



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 8E22  
BMRB ID : 31039  
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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

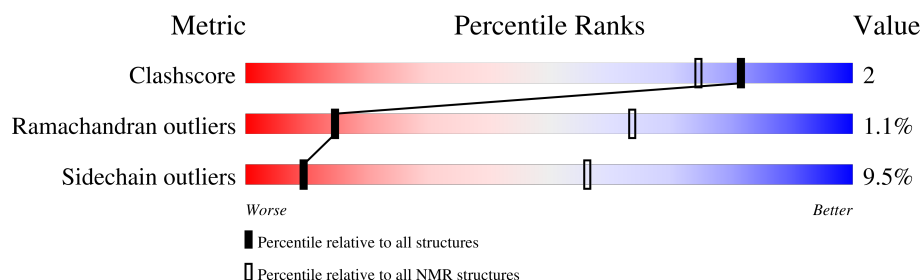
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	X	128	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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	X:25-X:130 (106)	0.46	1

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

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

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

Cluster number	Models
1	1, 3, 4, 7, 8, 9
2	5, 10
3	2, 6

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

There is only 1 type of molecule in this entry. The entry contains 2072 atoms, of which 1044 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vacuolar protein sorting-associated protein 37A.

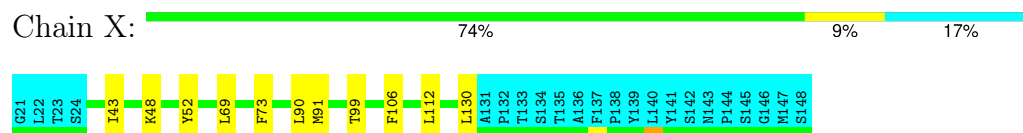
Mol	Chain	Residues	Atoms						Trace
1	X	128	Total	C	H	N	O	S	0
			2072	662	1044	173	190	3	

## 4 Residue-property plots

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

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

- Molecule 1: Vacuolar protein sorting-associated protein 37A

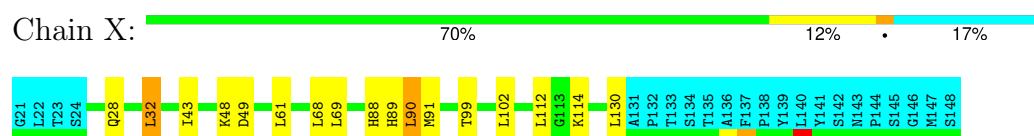


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

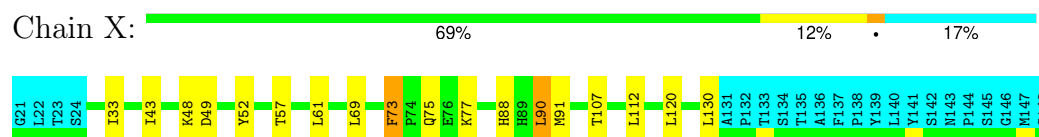
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Vacuolar protein sorting-associated protein 37A



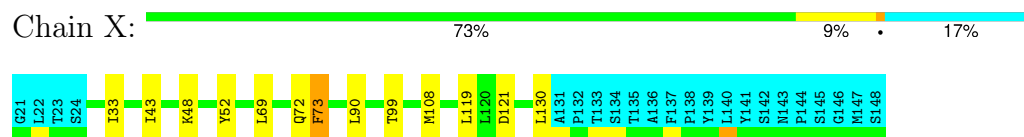
#### 4.2.2 Score per residue for model 2

