	0.22
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	16	0.22
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	16	0.22
(2,286)	1:17:A:ALA:HA	1:21:A:GLU:HB3	12	0.22
(2,277)	1:16:A:SER:HA	1:17:A:ALA:H	3	0.22
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	7	0.22
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	6	0.22
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	6	0.22
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	6	0.22
(2,110)	1:7:A:LEU:HG	1:54:A:ILE:HB	19	0.22
(2,36)	1:3:A:LYS:HB2	1:3:A:LYS:H	18	0.22
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	15	0.22
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	19	0.22
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	5	0.22
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	18	0.22
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	17	0.22
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	6	0.22
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	12	0.22
(1,380)	1:54:A:ILE:HD11	1:73:A:ARG:HD3	3	0.22
(1,380)	1:54:A:ILE:HD12	1:73:A:ARG:HD3	3	0.22
(1,380)	1:54:A:ILE:HD13	1:73:A:ARG:HD3	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	3	0.22
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	6	0.22
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	15	0.22
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	19	0.22
(1,294)	1:6:A:LYS:HG2	1:6:A:LYS:HD2	9	0.22
(1,286)	1:45:A:PHE:HA	1:48:A:ILE:H	17	0.22
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	7	0.22
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	9	0.22
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	2	0.22
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	3	0.22
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	14	0.22
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	15	0.22
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	19	0.22
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	10	0.22
(1,181)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	11	0.22
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	13	0.22
(1,110)	1:4:A:GLU:HG3	1:3:A:LYS:HD3	20	0.22
(1,103)	1:62:A:GLU:HA	1:62:A:GLU:HG2	5	0.22
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	11	0.22
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	19	0.22
(1,79)	1:6:A:LYS:H	1:9:A:ASP:H	5	0.22
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	12	0.22
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	4	0.22
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	3	0.22
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	3	0.22
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	3	0.22
(1,51)	1:62:A:GLU:HB2	1:62:A:GLU:HG2	2	0.22
(1,51)	1:19:A:GLU:HB2	1:19:A:GLU:HG3	9	0.22
(1,51)	1:19:A:GLU:HB2	1:19:A:GLU:HG3	13	0.22
(1,43)	1:72:A:ALA:H	1:69:A:LEU:HA	18	0.22
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	4	0.22
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	10	0.22
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	20	0.22
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	20	0.22
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	20	0.22
(1,11)	1:38:A:PRO:HB3	1:38:A:PRO:HG2	1	0.22
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	3	0.21
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	3	0.21
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	3	0.21
(2,2450)	1:58:A:PRO:HD3	1:57:A:ASP:H	19	0.21
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	6	0.21
(2,2401)	1:53:A:GLU:HG2	1:56:A:ASN:HB2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	7	0.21
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	9	0.21
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	11	0.21
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	11	0.21
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	11	0.21
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	13	0.21
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	13	0.21
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	13	0.21
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	4	0.21
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	4	0.21
(2,2279)	1:-1:A:MET:HB3	1:-1:A:MET:H	7	0.21
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	7	0.21
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	11	0.21
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	16	0.21
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	7	0.21
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	8	0.21
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	9	0.21
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	9	0.21
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	9	0.21
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	12	0.21
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	12	0.21
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	12	0.21
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	3	0.21
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	12	0.21
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	15	0.21
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	17	0.21
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	18	0.21
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	1	0.21
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	17	0.21
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	5	0.21
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	7	0.21
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	7	0.21
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	7	0.21
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	5	0.21
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	14	0.21
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	11	0.21
(2,1991)	1:52:A:PHE:HA	1:56:A:ASN:H	16	0.21
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	15	0.21
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	3	0.21
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	3	0.21
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	3	0.21
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	18	0.21
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	14	0.21
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	15	0.21
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	2	0.21
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	5	0.21
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	8	0.21
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	13	0.21
(2,1872)	1:46:A:LYS:H	1:45:A:PHE:HA	15	0.21
(2,1836)	1:43:A:GLU:H	1:42:A:THR:HG21	20	0.21
(2,1836)	1:43:A:GLU:H	1:42:A:THR:HG22	20	0.21
(2,1836)	1:43:A:GLU:H	1:42:A:THR:HG23	20	0.21
(2,1807)	1:39:A:THR:H	1:38:A:PRO:HG2	8	0.21
(2,1804)	1:39:A:THR:H	1:37:A:LYS:HG2	3	0.21
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	5	0.21
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	7	0.21
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	7	0.21
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	7	0.21
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	4	0.21
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	13	0.21
(2,1739)	1:29:A:ALA:H	1:28:A:LYS:HG3	5	0.21
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	7	0.21
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	16	0.21
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	19	0.21
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	11	0.21
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	14	0.21
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	9	0.21
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	16	0.21
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	6	0.21
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	18	0.21
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	1	0.21
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	12	0.21
(2,1553)	1:10:A:LEU:HB3	1:12:A:GLY:H	11	0.21
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	18	0.21
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	18	0.21
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	18	0.21
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	6	0.21
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	13	0.21
(2,1521)	1:6:A:LYS:HA	1:10:A:LEU:H	15	0.21
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	20	0.21
(2,1455)	1:3:A:LYS:HB2	1:4:A:GLU:H	1	0.21
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	15	0.21
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	20	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	4	0.21
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	18	0.21
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	4	0.21
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	6	0.21
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	12	0.21
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	12	0.21
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	12	0.21
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	14	0.21
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	12	0.21
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	12	0.21
(2,1211)	1:66:A:GLN:HB3	1:66:A:GLN:H	1	0.21
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	9	0.21
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	9	0.21
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	9	0.21
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	19	0.21
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	4	0.21
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	2	0.21
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	13	0.21
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	17	0.21
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	20	0.21
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	11	0.21
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	14	0.21
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	14	0.21
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	14	0.21
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	2	0.21
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	2	0.21
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	2	0.21
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	2	0.21
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	2	0.21
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	2	0.21
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG21	7	0.21
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG22	7	0.21
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG23	7	0.21
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG21	7	0.21
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG22	7	0.21
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG23	7	0.21
(2,835)	1:4:A:GLU:H	1:6:A:LYS:HE2	12	0.21
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	18	0.21
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	13	0.21
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	13	0.21
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	13	0.21
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	1	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	2	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	3	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	4	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	5	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	12	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	13	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	15	0.21
(2,739)	1:42:A:THR:HA	1:42:A:THR:HB	19	0.21
(2,730)	1:46:A:LYS:HG2	1:42:A:THR:HA	2	0.21
(2,689)	1:39:A:THR:H	1:38:A:PRO:HA	11	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	2	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	2	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	2	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	5	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	5	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	5	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	7	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	7	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	7	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	18	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	18	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	18	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	19	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	19	0.21
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	19	0.21
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	10	0.21
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	10	0.21
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	10	0.21
(2,536)	1:29:A:ALA:H	1:27:A:ARG:HA	16	0.21
(2,458)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	13	0.21
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	1	0.21
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	5	0.21
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	7	0.21
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	19	0.21
(2,426)	1:10:A:LEU:HD11	1:11:A:LEU:HA	5	0.21
(2,426)	1:10:A:LEU:HD12	1:11:A:LEU:HA	5	0.21
(2,426)	1:10:A:LEU:HD13	1:11:A:LEU:HA	5	0.21
(2,348)	1:19:A:GLU:HA	1:19:A:GLU:HG2	2	0.21
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE2	6	0.21
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	17	0.21
(2,230)	1:15:A:PRO:HD3	1:14:A:SER:HB2	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	10	0.21
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	10	0.21
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	10	0.21
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	11	0.21
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	11	0.21
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	11	0.21
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	3	0.21
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	3	0.21
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	3	0.21
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	11	0.21
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	1	0.21
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	1	0.21
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	1	0.21
(2,100)	1:0:A:THR:HG21	1:7:A:LEU:HA	15	0.21
(2,100)	1:0:A:THR:HG22	1:7:A:LEU:HA	15	0.21
(2,100)	1:0:A:THR:HG23	1:7:A:LEU:HA	15	0.21
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	14	0.21
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	13	0.21
(2,16)	1:2:A:VAL:HA	1:65:A:ASP:HB2	5	0.21
(2,8)	1:1:A:SER:H	1:1:A:SER:HB2	15	0.21
(2,2)	1:0:A:THR:HA	1:1:A:SER:H	6	0.21
(1,463)	1:53:A:GLU:H	1:55:A:LEU:HB2	13	0.21
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	6	0.21
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	1	0.21
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	11	0.21
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	13	0.21
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	8	0.21
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	15	0.21
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	15	0.21
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	15	0.21
(1,294)	1:24:A:LYS:HD3	1:24:A:LYS:HG2	3	0.21
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	7	0.21
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	11	0.21
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	8	0.21
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	2	0.21
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	7	0.21
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB1	5	0.21
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB2	5	0.21
(1,226)	1:22:A:LEU:HA	1:17:A:ALA:HB3	5	0.21
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	17	0.21
(1,205)	1:72:A:ALA:H	1:63:A:ILE:HB	18	0.21
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	2	0.21
(1,79)	1:17:A:ALA:H	1:18:A:ASN:H	7	0.21
(1,66)	1:60:A:LYS:HG2	1:60:A:LYS:HE2	5	0.21
(1,51)	1:19:A:GLU:HB2	1:19:A:GLU:HG3	8	0.21
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	6	0.21
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	11	0.21
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	14	0.21
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	16	0.21
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	17	0.21
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	20	0.21
(2,2460)	1:33:A:TYR:HD1	1:41:A:ASP:HB3	13	0.2
(2,2460)	1:33:A:TYR:HD2	1:41:A:ASP:HB3	13	0.2
(2,2455)	1:75:A:GLY:H	1:75:A:GLY:HA3	10	0.2
(2,2448)	1:42:A:THR:HA	1:35:A:PRO:HG3	14	0.2
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	16	0.2
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	17	0.2
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	17	0.2
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	17	0.2
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	13	0.2
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	13	0.2
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	13	0.2
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	13	0.2
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	13	0.2
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	13	0.2
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	6	0.2
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	6	0.2
(2,2343)	1:31:A:LEU:HB2	1:34:A:HIS:HD2	16	0.2
(2,2264)	1:77:A:PRO:HB2	1:79:A:PHE:H	13	0.2
(2,2261)	1:77:A:PRO:HA	1:78:A:SER:H	13	0.2
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	15	0.2
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	3	0.2
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	13	0.2
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	10	0.2
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	20	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	4	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	4	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	4	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	11	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	11	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	11	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	18	0.2
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	18	0.2
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	4	0.2
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	6	0.2
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	9	0.2
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	3	0.2
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	6	0.2
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	14	0.2
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	14	0.2
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	14	0.2
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	6	0.2
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	13	0.2
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	9	0.2
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	14	0.2
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	14	0.2
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	14	0.2
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	20	0.2
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	20	0.2
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	9	0.2
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	12	0.2
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	12	0.2
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	12	0.2
(2,2039)	1:55:A:LEU:HD11	1:61:A:ARG:H	16	0.2
(2,2039)	1:55:A:LEU:HD12	1:61:A:ARG:H	16	0.2
(2,2039)	1:55:A:LEU:HD13	1:61:A:ARG:H	16	0.2
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	11	0.2
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	12	0.2
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	15	0.2
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	6	0.2
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	6	0.2
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	6	0.2
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	7	0.2
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	12	0.2
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	12	0.2
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	20	0.2
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	9	0.2
(2,1838)	1:43:A:GLU:H	1:43:A:GLU:HG2	2	0.2
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	10	0.2
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	11	0.2
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	15	0.2
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG21	1	0.2
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG22	1	0.2
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG23	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1719)	1:27:A:ARG:H	1:23:A:LYS:HB3	17	0.2
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	4	0.2
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	13	0.2
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	19	0.2
(2,1683)	1:24:A:LYS:HD2	1:24:A:LYS:H	11	0.2
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	2	0.2
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	6	0.2
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	17	0.2
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	11	0.2
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	12	0.2
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	11	0.2
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	11	0.2
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	11	0.2
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	17	0.2
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	17	0.2
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	17	0.2
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	20	0.2