- Molecule 1: Vacuolar protein sorting-associated protein 37A



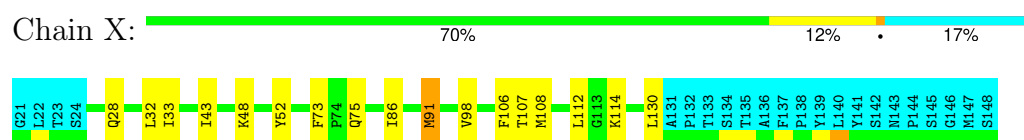
### 4.2.3 Score per residue for model 3

- Molecule 1: Vacuolar protein sorting-associated protein 37A



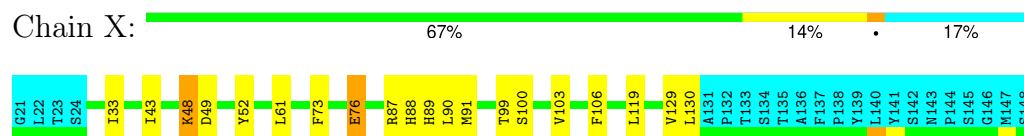
### 4.2.4 Score per residue for model 4

- Molecule 1: Vacuolar protein sorting-associated protein 37A



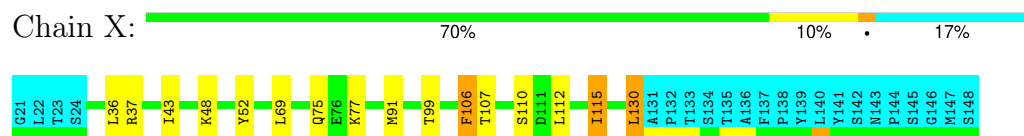
### 4.2.5 Score per residue for model 5

- Molecule 1: Vacuolar protein sorting-associated protein 37A



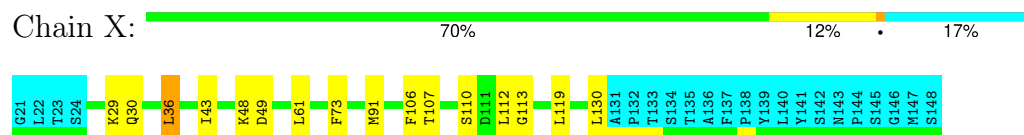
### 4.2.6 Score per residue for model 6

- Molecule 1: Vacuolar protein sorting-associated protein 37A



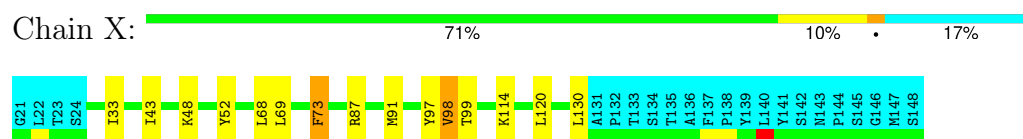
### 4.2.7 Score per residue for model 7

- Molecule 1: Vacuolar protein sorting-associated protein 37A



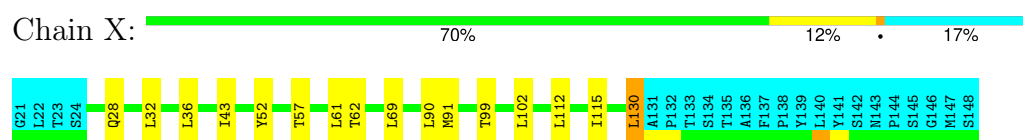
### 4.2.8 Score per residue for model 8

- Molecule 1: Vacuolar protein sorting-associated protein 37A



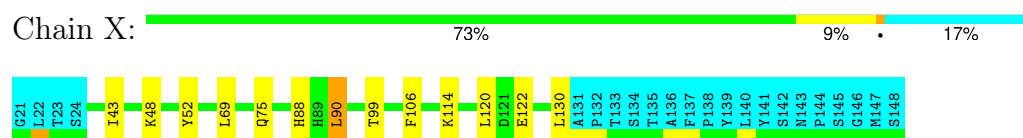
### 4.2.9 Score per residue for model 9

- Molecule 1: Vacuolar protein sorting-associated protein 37A



### 4.2.10 Score per residue for model 10

- Molecule 1: Vacuolar protein sorting-associated protein 37A



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	
CYANA	structure calculation	

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	1480
Number of shifts mapped to atoms	1480
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%