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	7	0.2
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	7	0.2
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	7	0.2
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	12	0.2
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	4	0.2
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD11	16	0.2
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD12	16	0.2
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD13	16	0.2
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	4	0.2
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	14	0.2
(2,1434)	1:1:A:SER:HA	1:2:A:VAL:H	10	0.2
(2,1422)	1:27:A:ARG:H	1:23:A:LYS:HB3	17	0.2
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	10	0.2
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	3	0.2
(2,1300)	1:24:A:LYS:HE2	1:21:A:GLU:HA	17	0.2
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	11	0.2
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	11	0.2
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	11	0.2
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	11	0.2
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	11	0.2
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	11	0.2
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	11	0.2
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	11	0.2
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	11	0.2
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	1	0.2
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	1	0.2
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	15	0.2
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	15	0.2
(2,1211)	1:66:A:GLN:HB3	1:66:A:GLN:H	2	0.2
(2,1211)	1:66:A:GLN:HB3	1:66:A:GLN:H	4	0.2
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	10	0.2
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	10	0.2
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	10	0.2
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	5	0.2
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	6	0.2
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	7	0.2
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	9	0.2
(2,1056)	1:61:A:ARG:HD2	1:58:A:PRO:HA	10	0.2
(2,1012)	1:61:A:ARG:HB2	1:55:A:LEU:HA	12	0.2
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	16	0.2
(2,909)	1:8:A:TYR:HD1	1:52:A:PHE:HA	18	0.2
(2,909)	1:8:A:TYR:HD2	1:52:A:PHE:HA	18	0.2
(2,869)	1:50:A:GLU:HA	1:50:A:GLU:HG3	12	0.2
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	9	0.2
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	20	0.2
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	20	0.2
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	20	0.2
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	13	0.2
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	15	0.2
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	1	0.2
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	1	0.2
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	1	0.2
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	17	0.2
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	17	0.2
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	17	0.2
(2,610)	1:30:A:ALA:HA	1:33:A:TYR:H	9	0.2
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	1	0.2
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	1	0.2
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	1	0.2
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	13	0.2
(2,542)	1:27:A:ARG:HB3	1:28:A:LYS:H	9	0.2
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	3	0.2
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	3	0.2
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	9	0.2
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	14	0.2
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	16	0.2
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	5	0.2
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	6	0.2
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	6	0.2
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	6	0.2
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	6	0.2
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	6	0.2
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	6	0.2
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	6	0.2
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	6	0.2
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	6	0.2
(2,399)	1:21:A:GLU:H	1:21:A:GLU:HG3	5	0.2
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	5	0.2
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	20	0.2
(2,384)	1:17:A:ALA:HA	1:21:A:GLU:HB3	6	0.2
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	16	0.2
(2,285)	1:17:A:ALA:HA	1:18:A:ASN:HB2	3	0.2
(2,278)	1:15:A:PRO:HD3	1:14:A:SER:HB2	14	0.2
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	6	0.2
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	11	0.2
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	7	0.2
(2,235)	1:5:A:THR:HG21	1:15:A:PRO:HA	9	0.2
(2,235)	1:5:A:THR:HG22	1:15:A:PRO:HA	9	0.2
(2,235)	1:5:A:THR:HG23	1:15:A:PRO:HA	9	0.2
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD11	5	0.2
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD12	5	0.2
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD13	5	0.2
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD11	5	0.2
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD12	5	0.2
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD13	5	0.2
(2,176)	1:11:A:LEU:HB2	1:10:A:LEU:HB2	4	0.2
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD11	6	0.2
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD12	6	0.2
(2,165)	1:7:A:LEU:HA	1:10:A:LEU:HD13	6	0.2
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	9	0.2
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	14	0.2
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	6	0.2
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG21	18	0.2
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG22	18	0.2
(2,91)	1:7:A:LEU:HD21	1:0:A:THR:HG23	18	0.2
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG21	18	0.2
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG22	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,91)	1:7:A:LEU:HD22	1:0:A:THR:HG23	18	0.2
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG21	18	0.2
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG22	18	0.2
(2,91)	1:7:A:LEU:HD23	1:0:A:THR:HG23	18	0.2
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	4	0.2
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	10	0.2
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	17	0.2
(2,10)	1:2:A:VAL:HG21	1:2:A:VAL:HA	19	0.2
(2,10)	1:2:A:VAL:HG22	1:2:A:VAL:HA	19	0.2
(2,10)	1:2:A:VAL:HG23	1:2:A:VAL:HA	19	0.2
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	19	0.2
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	19	0.2
(1,472)	1:72:A:ALA:H	1:67:A:TYR:HB2	14	0.2
(1,457)	1:45:A:PHE:H	1:46:A:LYS:HB2	15	0.2
(1,454)	1:72:A:ALA:H	1:64:A:TYR:H	18	0.2
(1,435)	1:47:A:GLU:HG3	1:47:A:GLU:HA	5	0.2
(1,389)	1:30:A:ALA:HB1	1:31:A:LEU:HB2	14	0.2
(1,389)	1:30:A:ALA:HB2	1:31:A:LEU:HB2	14	0.2
(1,389)	1:30:A:ALA:HB3	1:31:A:LEU:HB2	14	0.2
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	9	0.2
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	9	0.2
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	17	0.2
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	20	0.2
(1,320)	1:77:A:PRO:HD3	1:76:A:GLY:H	17	0.2
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	6	0.2
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	16	0.2
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	20	0.2
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	1	0.2
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	7	0.2
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	11	0.2
(1,246)	1:60:A:LYS:HE3	1:60:A:LYS:HB2	14	0.2
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	14	0.2
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	17	0.2
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	13	0.2
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	16	0.2
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	17	0.2
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	18	0.2
(1,164)	1:41:A:ASP:HB2	1:44:A:LYS:HG2	8	0.2
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	17	0.2
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	9	0.2
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	8	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	7	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	8	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	9	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	15	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	18	0.2
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	19	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	6	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	6	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	6	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	17	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	17	0.2
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	17	0.2
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	19	0.19
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	19	0.19
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	19	0.19
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	19	0.19
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	8	0.19
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	8	0.19
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	8	0.19
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	8	0.19
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	8	0.19
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	8	0.19
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	17	0.19
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	17	0.19
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	17	0.19
(2,2258)	1:77:A:PRO:HD3	1:78:A:SER:H	6	0.19
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	1	0.19
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	5	0.19
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	9	0.19
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	17	0.19
(2,2250)	1:76:A:GLY:HA2	1:76:A:GLY:H	14	0.19
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	17	0.19
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	19	0.19
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	18	0.19
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	20	0.19
(2,2181)	1:70:A:GLU:H	1:70:A:GLU:HG3	13	0.19
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	13	0.19
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	14	0.19
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	3	0.19
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	4	0.19
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	6	0.19
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	17	0.19
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	17	0.19
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	17	0.19
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	16	0.19
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB1	15	0.19
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB2	15	0.19
(2,2076)	1:63:A:ILE:H	1:71:A:ALA:HB3	15	0.19
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	7	0.19
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	17	0.19
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	5	0.19
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	5	0.19
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	5	0.19
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	16	0.19
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	16	0.19
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	16	0.19
(2,2039)	1:55:A:LEU:HD21	1:61:A:ARG:H	12	0.19
(2,2039)	1:55:A:LEU:HD22	1:61:A:ARG:H	12	0.19
(2,2039)	1:55:A:LEU:HD23	1:61:A:ARG:H	12	0.19
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	20	0.19
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	20	0.19
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	9	0.19
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	9	0.19
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	9	0.19
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	15	0.19
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	15	0.19
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	15	0.19
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	13	0.19
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	7	0.19
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD11	5	0.19
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD12	5	0.19
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD13	5	0.19
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	4	0.19
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	4	0.19
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	4	0.19
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB1	13	0.19
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB2	13	0.19
(2,1768)	1:32:A:LYS:H	1:29:A:ALA:HB3	13	0.19
(2,1754)	1:26:A:TYR:HE1	1:30:A:ALA:H	5	0.19
(2,1754)	1:26:A:TYR:HE2	1:30:A:ALA:H	5	0.19
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	20	0.19
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD11	11	0.19
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD12	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1726)	1:53:A:GLU:H	1:11:A:LEU:HD13	11	0.19
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	2	0.19
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	10	0.19
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	17	0.19
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	10	0.19
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	13	0.19
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	13	0.19
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	13	0.19
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	18	0.19
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	18	0.19
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	18	0.19
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	13	0.19
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	2	0.19
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	9	0.19
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	11	0.19
(2,1504)	1:10:A:LEU:HB3	1:9:A:ASP:H	20	0.19
(2,1484)	1:55:A:LEU:HD21	1:8:A:TYR:H	16	0.19
(2,1484)	1:55:A:LEU:HD22	1:8:A:TYR:H	16	0.19
(2,1484)	1:55:A:LEU:HD23	1:8:A:TYR:H	16	0.19
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	18	0.19
(2,1413)	1:0:A:THR:HB	1:0:A:THR:H	4	0.19
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	5	0.19
(2,1339)	1:67:A:TYR:HD1	1:77:A:PRO:HA	7	0.19
(2,1339)	1:67:A:TYR:HD2	1:77:A:PRO:HA	7	0.19
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	1	0.19
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	7	0.19
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	13	0.19
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	17	0.19
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	20	0.19
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	7	0.19
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	7	0.19
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	7	0.19
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	6	0.19
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	6	0.19
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	6	0.19
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	6	0.19
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	6	0.19
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	6	0.19
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	6	0.19
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	6	0.19
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	6	0.19
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	13	0.19
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	13	0.19
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	13	0.19
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	13	0.19
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	13	0.19
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	13	0.19
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	13	0.19
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	13	0.19
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	18	0.19
(2,1251)	1:70:A:GLU:HA	1:70:A:GLU:HG3	19	0.19
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	5	0.19
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	5	0.19
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	11	0.19
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	11	0.19
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	7	0.19
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	7	0.19
(2,1119)	1:73:A:ARG:HD2	1:69:A:LEU:HG	16	0.19
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	8	0.19
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	18	0.19
(2,1107)	1:50:A:GLU:HA	1:54:A:ILE:HG13	16	0.19
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	18	0.19
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	5	0.19
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	16	0.19
(2,1035)	1:55:A:LEU:HB2	1:56:A:ASN:HA	12	0.19
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	2	0.19
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	18	0.19
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	19	0.19
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE3	15	0.19
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	16	0.19
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	16	0.19
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	16	0.19
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	7	0.19
(2,747)	1:47:A:GLU:HG2	1:48:A:ILE:HB	11	0.19
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	12	0.19
(2,731)	1:45:A:PHE:HB2	1:42:A:THR:HA	2	0.19
(2,693)	1:37:A:LYS:HD3	1:38:A:PRO:HD2	13	0.19
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	9	0.19
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	9	0.19
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	9	0.19
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	15	0.19
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	15	0.19
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	13	0.19
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	13	0.19
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	13	0.19
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	15	0.19
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	17	0.19
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB3	19	0.19
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	18	0.19
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	13	0.19
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	6	0.19
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	6	0.19
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	6	0.19
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	7	0.19
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	7	0.19
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	1	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	3	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	3	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	3	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	3	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	3	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	3	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	3	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	3	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	3	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	9	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	9	0.19
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	9	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	9	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	9	0.19
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	9	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	9	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	9	0.19
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	9	0.19
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	19	0.19
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	19	0.19
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	19	0.19
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	3	0.19
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	2	0.19
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	19	0.19
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	5	0.19
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	5	0.19
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	11	0.19
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD1	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:22:A:LEU:HB2	1:52:A:PHE:HD2	7	0.19
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	4	0.19
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	7	0.19
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	14	0.19
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	18	0.19
(1,294)	1:28:A:LYS:HD3	1:28:A:LYS:HG2	12	0.19
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	4	0.19
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	4	0.19
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	4	0.19
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	16	0.19
(1,245)	1:58:A:PRO:HB2	1:58:A:PRO:HA	2	0.19
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	5	0.19
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	12	0.19
(1,233)	1:22:A:LEU:HD21	1:19:A:GLU:HA	12	0.19
(1,233)	1:22:A:LEU:HD22	1:19:A:GLU:HA	12	0.19
(1,233)	1:22:A:LEU:HD23	1:19:A:GLU:HA	12	0.19
(1,220)	1:63:A:ILE:HD11	1:75:A:GLY:HA2	9	0.19
(1,220)	1:63:A:ILE:HD12	1:75:A:GLY:HA2	9	0.19
(1,220)	1:63:A:ILE:HD13	1:75:A:GLY:HA2	9	0.19
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	13	0.19
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	10	0.19
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	7	0.19
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	11	0.19
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	14	0.19
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	3	0.19
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	18	0.19
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	17	0.19
(1,43)	1:72:A:ALA:H	1:69:A:LEU:HA	3	0.19
(1,43)	1:72:A:ALA:H	1:69:A:LEU:HA	14	0.19
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	1	0.19
(1,30)	1:20:A:GLN:H	1:20:A:GLN:HA	12	0.19
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	7	0.18
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	10	0.18
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	11	0.18
(2,2401)	1:53:A:GLU:HG2	1:56:A:ASN:HB2	14	0.18
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	8	0.18
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	8	0.18
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	8	0.18
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	15	0.18
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	15	0.18
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	15	0.18
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	3	0.18
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	3	0.18
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	3	0.18
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	3	0.18
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	3	0.18
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB1	6	0.18
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB2	6	0.18
(2,2382)	1:26:A:TYR:HE1	1:29:A:ALA:HB3	6	0.18
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB1	6	0.18
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB2	6	0.18
(2,2382)	1:26:A:TYR:HE2	1:29:A:ALA:HB3	6	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	11	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	11	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	11	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	11	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	11	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	11	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	17	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	17	0.18
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	17	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	17	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	17	0.18
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	17	0.18
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	16	0.18
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	16	0.18
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	2	0.18
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	6	0.18
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	10	0.18
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	12	0.18
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	19	0.18
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	20	0.18
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	16	0.18
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	4	0.18
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	14	0.18
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	13	0.18
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	6	0.18
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	20	0.18
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	11	0.18
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	17	0.18
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	5	0.18
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	5	0.18
(2,2083)	1:62:A:GLU:HG3	1:63:A:ILE:H	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	10	0.18
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	20	0.18
(2,2029)	1:60:A:LYS:HE2	1:60:A:LYS:H	4	0.18
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	2	0.18
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	14	0.18
(2,2013)	1:57:A:ASP:H	1:61:A:ARG:H	16	0.18
(2,1991)	1:52:A:PHE:HA	1:56:A:ASN:H	13	0.18
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	16	0.18
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	16	0.18
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	18	0.18
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	18	0.18
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	6	0.18
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	11	0.18
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	15	0.18
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	10	0.18
(2,1888)	1:51:A:ALA:HB1	1:48:A:ILE:H	13	0.18
(2,1888)	1:51:A:ALA:HB2	1:48:A:ILE:H	13	0.18
(2,1888)	1:51:A:ALA:HB3	1:48:A:ILE:H	13	0.18
(2,1804)	1:39:A:THR:H	1:37:A:LYS:HG2	20	0.18
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	4	0.18
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG21	14	0.18
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG22	14	0.18
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG23	14	0.18
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	3	0.18
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	1	0.18
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	1	0.18
(2,1667)	1:22:A:LEU:H	1:21:A:GLU:HB3	20	0.18
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	19	0.18
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	19	0.18
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	8	0.18
(2,1611)	1:17:A:ALA:H	1:21:A:GLU:HB3	5	0.18
(2,1604)	1:16:A:SER:H	1:17:A:ALA:H	18	0.18
(2,1601)	1:15:A:PRO:HB3	1:16:A:SER:H	14	0.18
(2,1598)	1:15:A:PRO:HD3	1:16:A:SER:H	12	0.18
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	17	0.18
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	10	0.18
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	10	0.18
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	10	0.18
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	14	0.18
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	10	0.18
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	16	0.18
(2,1509)	1:9:A:ASP:H	1:15:A:PRO:HD2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	1	0.18
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	10	0.18
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	19	0.18
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	10	0.18
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	16	0.18
(2,1364)	1:77:A:PRO:HD2	1:76:A:GLY:HA3	14	0.18
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	5	0.18
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	10	0.18
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	12	0.18
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	14	0.18
(2,1300)	1:24:A:LYS:HE2	1:21:A:GLU:HA	1	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	9	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	9	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	9	0.18
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	9	0.18
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	9	0.18
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	9	0.18
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	9	0.18
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	9	0.18
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	9	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	17	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	17	0.18
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	17	0.18
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	17	0.18
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	17	0.18
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	17	0.18
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	17	0.18
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	17	0.18
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	17	0.18
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	6	0.18
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	6	0.18
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	6	0.18
(2,1251)	1:70:A:GLU:HA	1:70:A:GLU:HG3	17	0.18
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	18	0.18
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	2	0.18
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	2	0.18
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	4	0.18
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	4	0.18
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	7	0.18
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	7	0.18
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	20	0.18
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	1	0.18
(2,1122)	1:73:A:ARG:HD2	1:73:A:ARG:HB3	14	0.18
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	11	0.18
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	19	0.18
(2,1107)	1:50:A:GLU:HA	1:54:A:ILE:HG13	5	0.18
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	8	0.18
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	5	0.18
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	15	0.18
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	1	0.18
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	6	0.18
(2,869)	1:50:A:GLU:HA	1:50:A:GLU:HG3	16	0.18
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	14	0.18
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	1	0.18
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	3	0.18
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	3	0.18
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	3	0.18
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	12	0.18
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	12	0.18
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	12	0.18
(2,827)	1:24:A:LYS:HE2	1:20:A:GLN:HB3	6	0.18
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	20	0.18
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	4	0.18
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	9	0.18
(2,788)	1:10:A:LEU:HD11	1:44:A:LYS:HG3	15	0.18
(2,788)	1:10:A:LEU:HD12	1:44:A:LYS:HG3	15	0.18
(2,788)	1:10:A:LEU:HD13	1:44:A:LYS:HG3	15	0.18
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD21	19	0.18
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD22	19	0.18
(2,779)	1:70:A:GLU:HB2	1:69:A:LEU:HD23	19	0.18
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD21	19	0.18
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD22	19	0.18
(2,778)	1:70:A:GLU:HB2	1:69:A:LEU:HD23	19	0.18
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	16	0.18
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	9	0.18
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	12	0.18
(2,642)	1:69:A:LEU:HD21	1:73:A:ARG:HG2	19	0.18
(2,642)	1:69:A:LEU:HD22	1:73:A:ARG:HG2	19	0.18
(2,642)	1:69:A:LEU:HD23	1:73:A:ARG:HG2	19	0.18
(2,626)	1:31:A:LEU:HA	1:34:A:HIS:HB3	6	0.18
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	3	0.18
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	13	0.18
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	13	0.18
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	3	0.18
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	3	0.18
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	3	0.18
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	20	0.18
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	20	0.18
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	20	0.18
(2,542)	1:27:A:ARG:HB3	1:28:A:LYS:H	6	0.18
(2,538)	1:30:A:ALA:H	1:27:A:ARG:HA	16	0.18
(2,497)	1:25:A:GLY:HA3	1:28:A:LYS:HB2	10	0.18
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	4	0.18
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	4	0.18
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	4	0.18
(2,472)	1:24:A:LYS:HE2	1:21:A:GLU:HA	17	0.18
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	9	0.18
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	19	0.18
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	19	0.18
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	19	0.18
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	11	0.18
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	11	0.18
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	11	0.18
(2,331)	1:26:A:TYR:HE1	1:23:A:LYS:HA	20	0.18
(2,331)	1:26:A:TYR:HE2	1:23:A:LYS:HA	20	0.18
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	1	0.18
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	5	0.18
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	12	0.18
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	3	0.18
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	8	0.18
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	4	0.18
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	2	0.18
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	2	0.18
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	2	0.18
(2,174)	1:10:A:LEU:HB2	1:10:A:LEU:HD11	10	0.18
(2,174)	1:10:A:LEU:HB2	1:10:A:LEU:HD12	10	0.18
(2,174)	1:10:A:LEU:HB2	1:10:A:LEU:HD13	10	0.18
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	15	0.18
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	4	0.18
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	8	0.18
(2,54)	1:4:A:GLU:HG2	1:3:A:LYS:HD2	5	0.18
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	2	0.18
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	15	0.18
(1,483)	1:53:A:GLU:HG2	1:53:A:GLU:H	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	18	0.18
(1,357)	1:28:A:LYS:HA	1:28:A:LYS:HB2	18	0.18
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	19	0.18
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	18	0.18
(1,309)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	20	0.18
(1,294)	1:24:A:LYS:HD3	1:24:A:LYS:HG2	4	0.18
(1,294)	1:24:A:LYS:HD3	1:24:A:LYS:HG2	5	0.18
(1,279)	1:24:A:LYS:HE3	1:21:A:GLU:HG3	18	0.18
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	8	0.18
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	19	0.18
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	1	0.18
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	9	0.18
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	14	0.18
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	19	0.18
(1,250)	1:51:A:ALA:HB1	1:10:A:LEU:H	19	0.18
(1,250)	1:51:A:ALA:HB2	1:10:A:LEU:H	19	0.18
(1,250)	1:51:A:ALA:HB3	1:10:A:LEU:H	19	0.18
(1,245)	1:58:A:PRO:HB2	1:58:A:PRO:HA	3	0.18
(1,245)	1:58:A:PRO:HB2	1:58:A:PRO:HA	7	0.18
(1,245)	1:58:A:PRO:HB2	1:58:A:PRO:HA	11	0.18
(1,238)	1:10:A:LEU:HB3	1:10:A:LEU:HA	11	0.18
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	5	0.18
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	12	0.18
(1,121)	1:64:A:TYR:HD1	1:65:A:ASP:H	18	0.18
(1,121)	1:64:A:TYR:HD2	1:65:A:ASP:H	18	0.18
(1,110)	1:50:A:GLU:HG2	1:54:A:ILE:HB	17	0.18
(1,103)	1:62:A:GLU:HA	1:62:A:GLU:HG2	6	0.18
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	6	0.18
(1,80)	1:28:A:LYS:HA	1:28:A:LYS:HG3	16	0.18
(1,68)	1:72:A:ALA:HB1	1:76:A:GLY:H	18	0.18
(1,68)	1:72:A:ALA:HB2	1:76:A:GLY:H	18	0.18
(1,68)	1:72:A:ALA:HB3	1:76:A:GLY:H	18	0.18
(1,66)	1:60:A:LYS:HG2	1:60:A:LYS:HE2	8	0.18
(1,57)	1:24:A:LYS:HB2	1:24:A:LYS:HE2	7	0.18
(2,2450)	1:58:A:PRO:HD3	1:57:A:ASP:H	15	0.17
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	11	0.17
(2,2411)	1:27:A:ARG:H	1:27:A:ARG:HD3	1	0.17
(2,2411)	1:27:A:ARG:H	1:27:A:ARG:HD2	6	0.17
(2,2401)	1:53:A:GLU:HG2	1:56:A:ASN:HB2	11	0.17
(2,2397)	1:68:A:GLY:H	1:66:A:GLN:HG3	15	0.17
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	5	0.17
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	10	0.17
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	10	0.17
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD1	19	0.17
(2,2293)	1:45:A:PHE:HB3	1:33:A:TYR:HD2	19	0.17
(2,2252)	1:74:A:SER:HA	1:76:A:GLY:H	20	0.17
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	8	0.17
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	15	0.17
(2,2237)	1:74:A:SER:H	1:75:A:GLY:HA2	6	0.17
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	14	0.17
(2,2219)	1:73:A:ARG:H	1:69:A:LEU:HG	13	0.17
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	8	0.17
(2,2178)	1:70:A:GLU:H	1:69:A:LEU:HB2	10	0.17
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	16	0.17
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	19	0.17
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	13	0.17
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	20	0.17
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	11	0.17
(2,2078)	1:72:A:ALA:HB1	1:63:A:ILE:H	14	0.17
(2,2078)	1:72:A:ALA:HB2	1:63:A:ILE:H	14	0.17
(2,2078)	1:72:A:ALA:HB3	1:63:A:ILE:H	14	0.17
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	1	0.17
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	4	0.17
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	9	0.17
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	2	0.17
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	2	0.17
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	4	0.17
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	20	0.17
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	20	0.17
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	20	0.17
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	20	0.17
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	20	0.17
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	1	0.17
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	1	0.17
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	11	0.17
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	20	0.17
(2,1933)	1:52:A:PHE:H	1:8:A:TYR:HA	19	0.17
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	19	0.17
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	19	0.17
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	19	0.17
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	4	0.17
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	8	0.17
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	1	0.17
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	10	0.17
(2,1691)	1:25:A:GLY:H	1:24:A:LYS:HG2	5	0.17
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	15	0.17
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	11	0.17
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	8	0.17
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	8	0.17
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	8	0.17
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	4	0.17
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	18	0.17
(2,1564)	1:13:A:VAL:HG11	1:13:A:VAL:H	20	0.17
(2,1564)	1:13:A:VAL:HG12	1:13:A:VAL:H	20	0.17
(2,1564)	1:13:A:VAL:HG13	1:13:A:VAL:H	20	0.17
(2,1553)	1:10:A:LEU:HB3	1:12:A:GLY:H	5	0.17
(2,1527)	1:9:A:ASP:HB2	1:10:A:LEU:H	1	0.17
(2,1521)	1:6:A:LYS:HA	1:10:A:LEU:H	18	0.17
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	12	0.17
(2,1489)	1:10:A:LEU:HB3	1:8:A:TYR:H	18	0.17
(2,1484)	1:55:A:LEU:HD21	1:8:A:TYR:H	15	0.17
(2,1484)	1:55:A:LEU:HD22	1:8:A:TYR:H	15	0.17
(2,1484)	1:55:A:LEU:HD23	1:8:A:TYR:H	15	0.17
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	2	0.17
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	2	0.17
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	5	0.17
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	14	0.17
(2,1451)	1:4:A:GLU:HG3	1:4:A:GLU:H	6	0.17
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	2	0.17
(2,1450)	1:2:A:VAL:HB	1:4:A:GLU:H	6	0.17
(2,1435)	1:53:A:GLU:H	1:56:A:ASN:H	20	0.17
(2,1432)	1:0:A:THR:HA	1:2:A:VAL:H	12	0.17
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	3	0.17
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	3	0.17
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	3	0.17
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	3	0.17
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	3	0.17
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	3	0.17
(2,1362)	1:77:A:PRO:HD2	1:76:A:GLY:HA2	16	0.17
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	4	0.17
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	15	0.17
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	19	0.17
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	17	0.17
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	2	0.17
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	2	0.17
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	2	0.17
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	2	0.17
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	2	0.17
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	2	0.17
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	2	0.17
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	2	0.17
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	18	0.17
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	18	0.17
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	18	0.17
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	18	0.17
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	18	0.17
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	18	0.17
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	18	0.17
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	18	0.17
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	18	0.17
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	8	0.17
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	8	0.17
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	8	0.17
(2,1261)	1:70:A:GLU:HA	1:70:A:GLU:HG3	7	0.17
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	5	0.17
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	13	0.17
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	13	0.17
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	17	0.17
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	17	0.17
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	10	0.17
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	10	0.17
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	4	0.17
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	17	0.17
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	1	0.17
(2,969)	1:50:A:GLU:HG2	1:54:A:ILE:HD11	10	0.17
(2,969)	1:50:A:GLU:HG2	1:54:A:ILE:HD12	10	0.17
(2,969)	1:50:A:GLU:HG2	1:54:A:ILE:HD13	10	0.17
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	10	0.17
(2,899)	1:55:A:LEU:HD11	1:52:A:PHE:HA	4	0.17
(2,899)	1:55:A:LEU:HD12	1:52:A:PHE:HA	4	0.17
(2,899)	1:55:A:LEU:HD13	1:52:A:PHE:HA	4	0.17
(2,883)	1:51:A:ALA:HA	1:54:A:ILE:HG21	18	0.17
(2,883)	1:51:A:ALA:HA	1:54:A:ILE:HG22	18	0.17
(2,883)	1:51:A:ALA:HA	1:54:A:ILE:HG23	18	0.17
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	16	0.17
(2,869)	1:50:A:GLU:HA	1:50:A:GLU:HG3	4	0.17
(2,825)	1:60:A:LYS:HE2	1:60:A:LYS:H	14	0.17
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	20	0.17
(2,795)	1:48:A:ILE:HG21	1:45:A:PHE:HA	4	0.17
(2,795)	1:48:A:ILE:HG22	1:45:A:PHE:HA	4	0.17
(2,795)	1:48:A:ILE:HG23	1:45:A:PHE:HA	4	0.17
(2,789)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	15	0.17
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	19	0.17
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	19	0.17
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	19	0.17
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	5	0.17
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	16	0.17
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	10	0.17
(2,688)	1:40:A:GLY:H	1:38:A:PRO:HA	17	0.17
(2,665)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	14	0.17
(2,665)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	14	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	11	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	11	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	11	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	14	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	14	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	14	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	20	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	20	0.17
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	20	0.17
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	12	0.17
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	12	0.17
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	12	0.17
(2,567)	1:24:A:LYS:HE2	1:24:A:LYS:H	15	0.17
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	15	0.17
(2,542)	1:27:A:ARG:HB3	1:28:A:LYS:H	2	0.17
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	7	0.17
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	6	0.17
(2,429)	1:22:A:LEU:HD11	1:22:A:LEU:HB3	12	0.17
(2,429)	1:22:A:LEU:HD12	1:22:A:LEU:HB3	12	0.17
(2,429)	1:22:A:LEU:HD13	1:22:A:LEU:HB3	12	0.17
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	17	0.17
(2,389)	1:13:A:VAL:HG21	1:21:A:GLU:HG2	15	0.17
(2,389)	1:13:A:VAL:HG22	1:21:A:GLU:HG2	15	0.17
(2,389)	1:13:A:VAL:HG23	1:21:A:GLU:HG2	15	0.17
(2,368)	1:21:A:GLU:H	1:20:A:GLN:HG3	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,351)	1:24:A:LYS:HE2	1:21:A:GLU:HA	17	0.17
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	6	0.17
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	7	0.17
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	8	0.17
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	11	0.17
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	7	0.17
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	16	0.17
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	17	0.17
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	18	0.17
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	4	0.17
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	9	0.17
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	12	0.17
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	12	0.17
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	12	0.17
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	10	0.17
(2,142)	1:10:A:LEU:HB3	1:9:A:ASP:HA	8	0.17
(2,77)	1:3:A:LYS:HB2	1:6:A:LYS:HB3	20	0.17
(2,21)	1:39:A:THR:HA	1:40:A:GLY:H	14	0.17
(1,483)	1:20:A:GLN:H	1:20:A:GLN:HB3	16	0.17
(1,454)	1:72:A:ALA:H	1:64:A:TYR:H	14	0.17
(1,449)	1:46:A:LYS:HB2	1:47:A:GLU:H	5	0.17
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	11	0.17
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	9	0.17
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	19	0.17
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	19	0.17
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	10	0.17
(1,309)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	17	0.17
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	2	0.17
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	14	0.17
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	16	0.17
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	3	0.17
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	4	0.17
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	12	0.17
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	17	0.17
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	20	0.17
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	1	0.17
(1,205)	1:72:A:ALA:H	1:63:A:ILE:HB	13	0.17
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	6	0.17
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	9	0.17
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	19	0.17
(1,116)	1:33:A:TYR:HD1	1:32:A:LYS:HE3	2	0.17
(1,116)	1:33:A:TYR:HD2	1:32:A:LYS:HE3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:59:A:GLN:H	1:60:A:LYS:HB2	6	0.17
(1,57)	1:24:A:LYS:HB3	1:24:A:LYS:HE2	6	0.17
(1,57)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	20	0.17
(1,5)	1:63:A:ILE:HG21	1:75:A:GLY:H	19	0.17
(1,5)	1:63:A:ILE:HG22	1:75:A:GLY:H	19	0.17
(1,5)	1:63:A:ILE:HG23	1:75:A:GLY:H	19	0.17
(2,2464)	1:28:A:LYS:HG3	1:28:A:LYS:HE2	9	0.16
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	18	0.16
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	7	0.16
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	7	0.16
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	7	0.16
(2,2317)	1:64:A:TYR:HD1	1:72:A:ALA:HB1	18	0.16
(2,2317)	1:64:A:TYR:HD1	1:72:A:ALA:HB2	18	0.16
(2,2317)	1:64:A:TYR:HD1	1:72:A:ALA:HB3	18	0.16
(2,2317)	1:64:A:TYR:HD2	1:72:A:ALA:HB1	18	0.16
(2,2317)	1:64:A:TYR:HD2	1:72:A:ALA:HB2	18	0.16
(2,2317)	1:64:A:TYR:HD2	1:72:A:ALA:HB3	18	0.16
(2,2268)	1:78:A:SER:HB3	1:79:A:PHE:H	20	0.16
(2,2259)	1:77:A:PRO:HD2	1:78:A:SER:H	6	0.16
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	7	0.16
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	10	0.16
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	17	0.16
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	6	0.16
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	7	0.16
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	5	0.16
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	9	0.16
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	12	0.16
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	14	0.16
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	16	0.16
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	20	0.16
(2,2133)	1:67:A:TYR:H	1:66:A:GLN:HB3	4	0.16
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	13	0.16
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	17	0.16
(2,2079)	1:66:A:GLN:HB3	1:63:A:ILE:H	5	0.16
(2,2068)	1:65:A:ASP:HB3	1:62:A:GLU:H	7	0.16
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	1	0.16
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	4	0.16
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	10	0.16
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	16	0.16
(2,2035)	1:57:A:ASP:H	1:60:A:LYS:H	12	0.16
(2,2029)	1:60:A:LYS:H	1:60:A:LYS:HE3	12	0.16
(2,1985)	1:55:A:LEU:HB2	1:56:A:ASN:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	12	0.16
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	11	0.16
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	13	0.16
(2,1968)	1:55:A:LEU:H	1:56:A:ASN:HB3	3	0.16
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	11	0.16
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	3	0.16
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	3	0.16
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	2	0.16
(2,1923)	1:55:A:LEU:HD21	1:52:A:PHE:H	3	0.16
(2,1923)	1:55:A:LEU:HD22	1:52:A:PHE:H	3	0.16
(2,1923)	1:55:A:LEU:HD23	1:52:A:PHE:H	3	0.16
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	14	0.16
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	14	0.16
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	14	0.16
(2,1900)	1:54:A:ILE:HD11	1:50:A:GLU:H	16	0.16
(2,1900)	1:54:A:ILE:HD12	1:50:A:GLU:H	16	0.16
(2,1900)	1:54:A:ILE:HD13	1:50:A:GLU:H	16	0.16
(2,1831)	1:45:A:PHE:HB2	1:42:A:THR:H	8	0.16
(2,1807)	1:39:A:THR:H	1:38:A:PRO:HG2	4	0.16
(2,1807)	1:39:A:THR:H	1:38:A:PRO:HG2	13	0.16
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	7	0.16
(2,1784)	1:34:A:HIS:HB3	1:33:A:TYR:H	10	0.16
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	9	0.16
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	6	0.16
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	14	0.16
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG21	9	0.16
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG22	9	0.16
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG23	9	0.16
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	9	0.16
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	13	0.16
(2,1673)	1:22:A:LEU:HD21	1:23:A:LYS:H	3	0.16
(2,1673)	1:22:A:LEU:HD22	1:23:A:LYS:H	3	0.16
(2,1673)	1:22:A:LEU:HD23	1:23:A:LYS:H	3	0.16
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	4	0.16
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	14	0.16
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	15	0.16
(2,1603)	1:15:A:PRO:HG3	1:16:A:SER:H	13	0.16
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	8	0.16
(2,1553)	1:10:A:LEU:HB3	1:12:A:GLY:H	7	0.16
(2,1553)	1:10:A:LEU:HB3	1:12:A:GLY:H	12	0.16
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	6	0.16
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	3	0.16
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	13	0.16
(2,1407)	1:33:A:TYR:HD1	1:41:A:ASP:H	4	0.16
(2,1407)	1:33:A:TYR:HD2	1:41:A:ASP:H	4	0.16
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	2	0.16
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	3	0.16
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	9	0.16
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	11	0.16
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	6	0.16
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	18	0.16
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	5	0.16
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	20	0.16
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	20	0.16
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	20	0.16
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	19	0.16
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	19	0.16
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	19	0.16
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	19	0.16
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	19	0.16
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	19	0.16
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	19	0.16
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	19	0.16
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	19	0.16
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	12	0.16
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	12	0.16
(2,1173)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	2	0.16
(2,1173)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	2	0.16
(2,1173)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	2	0.16
(2,1173)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	18	0.16
(2,1173)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	18	0.16
(2,1173)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	18	0.16
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	6	0.16
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	1	0.16
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	16	0.16
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	6	0.16
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	9	0.16
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	12	0.16
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	17	0.16
(2,943)	1:60:A:LYS:HG2	1:54:A:ILE:HA	7	0.16
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	5	0.16
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	11	0.16
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	20	0.16
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	4	0.16
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	4	0.16
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	4	0.16
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	4	0.16
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	4	0.16
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	4	0.16
(2,842)	1:51:A:ALA:HB1	1:48:A:ILE:HA	17	0.16
(2,842)	1:51:A:ALA:HB2	1:48:A:ILE:HA	17	0.16
(2,842)	1:51:A:ALA:HB3	1:48:A:ILE:HA	17	0.16
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	4	0.16
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	11	0.16
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	11	0.16
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	11	0.16
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	4	0.16
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	2	0.16
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	17	0.16
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	9	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	4	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	6	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	7	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	11	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	13	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	16	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	18	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	19	0.16
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	20	0.16
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	3	0.16
(2,688)	1:40:A:GLY:H	1:38:A:PRO:HA	6	0.16
(2,627)	1:31:A:LEU:HA	1:34:A:HIS:HB2	20	0.16
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	4	0.16
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	4	0.16
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	4	0.16
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	7	0.16
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	7	0.16
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	7	0.16
(2,552)	1:69:A:LEU:HD21	1:73:A:ARG:HG3	4	0.16
(2,552)	1:69:A:LEU:HD22	1:73:A:ARG:HG3	4	0.16
(2,552)	1:69:A:LEU:HD23	1:73:A:ARG:HG3	4	0.16
(2,472)	1:24:A:LYS:HE2	1:21:A:GLU:HA	1	0.16
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	4	0.16
(2,463)	1:57:A:ASP:H	1:60:A:LYS:HG2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	20	0.16
(2,444)	1:23:A:LYS:HE2	1:23:A:LYS:HB2	11	0.16
(2,429)	1:22:A:LEU:HD11	1:22:A:LEU:HB3	3	0.16
(2,429)	1:22:A:LEU:HD12	1:22:A:LEU:HB3	3	0.16
(2,429)	1:22:A:LEU:HD13	1:22:A:LEU:HB3	3	0.16
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	2	0.16
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	6	0.16
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	8	0.16
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	3	0.16
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	3	0.16
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	3	0.16
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	10	0.16
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	5	0.16
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	2	0.16
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	4	0.16
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	8	0.16
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	19	0.16
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	20	0.16
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	6	0.16
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	6	0.16
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	6	0.16
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	6	0.16
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	6	0.16
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	6	0.16
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	6	0.16
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	6	0.16
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	6	0.16
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	15	0.16
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	15	0.16
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	15	0.16
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	15	0.16
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	15	0.16
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	15	0.16
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	15	0.16
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	15	0.16
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	15	0.16
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	8	0.16
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	8	0.16
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	8	0.16
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	1	0.16
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	16	0.16
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD11	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD12	12	0.16
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD13	12	0.16
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	15	0.16
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	9	0.16
(2,47)	1:6:A:LYS:HG3	1:4:A:GLU:HA	1	0.16
(2,42)	1:4:A:GLU:HG2	1:3:A:LYS:HG2	20	0.16
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	4	0.16
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	1	0.16
(1,435)	1:47:A:GLU:HG3	1:47:A:GLU:HA	15	0.16
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	17	0.16
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	17	0.16
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	17	0.16
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	1	0.16
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	1	0.16
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	1	0.16
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	19	0.16
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	3	0.16
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	6	0.16
(1,332)	1:28:A:LYS:HA	1:31:A:LEU:HB2	2	0.16
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	3	0.16
(1,309)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	3	0.16
(1,309)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	12	0.16
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	6	0.16
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	6	0.16
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	7	0.16
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	8	0.16
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	18	0.16
(1,250)	1:72:A:ALA:HB1	1:71:A:ALA:H	6	0.16
(1,250)	1:72:A:ALA:HB2	1:71:A:ALA:H	6	0.16
(1,250)	1:72:A:ALA:HB3	1:71:A:ALA:H	6	0.16
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	8	0.16
(1,231)	1:60:A:LYS:HE3	1:60:A:LYS:HD2	11	0.16
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	3	0.16
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	13	0.16
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	15	0.16
(1,191)	1:23:A:LYS:H	1:20:A:GLN:HA	20	0.16
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	3	0.16
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	3	0.16
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	3	0.16
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	1	0.16
(1,86)	1:62:A:GLU:H	1:60:A:LYS:H	11	0.16
(1,80)	1:46:A:LYS:HA	1:46:A:LYS:HG3	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	20	0.16
(1,57)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	16	0.16
(1,24)	1:37:A:LYS:HE2	1:34:A:HIS:H	15	0.16
(2,2464)	1:28:A:LYS:HG3	1:28:A:LYS:HE3	6	0.15
(2,2427)	1:13:A:VAL:HB	1:18:A:ASN:H	3	0.15
(2,2408)	1:24:A:LYS:HB2	1:24:A:LYS:H	5	0.15
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	13	0.15
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	13	0.15
(2,2366)	1:33:A:TYR:HE1	1:32:A:LYS:HE3	16	0.15
(2,2366)	1:33:A:TYR:HE2	1:32:A:LYS:HE3	16	0.15
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	3	0.15
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	3	0.15
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	3	0.15
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	3	0.15
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	3	0.15
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	3	0.15
(2,2259)	1:77:A:PRO:HD2	1:78:A:SER:H	18	0.15
(2,2216)	1:54:A:ILE:HG21	1:73:A:ARG:H	19	0.15
(2,2216)	1:54:A:ILE:HG22	1:73:A:ARG:H	19	0.15
(2,2216)	1:54:A:ILE:HG23	1:73:A:ARG:H	19	0.15
(2,2211)	1:64:A:TYR:HE1	1:72:A:ALA:H	17	0.15
(2,2211)	1:64:A:TYR:HE2	1:72:A:ALA:H	17	0.15
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	11	0.15
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	10	0.15
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	10	0.15
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	10	0.15
(2,2159)	1:68:A:GLY:H	1:66:A:GLN:H	10	0.15
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	19	0.15
(2,2133)	1:67:A:TYR:H	1:66:A:GLN:HB3	1	0.15
(2,2126)	1:68:A:GLY:H	1:66:A:GLN:H	19	0.15
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	19	0.15
(2,2094)	1:63:A:ILE:HG21	1:64:A:TYR:H	3	0.15
(2,2094)	1:63:A:ILE:HG22	1:64:A:TYR:H	3	0.15
(2,2094)	1:63:A:ILE:HG23	1:64:A:TYR:H	3	0.15
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	8	0.15
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	13	0.15
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	20	0.15
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	2	0.15
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	13	0.15
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	13	0.15
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	11	0.15
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	16	0.15
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	18	0.15
(2,1963)	1:55:A:LEU:HD11	1:55:A:LEU:H	17	0.15
(2,1963)	1:55:A:LEU:HD12	1:55:A:LEU:H	17	0.15
(2,1963)	1:55:A:LEU:HD13	1:55:A:LEU:H	17	0.15
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	6	0.15
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	13	0.15
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	18	0.15
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	8	0.15
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	10	0.15
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	13	0.15
(2,1939)	1:53:A:GLU:H	1:54:A:ILE:HB	16	0.15
(2,1923)	1:55:A:LEU:HD21	1:52:A:PHE:H	6	0.15
(2,1923)	1:55:A:LEU:HD22	1:52:A:PHE:H	6	0.15
(2,1923)	1:55:A:LEU:HD23	1:52:A:PHE:H	6	0.15
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	1	0.15
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	1	0.15
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	1	0.15
(2,1829)	1:41:A:ASP:HB2	1:42:A:THR:H	9	0.15
(2,1829)	1:41:A:ASP:HB2	1:42:A:THR:H	14	0.15
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	7	0.15
(2,1781)	1:32:A:LYS:HB2	1:33:A:TYR:H	14	0.15
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	1	0.15
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG21	16	0.15
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG22	16	0.15
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG23	16	0.15
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	8	0.15
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	9	0.15
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	8	0.15
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	9	0.15
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	18	0.15
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	9	0.15
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	12	0.15
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	13	0.15
(2,1613)	1:17:A:ALA:H	1:16:A:SER:HB3	11	0.15
(2,1602)	1:15:A:PRO:HB2	1:16:A:SER:H	2	0.15
(2,1602)	1:15:A:PRO:HB2	1:16:A:SER:H	19	0.15
(2,1601)	1:15:A:PRO:HB3	1:16:A:SER:H	2	0.15
(2,1601)	1:15:A:PRO:HB3	1:16:A:SER:H	19	0.15
(2,1595)	1:14:A:SER:HB2	1:16:A:SER:H	15	0.15
(2,1583)	1:14:A:SER:H	1:21:A:GLU:HG3	4	0.15
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	16	0.15
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	16	0.15
(2,1568)	1:8:A:TYR:HB2	1:13:A:VAL:H	5	0.15
(2,1568)	1:8:A:TYR:HB2	1:13:A:VAL:H	6	0.15
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD11	10	0.15
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD12	10	0.15
(2,1532)	1:11:A:LEU:H	1:11:A:LEU:HD13	10	0.15
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	8	0.15
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	16	0.15
(2,1484)	1:55:A:LEU:HD21	1:8:A:TYR:H	18	0.15
(2,1484)	1:55:A:LEU:HD22	1:8:A:TYR:H	18	0.15
(2,1484)	1:55:A:LEU:HD23	1:8:A:TYR:H	18	0.15
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	6	0.15
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	14	0.15
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	16	0.15
(2,1407)	1:33:A:TYR:HD1	1:41:A:ASP:H	15	0.15
(2,1407)	1:33:A:TYR:HD2	1:41:A:ASP:H	15	0.15
(2,1340)	1:77:A:PRO:HA	1:78:A:SER:H	13	0.15
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	7	0.15
(2,1309)	1:54:A:ILE:HD11	1:73:A:ARG:HG3	16	0.15
(2,1309)	1:54:A:ILE:HD12	1:73:A:ARG:HG3	16	0.15
(2,1309)	1:54:A:ILE:HD13	1:73:A:ARG:HG3	16	0.15
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	9	0.15
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	13	0.15
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	7	0.15
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	7	0.15
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	7	0.15
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	7	0.15
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	7	0.15
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	7	0.15
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	7	0.15
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	7	0.15
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	7	0.15
(2,1257)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	3	0.15
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD21	5	0.15
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD22	5	0.15
(2,1255)	1:70:A:GLU:HB3	1:69:A:LEU:HD23	5	0.15
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	17	0.15
(2,1110)	1:55:A:LEU:HD21	1:61:A:ARG:HA	12	0.15
(2,1110)	1:55:A:LEU:HD22	1:61:A:ARG:HA	12	0.15
(2,1110)	1:55:A:LEU:HD23	1:61:A:ARG:HA	12	0.15
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	11	0.15
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	2	0.15
(2,1046)	1:52:A:PHE:HE1	1:56:A:ASN:HB3	7	0.15
(2,1046)	1:52:A:PHE:HE2	1:56:A:ASN:HB3	7	0.15
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	6	0.15
(2,931)	1:53:A:GLU:HA	1:52:A:PHE:HB3	7	0.15
(2,856)	1:45:A:PHE:HA	1:48:A:ILE:HG12	16	0.15
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	3	0.15
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	7	0.15
(2,831)	1:6:A:LYS:HA	1:6:A:LYS:HE2	7	0.15
(2,787)	1:10:A:LEU:HD11	1:44:A:LYS:HG2	16	0.15
(2,787)	1:10:A:LEU:HD12	1:44:A:LYS:HG2	16	0.15
(2,787)	1:10:A:LEU:HD13	1:44:A:LYS:HG2	16	0.15
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	4	0.15
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	16	0.15
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	9	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	1	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	3	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	4	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	5	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	6	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	7	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	8	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	10	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	11	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	12	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	14	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	15	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	16	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	17	0.15
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	18	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	1	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	2	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	5	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	8	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	9	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	10	0.15
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	17	0.15
(2,714)	1:43:A:GLU:HG3	1:41:A:ASP:HA	3	0.15
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	15	0.15
(2,607)	1:45:A:PHE:HB3	1:30:A:ALA:HA	12	0.15
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	6	0.15
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	6	0.15
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	20	0.15
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	20	0.15
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	20	0.15
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	7	0.15
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	7	0.15
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	7	0.15
(2,579)	1:28:A:LYS:HB3	1:29:A:ALA:HA	5	0.15
(2,467)	1:60:A:LYS:HA	1:63:A:ILE:HG12	20	0.15
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	19	0.15
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	19	0.15
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	19	0.15
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	19	0.15
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	19	0.15
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	19	0.15
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	19	0.15
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	19	0.15
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	19	0.15
(2,351)	1:24:A:LYS:HE2	1:21:A:GLU:HA	1	0.15
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	4	0.15
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	4	0.15
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	4	0.15
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	14	0.15
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	10	0.15
(2,280)	1:14:A:SER:HB2	1:16:A:SER:H	16	0.15
(2,277)	1:16:A:SER:HA	1:17:A:ALA:H	9	0.15
(2,271)	1:70:A:GLU:HB3	1:71:A:ALA:H	12	0.15
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	17	0.15
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	18	0.15
(2,238)	1:22:A:LEU:HD21	1:15:A:PRO:HA	5	0.15
(2,238)	1:22:A:LEU:HD22	1:15:A:PRO:HA	5	0.15
(2,238)	1:22:A:LEU:HD23	1:15:A:PRO:HA	5	0.15
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	4	0.15
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	4	0.15
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	4	0.15
(2,190)	1:11:A:LEU:HD11	1:11:A:LEU:HA	20	0.15
(2,190)	1:11:A:LEU:HD12	1:11:A:LEU:HA	20	0.15
(2,190)	1:11:A:LEU:HD13	1:11:A:LEU:HA	20	0.15
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	10	0.15
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	18	0.15
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:0:A:THR:HA	1:1:A:SER:H	8	0.15
(1,481)	1:-1:A:MET:HA	1:0:A:THR:H	18	0.15
(1,454)	1:72:A:ALA:H	1:64:A:TYR:H	13	0.15
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	1	0.15
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	13	0.15
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	14	0.15
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	14	0.15
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	14	0.15
(1,406)	1:37:A:LYS:HD3	1:38:A:PRO:HD2	13	0.15
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD11	11	0.15
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD12	11	0.15
(1,380)	1:60:A:LYS:HE3	1:54:A:ILE:HD13	11	0.15
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	7	0.15
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	13	0.15
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	8	0.15
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	10	0.15
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	13	0.15
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	17	0.15
(1,326)	1:78:A:SER:HA	1:79:A:PHE:H	1	0.15
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	7	0.15
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	13	0.15
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	2	0.15
(1,309)	1:58:A:PRO:HD2	1:58:A:PRO:HB3	5	0.15
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	11	0.15
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	18	0.15
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	6	0.15
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	8	0.15
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	2	0.15
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	5	0.15
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	10	0.15
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	13	0.15
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	15	0.15
(1,250)	1:72:A:ALA:HB1	1:71:A:ALA:H	9	0.15
(1,250)	1:72:A:ALA:HB2	1:71:A:ALA:H	9	0.15
(1,250)	1:72:A:ALA:HB3	1:71:A:ALA:H	9	0.15
(1,249)	1:23:A:LYS:HE2	1:23:A:LYS:HG2	7	0.15
(1,246)	1:24:A:LYS:HE3	1:24:A:LYS:HD2	3	0.15
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	4	0.15
(1,144)	1:62:A:GLU:HA	1:62:A:GLU:HG3	12	0.15
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	6	0.15
(1,136)	1:6:A:LYS:HG3	1:6:A:LYS:HA	7	0.15
(1,103)	1:59:A:GLN:HA	1:59:A:GLN:HG3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:59:A:GLN:H	1:60:A:LYS:HB2	12	0.15
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	10	0.15
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	6	0.15
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	11	0.15
(1,43)	1:72:A:ALA:H	1:69:A:LEU:HA	20	0.15
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	15	0.15
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	15	0.15
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	15	0.15
(1,5)	1:63:A:ILE:HG21	1:75:A:GLY:H	14	0.15
(1,5)	1:63:A:ILE:HG22	1:75:A:GLY:H	14	0.15
(1,5)	1:63:A:ILE:HG23	1:75:A:GLY:H	14	0.15
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	2	0.14
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	2	0.14
(2,2470)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	2	0.14
(2,2464)	1:28:A:LYS:HG3	1:28:A:LYS:HE3	1	0.14
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	1	0.14
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	14	0.14
(2,2383)	1:11:A:LEU:HB2	1:52:A:PHE:HE1	7	0.14
(2,2383)	1:11:A:LEU:HB2	1:52:A:PHE:HE2	7	0.14
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	16	0.14
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	16	0.14
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	16	0.14
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	16	0.14
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	16	0.14
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	16	0.14
(2,2350)	1:32:A:LYS:H	1:34:A:HIS:HD2	19	0.14
(2,2338)	1:32:A:LYS:H	1:34:A:HIS:HD2	19	0.14
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	18	0.14
(2,2250)	1:76:A:GLY:HA2	1:76:A:GLY:H	4	0.14
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	2	0.14
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	9	0.14
(2,2225)	1:73:A:ARG:HD2	1:73:A:ARG:H	4	0.14
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	1	0.14
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	3	0.14
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	16	0.14
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	16	0.14
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	16	0.14
(2,2167)	1:64:A:TYR:HB2	1:69:A:LEU:H	18	0.14
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	13	0.14
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	10	0.14
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	15	0.14
(2,2133)	1:67:A:TYR:H	1:66:A:GLN:HB3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2094)	1:63:A:ILE:HG21	1:64:A:TYR:H	2	0.14
(2,2094)	1:63:A:ILE:HG22	1:64:A:TYR:H	2	0.14
(2,2094)	1:63:A:ILE:HG23	1:64:A:TYR:H	2	0.14
(2,2086)	1:64:A:TYR:HB2	1:63:A:ILE:H	7	0.14
(2,2086)	1:64:A:TYR:HB2	1:63:A:ILE:H	11	0.14
(2,2086)	1:64:A:TYR:HB2	1:63:A:ILE:H	13	0.14
(2,2085)	1:64:A:TYR:HB3	1:63:A:ILE:H	18	0.14
(2,2044)	1:72:A:ALA:HB1	1:65:A:ASP:H	4	0.14
(2,2044)	1:72:A:ALA:HB2	1:65:A:ASP:H	4	0.14
(2,2044)	1:72:A:ALA:HB3	1:65:A:ASP:H	4	0.14
(2,2026)	1:60:A:LYS:HG2	1:60:A:LYS:H	9	0.14
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	2	0.14
(2,1967)	1:55:A:LEU:H	1:55:A:LEU:HB3	12	0.14
(2,1967)	1:55:A:LEU:H	1:55:A:LEU:HB3	19	0.14
(2,1953)	1:54:A:ILE:HD11	1:54:A:ILE:H	15	0.14
(2,1953)	1:54:A:ILE:HD12	1:54:A:ILE:H	15	0.14
(2,1953)	1:54:A:ILE:HD13	1:54:A:ILE:H	15	0.14
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	14	0.14
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	9	0.14
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	11	0.14
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	11	0.14
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	11	0.14
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	12	0.14
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	12	0.14
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	12	0.14
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	20	0.14
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	20	0.14
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	20	0.14
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	13	0.14
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG21	17	0.14
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG22	17	0.14
(2,1737)	1:29:A:ALA:H	1:48:A:ILE:HG23	17	0.14
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	17	0.14
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	20	0.14
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	3	0.14
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	2	0.14
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	16	0.14
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	10	0.14
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	20	0.14
(2,1605)	1:14:A:SER:H	1:16:A:SER:H	5	0.14
(2,1603)	1:15:A:PRO:HG3	1:16:A:SER:H	2	0.14
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	15	0.14
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	15	0.14
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	2	0.14
(2,1553)	1:10:A:LEU:HB3	1:12:A:GLY:H	1	0.14
(2,1531)	1:7:A:LEU:HD21	1:10:A:LEU:H	1	0.14
(2,1531)	1:7:A:LEU:HD22	1:10:A:LEU:H	1	0.14
(2,1531)	1:7:A:LEU:HD23	1:10:A:LEU:H	1	0.14
(2,1531)	1:7:A:LEU:HD21	1:10:A:LEU:H	13	0.14
(2,1531)	1:7:A:LEU:HD22	1:10:A:LEU:H	13	0.14
(2,1531)	1:7:A:LEU:HD23	1:10:A:LEU:H	13	0.14
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	2	0.14
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	4	0.14
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	18	0.14
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	13	0.14
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	10	0.14
(2,1451)	1:4:A:GLU:HG3	1:4:A:GLU:H	9	0.14
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	8	0.14
(2,1412)	1:-1:A:MET:HB3	1:0:A:THR:H	2	0.14
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	17	0.14
(2,1377)	1:79:A:PHE:HA	1:79:A:PHE:HB2	1	0.14
(2,1377)	1:79:A:PHE:HA	1:79:A:PHE:HB2	7	0.14
(2,1377)	1:79:A:PHE:HA	1:79:A:PHE:HB2	19	0.14
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	5	0.14
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	8	0.14
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	19	0.14
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	13	0.14
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	3	0.14
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	8	0.14
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	17	0.14
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	5	0.14
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	5	0.14
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	5	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	14	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	14	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	14	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	14	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	14	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	14	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	14	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	14	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	14	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	15	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	15	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	15	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	15	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	15	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	15	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	15	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	15	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	16	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	16	0.14
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	16	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	16	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	16	0.14
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	16	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	16	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	16	0.14
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	16	0.14
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	3	0.14
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	7	0.14
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	16	0.14
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	20	0.14
(2,1136)	1:63:A:ILE:HA	1:67:A:TYR:HE1	3	0.14
(2,1136)	1:63:A:ILE:HA	1:67:A:TYR:HE2	3	0.14
(2,1075)	1:63:A:ILE:HD11	1:59:A:GLN:HG3	4	0.14
(2,1075)	1:63:A:ILE:HD12	1:59:A:GLN:HG3	4	0.14
(2,1075)	1:63:A:ILE:HD13	1:59:A:GLN:HG3	4	0.14
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	4	0.14
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	19	0.14
(2,1057)	1:62:A:GLU:H	1:58:A:PRO:HA	12	0.14
(2,931)	1:53:A:GLU:HA	1:52:A:PHE:HB3	4	0.14
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	8	0.14
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	18	0.14
(2,869)	1:50:A:GLU:HA	1:50:A:GLU:HG3	14	0.14
(2,789)	1:41:A:ASP:HB3	1:44:A:LYS:HG2	12	0.14
(2,763)	1:70:A:GLU:H	1:70:A:GLU:HG3	3	0.14
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	10	0.14
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	9	0.14
(2,743)	1:44:A:LYS:H	1:43:A:GLU:HB2	7	0.14
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	2	0.14
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	13	0.14
(2,733)	1:42:A:THR:HA	1:42:A:THR:HB	19	0.14
(2,731)	1:45:A:PHE:HB2	1:42:A:THR:HA	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,731)	1:45:A:PHE:HB2	1:42:A:THR:HA	13	0.14
(2,715)	1:41:A:ASP:HA	1:41:A:ASP:HB2	14	0.14
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	4	0.14
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	11	0.14
(2,706)	1:58:A:PRO:HA	1:58:A:PRO:HG3	1	0.14
(2,706)	1:58:A:PRO:HA	1:58:A:PRO:HG3	16	0.14
(2,706)	1:58:A:PRO:HA	1:58:A:PRO:HG3	19	0.14
(2,626)	1:31:A:LEU:HA	1:34:A:HIS:HB3	14	0.14
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	13	0.14
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	13	0.14
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	13	0.14
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	10	0.14
(2,436)	1:55:A:LEU:HD21	1:61:A:ARG:HG3	12	0.14
(2,436)	1:55:A:LEU:HD22	1:61:A:ARG:HG3	12	0.14
(2,436)	1:55:A:LEU:HD23	1:61:A:ARG:HG3	12	0.14
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	2	0.14
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	2	0.14
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	2	0.14
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	2	0.14
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	2	0.14
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	2	0.14
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	2	0.14
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	2	0.14
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	2	0.14
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	11	0.14
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	11	0.14
(2,430)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	11	0.14
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	11	0.14
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	11	0.14
(2,430)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	11	0.14
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	11	0.14
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	11	0.14
(2,430)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	11	0.14
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	3	0.14
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	3	0.14
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	2	0.14
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	4	0.14
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	6	0.14
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	10	0.14
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	15	0.14
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	20	0.14
(2,373)	1:13:A:VAL:HG21	1:21:A:GLU:HB2	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,373)	1:13:A:VAL:HG22	1:21:A:GLU:HB2	6	0.14
(2,373)	1:13:A:VAL:HG23	1:21:A:GLU:HB2	6	0.14
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	17	0.14
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	11	0.14
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	14	0.14
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	15	0.14
(2,295)	1:17:A:ALA:HB1	1:14:A:SER:HB2	14	0.14
(2,295)	1:17:A:ALA:HB2	1:14:A:SER:HB2	14	0.14
(2,295)	1:17:A:ALA:HB3	1:14:A:SER:HB2	14	0.14
(2,271)	1:70:A:GLU:HB3	1:71:A:ALA:H	15	0.14
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	12	0.14
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	15	0.14
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	19	0.14
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	14	0.14
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	8	0.14
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	15	0.14
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	16	0.14
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	14	0.14
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	16	0.14
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	16	0.14
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	16	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	1	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	2	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	3	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	6	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	7	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	10	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	11	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	12	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	13	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	15	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	17	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	19	0.14
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	20	0.14
(2,102)	1:7:A:LEU:HA	1:10:A:LEU:HB3	6	0.14
(2,95)	1:7:A:LEU:HD21	1:51:A:ALA:H	13	0.14
(2,95)	1:7:A:LEU:HD22	1:51:A:ALA:H	13	0.14
(2,95)	1:7:A:LEU:HD23	1:51:A:ALA:H	13	0.14
(2,50)	1:4:A:GLU:H	1:6:A:LYS:HB3	8	0.14
(2,30)	1:4:A:GLU:H	1:3:A:LYS:HA	19	0.14
(2,8)	1:1:A:SER:H	1:1:A:SER:HB2	18	0.14
(2,5)	1:1:A:SER:HA	1:2:A:VAL:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG21	8	0.14
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG22	8	0.14
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG23	8	0.14
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	18	0.14
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	11	0.14
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	11	0.14
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	11	0.14
(1,398)	1:69:A:LEU:HD21	1:73:A:ARG:H	11	0.14
(1,398)	1:69:A:LEU:HD22	1:73:A:ARG:H	11	0.14
(1,398)	1:69:A:LEU:HD23	1:73:A:ARG:H	11	0.14
(1,357)	1:50:A:GLU:HA	1:53:A:GLU:HB2	7	0.14
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	8	0.14
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	5	0.14
(1,332)	1:70:A:GLU:HA	1:73:A:ARG:HG3	8	0.14
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	7	0.14
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	9	0.14
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	13	0.14
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	14	0.14
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	18	0.14
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	13	0.14
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	13	0.14
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	13	0.14
(1,294)	1:6:A:LYS:HG3	1:6:A:LYS:HD2	1	0.14
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB1	2	0.14
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB2	2	0.14
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB3	2	0.14
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG21	15	0.14
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG22	15	0.14
(1,288)	1:26:A:TYR:HA	1:48:A:ILE:HG23	15	0.14
(1,266)	1:30:A:ALA:HA	1:33:A:TYR:H	13	0.14
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	1	0.14
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	11	0.14
(1,258)	1:28:A:LYS:HA	1:28:A:LYS:H	11	0.14
(1,250)	1:51:A:ALA:HB1	1:10:A:LEU:H	3	0.14
(1,250)	1:51:A:ALA:HB2	1:10:A:LEU:H	3	0.14
(1,250)	1:51:A:ALA:HB3	1:10:A:LEU:H	3	0.14
(1,245)	1:43:A:GLU:HA	1:46:A:LYS:HB2	10	0.14
(1,238)	1:66:A:GLN:HB3	1:66:A:GLN:HA	8	0.14
(1,205)	1:72:A:ALA:H	1:63:A:ILE:HB	12	0.14
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	9	0.14
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	17	0.14
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG21	6	0.14
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG22	6	0.14
(1,178)	1:26:A:TYR:HA	1:48:A:ILE:HG23	6	0.14
(1,155)	1:66:A:GLN:HA	1:66:A:GLN:HG3	11	0.14
(1,121)	1:64:A:TYR:HD1	1:65:A:ASP:H	5	0.14
(1,121)	1:64:A:TYR:HD2	1:65:A:ASP:H	5	0.14
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	7	0.14
(1,88)	1:61:A:ARG:H	1:60:A:LYS:HE2	2	0.14
(1,88)	1:60:A:LYS:HE3	1:61:A:ARG:H	13	0.14
(1,80)	1:28:A:LYS:HA	1:28:A:LYS:HG3	14	0.14
(1,68)	1:72:A:ALA:HB1	1:76:A:GLY:H	8	0.14
(1,68)	1:72:A:ALA:HB2	1:76:A:GLY:H	8	0.14
(1,68)	1:72:A:ALA:HB3	1:76:A:GLY:H	8	0.14
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	10	0.14
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	10	0.14
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	10	0.14
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG2	19	0.14
(1,5)	1:63:A:ILE:HD11	1:75:A:GLY:H	10	0.14
(1,5)	1:63:A:ILE:HD12	1:75:A:GLY:H	10	0.14
(1,5)	1:63:A:ILE:HD13	1:75:A:GLY:H	10	0.14
(2,2464)	1:28:A:LYS:HG3	1:28:A:LYS:HE3	3	0.13
(2,2411)	1:27:A:ARG:H	1:27:A:ARG:HD2	2	0.13
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	2	0.13
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	13	0.13
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	17	0.13
(2,2251)	1:76:A:GLY:HA3	1:76:A:GLY:H	4	0.13
(2,2250)	1:76:A:GLY:HA2	1:76:A:GLY:H	18	0.13
(2,2237)	1:74:A:SER:H	1:75:A:GLY:HA2	3	0.13
(2,2237)	1:74:A:SER:H	1:75:A:GLY:HA2	18	0.13
(2,2221)	1:73:A:ARG:HG2	1:73:A:ARG:H	8	0.13
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD2	2	0.13
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	16	0.13
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	18	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	1	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	1	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	1	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	5	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	5	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	5	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	19	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	19	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	20	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	20	0.13
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	20	0.13
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	14	0.13
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	19	0.13
(2,2136)	1:67:A:TYR:H	1:67:A:TYR:HB3	18	0.13
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	8	0.13
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	5	0.13
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	5	0.13
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	5	0.13
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	15	0.13
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	15	0.13
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	15	0.13
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	14	0.13
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	14	0.13
(2,2078)	1:72:A:ALA:HB1	1:63:A:ILE:H	19	0.13
(2,2078)	1:72:A:ALA:HB2	1:63:A:ILE:H	19	0.13
(2,2078)	1:72:A:ALA:HB3	1:63:A:ILE:H	19	0.13
(2,2077)	1:63:A:ILE:HG12	1:63:A:ILE:H	2	0.13
(2,2068)	1:65:A:ASP:HB3	1:62:A:GLU:H	15	0.13
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	5	0.13
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	14	0.13
(2,2029)	1:60:A:LYS:H	1:60:A:LYS:HE3	6	0.13
(2,2013)	1:57:A:ASP:H	1:61:A:ARG:H	12	0.13
(2,1991)	1:52:A:PHE:HA	1:56:A:ASN:H	20	0.13
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	4	0.13
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	6	0.13
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	19	0.13
(2,1968)	1:55:A:LEU:H	1:56:A:ASN:HB3	9	0.13
(2,1963)	1:55:A:LEU:HD21	1:55:A:LEU:H	7	0.13
(2,1963)	1:55:A:LEU:HD22	1:55:A:LEU:H	7	0.13
(2,1963)	1:55:A:LEU:HD23	1:55:A:LEU:H	7	0.13
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	3	0.13
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	10	0.13
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	20	0.13
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	10	0.13
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	10	0.13
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	3	0.13
(2,1914)	1:7:A:LEU:HG	1:51:A:ALA:H	6	0.13
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	7	0.13
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	7	0.13
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	11	0.13
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	5	0.13
(2,1720)	1:26:A:TYR:HB2	1:27:A:ARG:H	11	0.13
(2,1708)	1:26:A:TYR:H	1:27:A:ARG:HA	9	0.13
(2,1692)	1:25:A:GLY:H	1:24:A:LYS:HD2	20	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	1	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	2	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	6	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	7	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	10	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	11	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	14	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	15	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	17	0.13
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	20	0.13
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	6	0.13
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	7	0.13
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	15	0.13
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	20	0.13
(2,1643)	1:18:A:ASN:HB2	1:20:A:GLN:H	19	0.13
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	7	0.13
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	14	0.13
(2,1614)	1:14:A:SER:HB2	1:17:A:ALA:H	20	0.13
(2,1601)	1:15:A:PRO:HB3	1:16:A:SER:H	13	0.13
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	16	0.13
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	17	0.13
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	3	0.13
(2,1493)	1:8:A:TYR:HB3	1:8:A:TYR:H	18	0.13
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG21	13	0.13
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG22	13	0.13
(2,1476)	1:7:A:LEU:H	1:0:A:THR:HG23	13	0.13
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD21	1	0.13
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD22	1	0.13
(2,1474)	1:7:A:LEU:H	1:55:A:LEU:HD23	1	0.13
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	13	0.13
(2,1452)	1:4:A:GLU:HG2	1:4:A:GLU:H	18	0.13
(2,1445)	1:3:A:LYS:HB2	1:3:A:LYS:H	17	0.13
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	1	0.13
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	12	0.13
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG11	7	0.13
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG12	7	0.13
(2,1417)	1:1:A:SER:H	1:2:A:VAL:HG13	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	10	0.13
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	10	0.13
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	10	0.13
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	10	0.13
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	10	0.13
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	10	0.13
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD11	19	0.13
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD12	19	0.13
(2,1400)	1:26:A:TYR:HE1	1:48:A:ILE:HD13	19	0.13
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD11	19	0.13
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD12	19	0.13
(2,1400)	1:26:A:TYR:HE2	1:48:A:ILE:HD13	19	0.13
(2,1377)	1:79:A:PHE:HA	1:79:A:PHE:HB2	14	0.13
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	15	0.13
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	18	0.13
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	17	0.13
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	8	0.13
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	2	0.13
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	6	0.13
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	14	0.13
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	18	0.13
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	19	0.13
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	3	0.13
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	3	0.13
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	3	0.13
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	3	0.13
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	3	0.13
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	3	0.13
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	3	0.13
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	3	0.13
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	3	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	13	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	13	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	13	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	14	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	14	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	14	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	17	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	17	0.13
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	17	0.13
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	2	0.13
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	15	0.13
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	15	0.13
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	15	0.13
(2,1260)	1:43:A:GLU:HA	1:43:A:GLU:HG3	12	0.13
(2,1260)	1:43:A:GLU:HA	1:43:A:GLU:HG3	15	0.13
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	1	0.13
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	10	0.13
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	15	0.13
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	3	0.13
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	3	0.13
(2,1173)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	1	0.13
(2,1173)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	1	0.13
(2,1173)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	1	0.13
(2,1173)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	10	0.13
(2,1173)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	10	0.13
(2,1173)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	10	0.13
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	14	0.13
(2,1107)	1:50:A:GLU:HA	1:54:A:ILE:HG13	1	0.13
(2,1067)	1:15:A:PRO:HD2	1:14:A:SER:HA	5	0.13
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	18	0.13
(2,1017)	1:61:A:ARG:H	1:55:A:LEU:HA	7	0.13
(2,967)	1:54:A:ILE:HD11	1:72:A:ALA:HA	8	0.13
(2,967)	1:54:A:ILE:HD12	1:72:A:ALA:HA	8	0.13
(2,967)	1:54:A:ILE:HD13	1:72:A:ALA:HA	8	0.13
(2,967)	1:54:A:ILE:HD11	1:72:A:ALA:HA	11	0.13
(2,967)	1:54:A:ILE:HD12	1:72:A:ALA:HA	11	0.13
(2,967)	1:54:A:ILE:HD13	1:72:A:ALA:HA	11	0.13
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB2	5	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	12	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	12	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	14	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	14	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	16	0.13
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	16	0.13
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	2	0.13
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	14	0.13
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	11	0.13
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	17	0.13
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	17	0.13
(2,754)	1:70:A:GLU:HG3	1:73:A:ARG:HD2	2	0.13
(2,754)	1:70:A:GLU:HG3	1:73:A:ARG:HD2	17	0.13
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	8	0.13
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	20	0.13
(2,610)	1:30:A:ALA:HA	1:33:A:TYR:H	2	0.13
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	1	0.13
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	1	0.13
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	1	0.13
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	3	0.13
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	3	0.13
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	3	0.13
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	11	0.13
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	11	0.13
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	11	0.13
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	12	0.13
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	12	0.13
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	12	0.13
(2,557)	1:73:A:ARG:HG3	1:73:A:ARG:HA	11	0.13
(2,501)	1:25:A:GLY:HA2	1:24:A:LYS:HD3	16	0.13
(2,495)	1:13:A:VAL:HG21	1:25:A:GLY:HA3	8	0.13
(2,495)	1:13:A:VAL:HG22	1:25:A:GLY:HA3	8	0.13
(2,495)	1:13:A:VAL:HG23	1:25:A:GLY:HA3	8	0.13
(2,398)	1:21:A:GLU:HA	1:21:A:GLU:HG3	1	0.13
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	4	0.13
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	13	0.13
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	2	0.13
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	2	0.13
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	2	0.13
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	13	0.13
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	13	0.13
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	13	0.13
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	11	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	3	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	5	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	8	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	11	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	13	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	14	0.13
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	16	0.13
(2,347)	1:19:A:GLU:HG2	1:23:A:LYS:HE3	5	0.13
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	4	0.13
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	9	0.13
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	6	0.13
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	13	0.13
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	13	0.13
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	13	0.13
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	13	0.13
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	13	0.13
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	13	0.13
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	13	0.13
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	13	0.13
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	13	0.13
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	13	0.13
(2,264)	1:58:A:PRO:HD3	1:59:A:GLN:H	5	0.13
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	12	0.13
(2,244)	1:15:A:PRO:HA	1:16:A:SER:HA	5	0.13
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD11	18	0.13
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD12	18	0.13
(2,208)	1:26:A:TYR:HE1	1:11:A:LEU:HD13	18	0.13
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD11	18	0.13
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD12	18	0.13
(2,208)	1:26:A:TYR:HE2	1:11:A:LEU:HD13	18	0.13
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD11	1	0.13
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD12	1	0.13
(2,206)	1:11:A:LEU:H	1:11:A:LEU:HD13	1	0.13
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	17	0.13
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	17	0.13
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	17	0.13
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD11	9	0.13
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD12	9	0.13
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD13	9	0.13
(2,184)	1:11:A:LEU:HB2	1:10:A:LEU:HB3	14	0.13
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	4	0.13
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	5	0.13
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	9	0.13
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	14	0.13
(2,144)	1:9:A:ASP:HB3	1:9:A:ASP:HA	18	0.13
(2,118)	1:63:A:ILE:HG21	1:64:A:TYR:HA	3	0.13
(2,118)	1:63:A:ILE:HG22	1:64:A:TYR:HA	3	0.13
(2,118)	1:63:A:ILE:HG23	1:64:A:TYR:HA	3	0.13
(2,47)	1:6:A:LYS:HG2	1:4:A:GLU:HA	7	0.13
(2,38)	1:3:A:LYS:HB3	1:3:A:LYS:H	9	0.13
(2,27)	1:2:A:VAL:HB	1:65:A:ASP:HA	10	0.13
(2,27)	1:2:A:VAL:HB	1:65:A:ASP:HA	13	0.13
(2,26)	1:2:A:VAL:HA	1:2:A:VAL:HB	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:2:A:VAL:HA	1:4:A:GLU:HG3	10	0.13
(2,2)	1:0:A:THR:HA	1:1:A:SER:H	15	0.13
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	3	0.13
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	14	0.13
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	19	0.13
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	4	0.13
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	2	0.13
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	4	0.13
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	18	0.13
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	7	0.13
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	2	0.13
(1,338)	1:52:A:PHE:H	1:48:A:ILE:HA	20	0.13
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	5	0.13
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	4	0.13
(1,309)	1:38:A:PRO:HB3	1:38:A:PRO:HD2	8	0.13
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	10	0.13
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	14	0.13
(1,249)	1:60:A:LYS:HG3	1:57:A:ASP:HB3	5	0.13
(1,204)	1:51:A:ALA:H	1:52:A:PHE:H	13	0.13
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	8	0.13
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	10	0.13
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	11	0.13
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	1	0.13
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	17	0.13
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	20	0.13
(1,157)	1:61:A:ARG:HD2	1:55:A:LEU:HA	18	0.13
(1,155)	1:66:A:GLN:HA	1:66:A:GLN:HG3	16	0.13
(1,155)	1:66:A:GLN:HA	1:66:A:GLN:HG3	17	0.13
(1,150)	1:72:A:ALA:H	1:63:A:ILE:HB	9	0.13
(1,103)	1:59:A:GLN:HA	1:59:A:GLN:HG3	4	0.13
(1,68)	1:72:A:ALA:HB1	1:76:A:GLY:H	17	0.13
(1,68)	1:72:A:ALA:HB2	1:76:A:GLY:H	17	0.13
(1,68)	1:72:A:ALA:HB3	1:76:A:GLY:H	17	0.13
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD21	13	0.13
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD22	13	0.13
(1,59)	1:11:A:LEU:H	1:10:A:LEU:HD23	13	0.13
(1,57)	1:24:A:LYS:HE3	1:24:A:LYS:HB2	12	0.13
(1,43)	1:64:A:TYR:HA	1:72:A:ALA:H	5	0.13
(1,43)	1:72:A:ALA:H	1:69:A:LEU:HA	15	0.13
(1,8)	1:20:A:GLN:HA	1:20:A:GLN:HG3	8	0.13
(2,2461)	1:7:A:LEU:HG	1:54:A:ILE:H	19	0.12
(2,2394)	1:53:A:GLU:H	1:7:A:LEU:HB2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB1	13	0.12
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB2	13	0.12
(2,2355)	1:64:A:TYR:HE1	1:72:A:ALA:HB3	13	0.12
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB1	13	0.12
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB2	13	0.12
(2,2355)	1:64:A:TYR:HE2	1:72:A:ALA:HB3	13	0.12
(2,2321)	1:64:A:TYR:HD1	1:72:A:ALA:HA	2	0.12
(2,2321)	1:64:A:TYR:HD2	1:72:A:ALA:HA	2	0.12
(2,2272)	1:79:A:PHE:HD1	1:79:A:PHE:H	3	0.12
(2,2272)	1:79:A:PHE:HD2	1:79:A:PHE:H	3	0.12
(2,2259)	1:77:A:PRO:HD2	1:78:A:SER:H	3	0.12
(2,2237)	1:74:A:SER:H	1:75:A:GLY:HA2	13	0.12
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	11	0.12
(2,2211)	1:64:A:TYR:HE1	1:72:A:ALA:H	9	0.12
(2,2211)	1:64:A:TYR:HE2	1:72:A:ALA:H	9	0.12
(2,2209)	1:64:A:TYR:HB3	1:72:A:ALA:H	11	0.12
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	5	0.12
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	20	0.12
(2,2167)	1:64:A:TYR:HB2	1:69:A:LEU:H	15	0.12
(2,2162)	1:69:A:LEU:H	1:69:A:LEU:HG	10	0.12
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	6	0.12
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	6	0.12
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	6	0.12
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	6	0.12
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	6	0.12
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	11	0.12
(2,2094)	1:63:A:ILE:HG21	1:64:A:TYR:H	8	0.12
(2,2094)	1:63:A:ILE:HG22	1:64:A:TYR:H	8	0.12
(2,2094)	1:63:A:ILE:HG23	1:64:A:TYR:H	8	0.12
(2,2094)	1:63:A:ILE:HG21	1:64:A:TYR:H	20	0.12
(2,2094)	1:63:A:ILE:HG22	1:64:A:TYR:H	20	0.12
(2,2094)	1:63:A:ILE:HG23	1:64:A:TYR:H	20	0.12
(2,2057)	1:64:A:TYR:HE1	1:65:A:ASP:H	9	0.12
(2,2057)	1:64:A:TYR:HE2	1:65:A:ASP:H	9	0.12
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	1	0.12
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	7	0.12
(2,2019)	1:59:A:GLN:H	1:59:A:GLN:HG2	3	0.12
(2,2015)	1:59:A:GLN:H	1:60:A:LYS:HG2	5	0.12
(2,1991)	1:52:A:PHE:HA	1:56:A:ASN:H	2	0.12
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	8	0.12
(2,1968)	1:55:A:LEU:H	1:56:A:ASN:HB3	11	0.12
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1952)	1:54:A:ILE:HG21	1:54:A:ILE:H	12	0.12
(2,1952)	1:54:A:ILE:HG22	1:54:A:ILE:H	12	0.12
(2,1952)	1:54:A:ILE:HG23	1:54:A:ILE:H	12	0.12
(2,1951)	1:7:A:LEU:HG	1:54:A:ILE:H	19	0.12
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	16	0.12
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD11	17	0.12
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD12	17	0.12
(2,1916)	1:51:A:ALA:H	1:10:A:LEU:HD13	17	0.12
(2,1829)	1:41:A:ASP:HB2	1:42:A:THR:H	1	0.12
(2,1809)	1:39:A:THR:H	1:38:A:PRO:HD3	1	0.12
(2,1787)	1:33:A:TYR:H	1:45:A:PHE:HA	3	0.12
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	16	0.12
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	17	0.12
(2,1751)	1:22:A:LEU:H	1:22:A:LEU:HG	19	0.12
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	10	0.12
(2,1693)	1:25:A:GLY:H	1:24:A:LYS:HD3	17	0.12
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	12	0.12
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	13	0.12
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	18	0.12
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	19	0.12
(2,1684)	1:23:A:LYS:HB3	1:24:A:LYS:H	14	0.12
(2,1652)	1:21:A:GLU:H	1:20:A:GLN:HB3	18	0.12
(2,1634)	1:18:A:ASN:HB2	1:19:A:GLU:H	17	0.12
(2,1604)	1:16:A:SER:H	1:17:A:ALA:H	1	0.12
(2,1603)	1:15:A:PRO:HG3	1:16:A:SER:H	19	0.12
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	14	0.12
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	14	0.12
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	14	0.12
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	14	0.12
(2,1531)	1:7:A:LEU:HD21	1:10:A:LEU:H	9	0.12
(2,1531)	1:7:A:LEU:HD22	1:10:A:LEU:H	9	0.12
(2,1531)	1:7:A:LEU:HD23	1:10:A:LEU:H	9	0.12
(2,1480)	1:8:A:TYR:HD1	1:7:A:LEU:H	17	0.12
(2,1480)	1:8:A:TYR:HD2	1:7:A:LEU:H	17	0.12
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	17	0.12
(2,1464)	1:5:A:THR:H	1:6:A:LYS:HA	3	0.12
(2,1463)	1:3:A:LYS:HB2	1:5:A:THR:H	19	0.12
(2,1444)	1:3:A:LYS:HB3	1:3:A:LYS:H	7	0.12
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	11	0.12
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	13	0.12
(2,1415)	1:-1:A:MET:HA	1:0:A:THR:H	20	0.12
(2,1408)	1:5:A:THR:H	1:6:A:LYS:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1352)	1:77:A:PRO:HB3	1:78:A:SER:H	7	0.12
(2,1352)	1:77:A:PRO:HB3	1:78:A:SER:H	13	0.12
(2,1334)	1:77:A:PRO:HG3	1:77:A:PRO:HA	6	0.12
(2,1323)	1:77:A:PRO:HD3	1:76:A:GLY:HA3	3	0.12
(2,1315)	1:74:A:SER:HA	1:76:A:GLY:H	15	0.12
(2,1304)	1:73:A:ARG:HB3	1:73:A:ARG:H	15	0.12
(2,1300)	1:24:A:LYS:HE2	1:21:A:GLU:HA	19	0.12
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	11	0.12
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	11	0.12
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	11	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	6	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	6	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	6	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	19	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	19	0.12
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	19	0.12
(2,1270)	1:73:A:ARG:H	1:71:A:ALA:HA	3	0.12
(2,1261)	1:70:A:GLU:HA	1:70:A:GLU:HG3	19	0.12
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	11	0.12
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	14	0.12
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	19	0.12
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	3	0.12
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	3	0.12
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	3	0.12
(2,1187)	1:2:A:VAL:HG21	1:65:A:ASP:HA	14	0.12
(2,1187)	1:2:A:VAL:HG22	1:65:A:ASP:HA	14	0.12
(2,1187)	1:2:A:VAL:HG23	1:65:A:ASP:HA	14	0.12
(2,1128)	1:65:A:ASP:HB3	1:62:A:GLU:HA	15	0.12
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	2	0.12
(2,1127)	1:65:A:ASP:HB2	1:62:A:GLU:HA	3	0.12
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	20	0.12
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	5	0.12
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	20	0.12
(2,1112)	1:61:A:ARG:HG2	1:61:A:ARG:HA	14	0.12
(2,1093)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	16	0.12
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	9	0.12
(2,1013)	1:61:A:ARG:HD3	1:55:A:LEU:HA	11	0.12
(2,992)	1:54:A:ILE:HG21	1:60:A:LYS:HB2	6	0.12
(2,992)	1:54:A:ILE:HG22	1:60:A:LYS:HB2	6	0.12
(2,992)	1:54:A:ILE:HG23	1:60:A:LYS:HB2	6	0.12
(2,967)	1:54:A:ILE:HD11	1:72:A:ALA:HA	2	0.12
(2,967)	1:54:A:ILE:HD12	1:72:A:ALA:HA	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,967)	1:54:A:ILE:HD13	1:72:A:ALA:HA	2	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	9	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	9	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	10	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	10	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	19	0.12
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	19	0.12
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	4	0.12
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	17	0.12
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	1	0.12
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	1	0.12
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	1	0.12
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	1	0.12
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	1	0.12
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	1	0.12
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	19	0.12
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	19	0.12
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	19	0.12
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	19	0.12
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	19	0.12
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	19	0.12
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	8	0.12
(2,846)	1:51:A:ALA:H	1:48:A:ILE:HA	20	0.12
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	6	0.12
(2,797)	1:45:A:PHE:HA	1:48:A:ILE:HG12	18	0.12
(2,760)	1:13:A:VAL:HB	1:17:A:ALA:H	7	0.12
(2,754)	1:70:A:GLU:HG3	1:73:A:ARG:HD2	12	0.12
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	17	0.12
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	14	0.12
(2,746)	1:70:A:GLU:HB3	1:70:A:GLU:HG3	18	0.12
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	5	0.12
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	6	0.12
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	7	0.12
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	20	0.12
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	1	0.12
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	13	0.12
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	19	0.12
(2,706)	1:58:A:PRO:HA	1:58:A:PRO:HG3	6	0.12
(2,706)	1:58:A:PRO:HA	1:58:A:PRO:HG3	15	0.12
(2,696)	1:38:A:PRO:HD3	1:37:A:LYS:HB3	3	0.12
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB1	8	0.12
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,623)	1:31:A:LEU:HA	1:30:A:ALA:HB3	8	0.12
(2,610)	1:30:A:ALA:HA	1:33:A:TYR:H	10	0.12
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	12	0.12
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	12	0.12
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	12	0.12
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	14	0.12
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	14	0.12
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	14	0.12
(2,590)	1:29:A:ALA:HB1	1:48:A:ILE:HG13	7	0.12
(2,590)	1:29:A:ALA:HB2	1:48:A:ILE:HG13	7	0.12
(2,590)	1:29:A:ALA:HB3	1:48:A:ILE:HG13	7	0.12
(2,579)	1:28:A:LYS:HB3	1:29:A:ALA:HA	8	0.12
(2,579)	1:28:A:LYS:HB3	1:29:A:ALA:HA	10	0.12
(2,579)	1:28:A:LYS:HB3	1:29:A:ALA:HA	18	0.12
(2,563)	1:28:A:LYS:HA	1:32:A:LYS:H	1	0.12
(2,557)	1:73:A:ARG:HG3	1:73:A:ARG:HA	7	0.12
(2,513)	1:26:A:TYR:HA	1:30:A:ALA:H	2	0.12
(2,456)	1:20:A:GLN:HA	1:23:A:LYS:HD2	14	0.12
(2,454)	1:23:A:LYS:H	1:23:A:LYS:HB3	11	0.12
(2,393)	1:21:A:GLU:H	1:21:A:GLU:HG2	16	0.12
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	6	0.12
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	7	0.12
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	7	0.12
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	9	0.12
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	17	0.12
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	18	0.12
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	19	0.12
(2,368)	1:21:A:GLU:H	1:20:A:GLN:HG2	18	0.12
(2,330)	1:26:A:TYR:HD1	1:23:A:LYS:HA	19	0.12
(2,330)	1:26:A:TYR:HD2	1:23:A:LYS:HA	19	0.12
(2,311)	1:18:A:ASN:HA	1:20:A:GLN:H	18	0.12
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB1	15	0.12
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB2	15	0.12
(2,302)	1:22:A:LEU:HD11	1:17:A:ALA:HB3	15	0.12
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB1	15	0.12
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB2	15	0.12
(2,302)	1:22:A:LEU:HD12	1:17:A:ALA:HB3	15	0.12
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB1	15	0.12
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB2	15	0.12
(2,302)	1:22:A:LEU:HD13	1:17:A:ALA:HB3	15	0.12
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	4	0.12
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	8	0.12
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	16	0.12
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	18	0.12
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	19	0.12
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	6	0.12
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD11	8	0.12
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD12	8	0.12
(2,205)	1:52:A:PHE:H	1:11:A:LEU:HD13	8	0.12
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD11	4	0.12
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD12	4	0.12
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD13	4	0.12
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD11	14	0.12
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD12	14	0.12
(2,204)	1:53:A:GLU:H	1:11:A:LEU:HD13	14	0.12
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	12	0.12
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	12	0.12
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	12	0.12
(2,136)	1:8:A:TYR:HB3	1:15:A:PRO:HD2	16	0.12
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD1	5	0.12
(2,65)	1:5:A:THR:HA	1:8:A:TYR:HD2	5	0.12
(2,22)	1:2:A:VAL:HA	1:3:A:LYS:H	9	0.12
(1,435)	1:47:A:GLU:HG3	1:47:A:GLU:HA	18	0.12
(1,429)	1:6:A:LYS:HG3	1:7:A:LEU:H	11	0.12
(1,381)	1:22:A:LEU:H	1:20:A:GLN:H	13	0.12
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	5	0.12
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	7	0.12
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	10	0.12
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	11	0.12
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	13	0.12
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	15	0.12
(1,338)	1:48:A:ILE:HA	1:50:A:GLU:H	12	0.12
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD21	8	0.12
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD22	8	0.12
(1,295)	1:31:A:LEU:H	1:31:A:LEU:HD23	8	0.12
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	9	0.12
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	20	0.12
(1,250)	1:51:A:ALA:HB1	1:10:A:LEU:H	12	0.12
(1,250)	1:51:A:ALA:HB2	1:10:A:LEU:H	12	0.12
(1,250)	1:51:A:ALA:HB3	1:10:A:LEU:H	12	0.12
(1,249)	1:23:A:LYS:HE2	1:23:A:LYS:HG2	16	0.12
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	9	0.12
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	19	0.12
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	3	0.12
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	9	0.12
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	14	0.12
(1,142)	1:23:A:LYS:H	1:20:A:GLN:HA	4	0.12
(1,103)	1:59:A:GLN:HA	1:59:A:GLN:HG3	2	0.12
(1,99)	1:59:A:GLN:H	1:61:A:ARG:HB3	16	0.12
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	18	0.12
(1,86)	1:62:A:GLU:H	1:60:A:LYS:H	15	0.12
(1,61)	1:27:A:ARG:H	1:24:A:LYS:HA	3	0.12
(1,47)	1:2:A:VAL:HB	1:65:A:ASP:H	4	0.12
(1,20)	1:4:A:GLU:HG3	1:3:A:LYS:HG3	9	0.12
(2,2425)	1:8:A:TYR:HB2	1:15:A:PRO:HD2	14	0.11
(2,2408)	1:24:A:LYS:HB3	1:24:A:LYS:H	12	0.11
(2,2331)	1:26:A:TYR:HD1	1:48:A:ILE:HG21	16	0.11
(2,2331)	1:26:A:TYR:HD1	1:48:A:ILE:HG22	16	0.11
(2,2331)	1:26:A:TYR:HD1	1:48:A:ILE:HG23	16	0.11
(2,2331)	1:26:A:TYR:HD2	1:48:A:ILE:HG21	16	0.11
(2,2331)	1:26:A:TYR:HD2	1:48:A:ILE:HG22	16	0.11
(2,2331)	1:26:A:TYR:HD2	1:48:A:ILE:HG23	16	0.11
(2,2248)	1:77:A:PRO:HD3	1:76:A:GLY:H	5	0.11
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	1	0.11
(2,2236)	1:74:A:SER:H	1:75:A:GLY:HA3	16	0.11
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	8	0.11
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	16	0.11
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	9	0.11
(2,2152)	1:64:A:TYR:HB3	1:68:A:GLY:H	17	0.11
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	2	0.11
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	4	0.11
(2,2120)	1:64:A:TYR:HB2	1:66:A:GLN:H	16	0.11
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	7	0.11
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	7	0.11
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	7	0.11
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	12	0.11
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	12	0.11
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	1	0.11
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	5	0.11
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	12	0.11
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	15	0.11
(2,2063)	1:62:A:GLU:H	1:63:A:ILE:HG12	8	0.11
(2,1971)	1:55:A:LEU:H	1:56:A:ASN:HB2	20	0.11
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	4	0.11
(2,1968)	1:55:A:LEU:H	1:56:A:ASN:HB3	17	0.11
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	1	0.11
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	2	0.11
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	4	0.11
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	5	0.11
(2,1954)	1:54:A:ILE:HG12	1:54:A:ILE:H	19	0.11
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE1	2	0.11
(2,1947)	1:53:A:GLU:H	1:52:A:PHE:HE2	2	0.11
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	12	0.11
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD11	4	0.11
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD12	4	0.11
(2,1924)	1:52:A:PHE:H	1:54:A:ILE:HD13	4	0.11
(2,1809)	1:39:A:THR:H	1:38:A:PRO:HD3	5	0.11
(2,1729)	1:28:A:LYS:HB3	1:28:A:LYS:H	8	0.11
(2,1729)	1:28:A:LYS:HB2	1:28:A:LYS:H	20	0.11
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	15	0.11
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	17	0.11
(2,1718)	1:27:A:ARG:H	1:27:A:ARG:HG2	19	0.11
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	8	0.11
(2,1688)	1:24:A:LYS:HA	1:24:A:LYS:H	9	0.11
(2,1677)	1:23:A:LYS:H	1:23:A:LYS:HE2	15	0.11
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	1	0.11
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	4	0.11
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	6	0.11
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	16	0.11
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	17	0.11
(2,1663)	1:22:A:LEU:H	1:22:A:LEU:HB3	19	0.11
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	8	0.11
(2,1658)	1:17:A:ALA:HA	1:21:A:GLU:H	16	0.11
(2,1612)	1:15:A:PRO:HD3	1:17:A:ALA:H	5	0.11
(2,1604)	1:16:A:SER:H	1:17:A:ALA:H	8	0.11
(2,1604)	1:16:A:SER:H	1:17:A:ALA:H	15	0.11
(2,1603)	1:15:A:PRO:HG3	1:16:A:SER:H	16	0.11
(2,1597)	1:16:A:SER:H	1:16:A:SER:HB3	2	0.11
(2,1580)	1:13:A:VAL:HG11	1:14:A:SER:H	9	0.11
(2,1580)	1:13:A:VAL:HG12	1:14:A:SER:H	9	0.11
(2,1580)	1:13:A:VAL:HG13	1:14:A:SER:H	9	0.11
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	11	0.11
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	15	0.11
(2,1574)	1:11:A:LEU:H	1:13:A:VAL:H	17	0.11
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	13	0.11
(2,1514)	1:9:A:ASP:H	1:11:A:LEU:H	15	0.11
(2,1508)	1:8:A:TYR:HB3	1:9:A:ASP:H	2	0.11
(2,1490)	1:8:A:TYR:H	1:15:A:PRO:HA	1	0.11
(2,1437)	1:2:A:VAL:H	1:3:A:LYS:H	10	0.11
(2,1377)	1:79:A:PHE:HA	1:79:A:PHE:HB2	9	0.11
(2,1314)	1:74:A:SER:HA	1:75:A:GLY:H	16	0.11
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB1	8	0.11
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB2	8	0.11
(2,1288)	1:72:A:ALA:HB1	1:71:A:ALA:HB3	8	0.11
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB1	8	0.11
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB2	8	0.11
(2,1288)	1:72:A:ALA:HB2	1:71:A:ALA:HB3	8	0.11
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB1	8	0.11
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB2	8	0.11
(2,1288)	1:72:A:ALA:HB3	1:71:A:ALA:HB3	8	0.11
(2,1266)	1:63:A:ILE:HG21	1:71:A:ALA:HA	14	0.11
(2,1266)	1:63:A:ILE:HG22	1:71:A:ALA:HA	14	0.11
(2,1266)	1:63:A:ILE:HG23	1:71:A:ALA:HA	14	0.11
(2,1264)	1:43:A:GLU:H	1:43:A:GLU:HG2	15	0.11
(2,1261)	1:70:A:GLU:HA	1:70:A:GLU:HG3	17	0.11
(2,1258)	1:19:A:GLU:HB3	1:19:A:GLU:HG2	17	0.11
(2,1253)	1:70:A:GLU:HA	1:73:A:ARG:HD2	18	0.11
(2,1235)	1:68:A:GLY:HA2	1:70:A:GLU:HB2	19	0.11
(2,1216)	1:67:A:TYR:HD1	1:67:A:TYR:HA	15	0.11
(2,1216)	1:67:A:TYR:HD2	1:67:A:TYR:HA	15	0.11
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	9	0.11
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	9	0.11
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD1	17	0.11
(2,1212)	1:66:A:GLN:HB2	1:67:A:TYR:HD2	17	0.11
(2,1194)	1:2:A:VAL:HG21	1:65:A:ASP:HB2	4	0.11
(2,1194)	1:2:A:VAL:HG22	1:65:A:ASP:HB2	4	0.11
(2,1194)	1:2:A:VAL:HG23	1:65:A:ASP:HB2	4	0.11
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	1	0.11
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	4	0.11
(2,1116)	1:64:A:TYR:HB2	1:61:A:ARG:HA	8	0.11
(2,1092)	1:60:A:LYS:HB3	1:57:A:ASP:HB3	9	0.11
(2,1066)	1:15:A:PRO:HD2	1:14:A:SER:HA	6	0.11
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	3	0.11
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	7	0.11
(2,1059)	1:58:A:PRO:HA	1:60:A:LYS:H	10	0.11
(2,1012)	1:61:A:ARG:HB2	1:55:A:LEU:HA	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	2	0.11
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	1	0.11
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	1	0.11
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	5	0.11
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	5	0.11
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	8	0.11
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	8	0.11
(2,879)	1:50:A:GLU:HA	1:50:A:GLU:HG2	3	0.11
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD1	3	0.11
(2,866)	1:48:A:ILE:HG21	1:33:A:TYR:HD2	3	0.11
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD1	3	0.11
(2,866)	1:48:A:ILE:HG22	1:33:A:TYR:HD2	3	0.11
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD1	3	0.11
(2,866)	1:48:A:ILE:HG23	1:33:A:TYR:HD2	3	0.11
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG21	13	0.11
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG22	13	0.11
(2,865)	1:26:A:TYR:HE1	1:48:A:ILE:HG23	13	0.11
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG21	13	0.11
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG22	13	0.11
(2,865)	1:26:A:TYR:HE2	1:48:A:ILE:HG23	13	0.11
(2,852)	1:48:A:ILE:HB	1:45:A:PHE:HA	8	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	1	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	2	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	3	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	4	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	5	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	6	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	7	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	9	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	10	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	11	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	13	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	14	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	15	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	16	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	18	0.11
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	19	0.11
(2,761)	1:47:A:GLU:HG2	1:52:A:PHE:H	18	0.11
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	4	0.11
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	14	0.11
(2,745)	1:43:A:GLU:HG2	1:43:A:GLU:HB3	18	0.11
(2,734)	1:46:A:LYS:H	1:42:A:THR:HA	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	7	0.11
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	8	0.11
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	16	0.11
(2,713)	1:40:A:GLY:HA2	1:41:A:ASP:H	18	0.11
(2,610)	1:30:A:ALA:HA	1:33:A:TYR:H	3	0.11
(2,610)	1:30:A:ALA:HA	1:33:A:TYR:H	7	0.11
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	15	0.11
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	15	0.11
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	15	0.11
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	18	0.11
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	18	0.11
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	18	0.11
(2,604)	1:29:A:ALA:HB1	1:30:A:ALA:HA	19	0.11
(2,604)	1:29:A:ALA:HB2	1:30:A:ALA:HA	19	0.11
(2,604)	1:29:A:ALA:HB3	1:30:A:ALA:HA	19	0.11
(2,601)	1:48:A:ILE:HG21	1:30:A:ALA:HA	5	0.11
(2,601)	1:48:A:ILE:HG22	1:30:A:ALA:HA	5	0.11
(2,601)	1:48:A:ILE:HG23	1:30:A:ALA:HA	5	0.11
(2,573)	1:29:A:ALA:H	1:28:A:LYS:HG3	1	0.11
(2,557)	1:73:A:ARG:HG3	1:73:A:ARG:HA	5	0.11
(2,536)	1:29:A:ALA:H	1:27:A:ARG:HA	3	0.11
(2,536)	1:29:A:ALA:H	1:27:A:ARG:HA	7	0.11
(2,536)	1:29:A:ALA:H	1:27:A:ARG:HA	12	0.11
(2,468)	1:60:A:LYS:HA	1:60:A:LYS:HG3	13	0.11
(2,457)	1:23:A:LYS:H	1:23:A:LYS:HD2	6	0.11
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	1	0.11
(2,390)	1:17:A:ALA:HB1	1:21:A:GLU:HG2	9	0.11
(2,390)	1:17:A:ALA:HB2	1:21:A:GLU:HG2	9	0.11
(2,390)	1:17:A:ALA:HB3	1:21:A:GLU:HG2	9	0.11
(2,387)	1:18:A:ASN:H	1:21:A:GLU:HB3	1	0.11
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	1	0.11
(2,386)	1:21:A:GLU:HB3	1:21:A:GLU:H	12	0.11
(2,350)	1:72:A:ALA:HB1	1:69:A:LEU:HA	7	0.11
(2,350)	1:72:A:ALA:HB2	1:69:A:LEU:HA	7	0.11
(2,350)	1:72:A:ALA:HB3	1:69:A:LEU:HA	7	0.11
(2,331)	1:26:A:TYR:HE1	1:23:A:LYS:HA	17	0.11
(2,331)	1:26:A:TYR:HE2	1:23:A:LYS:HA	17	0.11
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	19	0.11
(2,309)	1:17:A:ALA:HA	1:18:A:ASN:HA	3	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	4	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	4	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	4	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	4	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	4	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	4	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	4	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	4	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	10	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	10	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	10	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	10	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	10	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	10	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	10	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	10	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	10	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	14	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	14	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	14	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	14	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	14	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	14	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	14	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	14	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	14	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB1	19	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB2	19	0.11
(2,300)	1:13:A:VAL:HG11	1:17:A:ALA:HB3	19	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB1	19	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB2	19	0.11
(2,300)	1:13:A:VAL:HG12	1:17:A:ALA:HB3	19	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB1	19	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB2	19	0.11
(2,300)	1:13:A:VAL:HG13	1:17:A:ALA:HB3	19	0.11
(2,277)	1:16:A:SER:HA	1:17:A:ALA:H	13	0.11
(2,258)	1:15:A:PRO:HD3	1:14:A:SER:HB2	14	0.11
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	1	0.11
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	2	0.11
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	9	0.11
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	13	0.11
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	15	0.11
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	17	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	4	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	5	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	8	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	11	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	15	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	17	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	18	0.11
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	20	0.11
(2,224)	1:13:A:VAL:HA	1:14:A:SER:H	18	0.11
(2,224)	1:13:A:VAL:HA	1:14:A:SER:H	20	0.11
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB1	5	0.11
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB2	5	0.11
(2,221)	1:13:A:VAL:HA	1:17:A:ALA:HB3	5	0.11
(2,181)	1:7:A:LEU:HD21	1:10:A:LEU:HB3	15	0.11
(2,181)	1:7:A:LEU:HD22	1:10:A:LEU:HB3	15	0.11
(2,181)	1:7:A:LEU:HD23	1:10:A:LEU:HB3	15	0.11
(2,176)	1:11:A:LEU:HB2	1:10:A:LEU:HB2	13	0.11
(2,101)	1:7:A:LEU:HA	1:11:A:LEU:HB2	15	0.11
(2,22)	1:2:A:VAL:HA	1:3:A:LYS:H	17	0.11
(2,14)	1:2:A:VAL:HA	1:4:A:GLU:HG3	12	0.11
(1,456)	1:0:A:THR:HB	1:1:A:SER:H	20	0.11
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	9	0.11
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	13	0.11
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG21	14	0.11
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG22	14	0.11
(1,422)	1:26:A:TYR:HB2	1:48:A:ILE:HG23	14	0.11
(1,415)	1:53:A:GLU:HG2	1:53:A:GLU:H	16	0.11
(1,378)	1:59:A:GLN:H	1:58:A:PRO:HB2	10	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	1	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	2	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	3	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	6	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	9	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	12	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	17	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	19	0.11
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	20	0.11
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	1	0.11
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	20	0.11
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB1	11	0.11
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB2	11	0.11
(1,289)	1:26:A:TYR:HA	1:29:A:ALA:HB3	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:20:A:GLN:H	1:23:A:LYS:HD3	4	0.11
(1,278)	1:1:A:SER:H	1:1:A:SER:HB3	8	0.11
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	10	0.11
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	13	0.11
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	3	0.11
(1,261)	1:47:A:GLU:HB3	1:47:A:GLU:HG2	19	0.11
(1,250)	1:72:A:ALA:HB1	1:71:A:ALA:H	4	0.11
(1,250)	1:72:A:ALA:HB2	1:71:A:ALA:H	4	0.11
(1,250)	1:72:A:ALA:HB3	1:71:A:ALA:H	4	0.11
(1,246)	1:60:A:LYS:HE3	1:60:A:LYS:HB2	16	0.11
(1,223)	1:15:A:PRO:HA	1:17:A:ALA:H	14	0.11
(1,215)	1:28:A:LYS:HA	1:28:A:LYS:H	16	0.11
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	2	0.11
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	3	0.11
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	14	0.11
(1,197)	1:34:A:HIS:H	1:34:A:HIS:HA	16	0.11
(1,196)	1:62:A:GLU:HG2	1:63:A:ILE:H	4	0.11
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	2	0.11
(1,155)	1:66:A:GLN:HA	1:66:A:GLN:HG3	5	0.11
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD11	5	0.11
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD12	5	0.11
(1,152)	1:45:A:PHE:HE1	1:48:A:ILE:HD13	5	0.11
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD11	5	0.11
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD12	5	0.11
(1,152)	1:45:A:PHE:HE2	1:48:A:ILE:HD13	5	0.11
(1,114)	1:24:A:LYS:HA	1:25:A:GLY:H	5	0.11
(1,114)	1:24:A:LYS:HA	1:25:A:GLY:H	8	0.11
(1,103)	1:62:A:GLU:HA	1:62:A:GLU:HG2	13	0.11
(1,91)	1:11:A:LEU:HB3	1:26:A:TYR:H	13	0.11
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	7	0.11
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	7	0.11
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	7	0.11
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	3	0.1
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	3	0.1
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	3	0.1
(2,2391)	1:48:A:ILE:HD11	1:49:A:SER:H	20	0.1
(2,2391)	1:48:A:ILE:HD12	1:49:A:SER:H	20	0.1
(2,2391)	1:48:A:ILE:HD13	1:49:A:SER:H	20	0.1
(2,2356)	1:64:A:TYR:HE1	1:69:A:LEU:HB2	7	0.1
(2,2356)	1:64:A:TYR:HE2	1:69:A:LEU:HB2	7	0.1
(2,2309)	1:45:A:PHE:HD1	1:46:A:LYS:HB2	18	0.1
(2,2309)	1:45:A:PHE:HD2	1:46:A:LYS:HB2	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2259)	1:77:A:PRO:HD2	1:78:A:SER:H	15	0.1
(2,2257)	1:77:A:PRO:HB3	1:78:A:SER:H	16	0.1
(2,2243)	1:40:A:GLY:H	1:37:A:LYS:HE3	12	0.1
(2,2241)	1:71:A:ALA:H	1:74:A:SER:H	9	0.1
(2,2211)	1:64:A:TYR:HE1	1:72:A:ALA:H	2	0.1
(2,2211)	1:64:A:TYR:HE2	1:72:A:ALA:H	2	0.1
(2,2207)	1:60:A:LYS:H	1:60:A:LYS:HD3	4	0.1
(2,2195)	1:71:A:ALA:H	1:70:A:GLU:HG3	2	0.1
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB1	6	0.1
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB2	6	0.1
(2,2174)	1:70:A:GLU:H	1:71:A:ALA:HB3	6	0.1
(2,2113)	1:63:A:ILE:HG21	1:66:A:GLN:H	4	0.1
(2,2113)	1:63:A:ILE:HG22	1:66:A:GLN:H	4	0.1
(2,2113)	1:63:A:ILE:HG23	1:66:A:GLN:H	4	0.1
(2,2112)	1:64:A:TYR:HE1	1:65:A:ASP:H	19	0.1
(2,2112)	1:64:A:TYR:HE2	1:65:A:ASP:H	19	0.1
(2,2095)	1:64:A:TYR:H	1:63:A:ILE:HG12	7	0.1
(2,2094)	1:63:A:ILE:HG21	1:64:A:TYR:H	1	0.1
(2,2094)	1:63:A:ILE:HG22	1:64:A:TYR:H	1	0.1
(2,2094)	1:63:A:ILE:HG23	1:64:A:TYR:H	1	0.1
(2,2085)	1:64:A:TYR:HB3	1:63:A:ILE:H	15	0.1
(2,2048)	1:60:A:LYS:HB3	1:61:A:ARG:H	18	0.1
(2,2013)	1:57:A:ASP:H	1:61:A:ARG:H	8	0.1
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	8	0.1
(2,1970)	1:54:A:ILE:HG13	1:55:A:LEU:H	9	0.1
(2,1968)	1:55:A:LEU:H	1:56:A:ASN:HB3	12	0.1
(2,1943)	1:53:A:GLU:H	1:52:A:PHE:HB2	9	0.1
(2,1903)	1:51:A:ALA:HB1	1:50:A:GLU:H	10	0.1
(2,1903)	1:51:A:ALA:HB2	1:50:A:GLU:H	10	0.1
(2,1903)	1:51:A:ALA:HB3	1:50:A:GLU:H	10	0.1
(2,1795)	1:34:A:HIS:HB3	1:34:A:HIS:H	8	0.1
(2,1782)	1:29:A:ALA:HB1	1:33:A:TYR:H	20	0.1
(2,1782)	1:29:A:ALA:HB2	1:33:A:TYR:H	20	0.1
(2,1782)	1:29:A:ALA:HB3	1:33:A:TYR:H	20	0.1
(2,1682)	1:44:A:LYS:HD3	1:44:A:LYS:H	5	0.1
(2,1603)	1:15:A:PRO:HG3	1:16:A:SER:H	9	0.1
(2,1540)	1:11:A:LEU:H	1:52:A:PHE:HA	12	0.1
(2,1538)	1:10:A:LEU:HB3	1:11:A:LEU:H	9	0.1
(2,1531)	1:7:A:LEU:HD21	1:10:A:LEU:H	16	0.1
(2,1531)	1:7:A:LEU:HD22	1:10:A:LEU:H	16	0.1
(2,1531)	1:7:A:LEU:HD23	1:10:A:LEU:H	16	0.1
(2,1497)	1:8:A:TYR:H	1:9:A:ASP:HA	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1465)	1:5:A:THR:H	1:6:A:LYS:H	9	0.1
(2,1312)	1:74:A:SER:HB2	1:74:A:SER:HA	17	0.1
(2,1289)	1:72:A:ALA:HB1	1:64:A:TYR:HB3	12	0.1
(2,1289)	1:72:A:ALA:HB2	1:64:A:TYR:HB3	12	0.1
(2,1289)	1:72:A:ALA:HB3	1:64:A:TYR:HB3	12	0.1
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	2	0.1
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	2	0.1
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	2	0.1
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB1	3	0.1
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB2	3	0.1
(2,1281)	1:72:A:ALA:HA	1:71:A:ALA:HB3	3	0.1
(2,1280)	1:63:A:ILE:HG21	1:72:A:ALA:HA	14	0.1
(2,1280)	1:63:A:ILE:HG22	1:72:A:ALA:HA	14	0.1
(2,1280)	1:63:A:ILE:HG23	1:72:A:ALA:HA	14	0.1
(2,1217)	1:63:A:ILE:HG21	1:67:A:TYR:HB3	1	0.1
(2,1217)	1:63:A:ILE:HG22	1:67:A:TYR:HB3	1	0.1
(2,1217)	1:63:A:ILE:HG23	1:67:A:TYR:HB3	1	0.1
(2,1126)	1:62:A:GLU:HA	1:62:A:GLU:HG2	18	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	1	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	2	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	3	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	5	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	6	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	7	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	9	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	10	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	11	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	12	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	13	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	14	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	15	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	16	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	17	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	18	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	19	0.1
(2,1080)	1:59:A:GLN:HG3	1:59:A:GLN:HG2	20	0.1
(2,1068)	1:15:A:PRO:HD2	1:14:A:SER:H	14	0.1
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	14	0.1
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	18	0.1
(2,945)	1:54:A:ILE:HA	1:53:A:GLU:HB3	19	0.1
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	11	0.1
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE1	17	0.1
(2,921)	1:52:A:PHE:HB3	1:52:A:PHE:HE2	17	0.1
(2,815)	1:46:A:LYS:H	1:46:A:LYS:HA	8	0.1
(2,806)	1:45:A:PHE:HB2	1:33:A:TYR:HB3	16	0.1
(2,805)	1:45:A:PHE:HB3	1:33:A:TYR:HB3	15	0.1
(2,748)	1:70:A:GLU:HG3	1:69:A:LEU:HB2	1	0.1
(2,579)	1:28:A:LYS:HB3	1:29:A:ALA:HA	7	0.1
(2,449)	1:23:A:LYS:HB3	1:23:A:LYS:HD2	13	0.1
(2,327)	1:19:A:GLU:HA	1:19:A:GLU:HG2	1	0.1
(2,271)	1:70:A:GLU:HB3	1:71:A:ALA:H	2	0.1
(2,255)	1:15:A:PRO:HD3	1:15:A:PRO:HB2	6	0.1
(2,236)	1:15:A:PRO:HA	1:15:A:PRO:HB2	7	0.1
(2,185)	1:7:A:LEU:HA	1:10:A:LEU:HB3	12	0.1
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD11	18	0.1
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD12	18	0.1
(2,163)	1:47:A:GLU:HB2	1:10:A:LEU:HD13	18	0.1
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	14	0.1
(1,465)	1:38:A:PRO:HA	1:38:A:PRO:HB2	18	0.1
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	1	0.1
(1,437)	1:23:A:LYS:HA	1:23:A:LYS:HB3	18	0.1
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD21	5	0.1
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD22	5	0.1
(1,412)	1:10:A:LEU:H	1:10:A:LEU:HD23	5	0.1
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	10	0.1
(1,375)	1:47:A:GLU:HA	1:50:A:GLU:H	11	0.1
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	14	0.1
(1,353)	1:29:A:ALA:H	1:29:A:ALA:HA	16	0.1
(1,339)	1:31:A:LEU:H	1:33:A:TYR:H	17	0.1
(1,326)	1:78:A:SER:HA	1:79:A:PHE:H	3	0.1
(1,321)	1:55:A:LEU:HB2	1:52:A:PHE:HA	7	0.1
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	10	0.1
(1,317)	1:47:A:GLU:HA	1:50:A:GLU:H	11	0.1
(1,269)	1:45:A:PHE:HA	1:47:A:GLU:H	12	0.1
(1,215)	1:28:A:LYS:HA	1:28:A:LYS:H	1	0.1
(1,215)	1:28:A:LYS:HA	1:28:A:LYS:H	14	0.1
(1,197)	1:34:A:HIS:H	1:34:A:HIS:HA	11	0.1
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	12	0.1
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	18	0.1
(1,197)	1:47:A:GLU:HA	1:47:A:GLU:H	19	0.1
(1,179)	1:20:A:GLN:H	1:21:A:GLU:HG3	11	0.1
(1,172)	1:59:A:GLN:HA	1:59:A:GLN:HB3	11	0.1
(1,121)	1:64:A:TYR:HD1	1:65:A:ASP:H	15	0.1

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<b>Key</b>	<b>Atom-1</b>	<b>Atom-2</b>	<b>Model ID</b>	<b>Violation (Å)</b>
(1,121)	1:64:A:TYR:HD2	1:65:A:ASP:H	15	0.1
(1,114)	1:24:A:LYS:HA	1:25:A:GLY:H	3	0.1
(1,113)	1:58:A:PRO:HB3	1:58:A:PRO:HG2	19	0.1
(1,98)	1:14:A:SER:H	1:21:A:GLU:HB2	3	0.1
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB1	1	0.1
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB2	1	0.1
(1,22)	1:70:A:GLU:HB2	1:71:A:ALA:HB3	1	0.1
(1,8)	1:43:A:GLU:HA	1:43:A:GLU:HG2	2	0.1

## 10 Dihedral-angle violation analysis

No dihedral-angle restraints found