## 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	X	870	895	891	4±1
All	All	8700	8950	8910	43

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:X:69:LEU:HD23	1:X:73:PHE:CZ	0.58	2.34	2	2
1:X:33:ILE:HG23	1:X:52:TYR:OH	0.56	2.00	8	4
1:X:107:THR:HG22	1:X:110:SER:OG	0.54	2.03	7	2
1:X:68:LEU:C	1:X:69:LEU:HD12	0.53	2.24	8	2
1:X:52:TYR:CE2	1:X:69:LEU:HD11	0.51	2.40	10	3
1:X:90:LEU:HD22	1:X:122:GLU:OE2	0.49	2.07	10	1
1:X:69:LEU:HD23	1:X:73:PHE:CE1	0.48	2.44	3	2
1:X:87:ARG:NH2	1:X:129:VAL:HG11	0.47	2.24	5	1
1:X:99:THR:O	1:X:99:THR:HG23	0.45	2.11	8	2
1:X:36:LEU:HD13	1:X:36:LEU:C	0.45	2.32	6	2
1:X:57:THR:HG22	1:X:62:THR:OG1	0.45	2.11	9	1
1:X:100:SER:O	1:X:103:VAL:HG12	0.44	2.12	5	1
1:X:33:ILE:HD12	1:X:52:TYR:OH	0.44	2.12	3	3
1:X:89:HIS:CE1	1:X:90:LEU:HD11	0.44	2.48	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:28:GLN:O	1:X:32:LEU:HD12	0.43	2.13	1	2
1:X:86:ILE:HD11	1:X:91:MET:HE1	0.43	1.90	4	1
1:X:119:LEU:HD13	1:X:119:LEU:C	0.43	2.34	7	2
1:X:102:LEU:O	1:X:115:ILE:HD12	0.42	2.15	9	1
1:X:69:LEU:HD12	1:X:69:LEU:N	0.42	2.29	1	2
1:X:28:GLN:O	1:X:32:LEU:HD13	0.41	2.15	4	1
1:X:88:HIS:ND1	1:X:90:LEU:HD12	0.41	2.31	2	1
1:X:90:LEU:N	1:X:90:LEU:HD12	0.41	2.31	5	1
1:X:36:LEU:HD22	1:X:113:GLY:HA2	0.40	1.93	7	1
1:X:73:PHE:CD2	1:X:76:GLU:O	0.40	2.75	5	1
1:X:106:PHE:CE2	1:X:115:ILE:HD13	0.40	2.52	6	1
1:X:97:TYR:O	1:X:98:VAL:O	0.40	2.39	8	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	106/128 (83%)	98±1 (93±1%)	6±1 (6±1%)	1±1 (1±1%)	15	64
All	All	1060/1280 (83%)	985 (93%)	63 (6%)	12 (1%)	15	64

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	X	48	LYS	8
1	X	98	VAL	2
1	X	130	LEU	2

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	103/121 (85%)	93±2 (90±2%)	10±2 (10±2%)	9	56
All	All	1030/1210 (85%)	932 (90%)	98 (10%)	9	56

All 31 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	X	43	ILE	10
1	X	130	LEU	10
1	X	91	MET	8
1	X	112	LEU	6
1	X	61	LEU	5
1	X	90	LEU	5
1	X	73	PHE	5
1	X	99	THR	5
1	X	106	PHE	5
1	X	49	ASP	4
1	X	114	LYS	4
1	X	75	GLN	4
1	X	88	HIS	3
1	X	120	LEU	3
1	X	48	LYS	2
1	X	77	LYS	2
1	X	107	THR	2
1	X	108	MET	2
1	X	32	LEU	1
1	X	102	LEU	1
1	X	57	THR	1
1	X	72	GLN	1
1	X	121	ASP	1
1	X	76	GLU	1
1	X	119	LEU	1
1	X	37	ARG	1
1	X	115	ILE	1
1	X	29	LYS	1
1	X	30	GLN	1
1	X	36	LEU	1
1	X	87	ARG	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1480
Number of shifts mapped to atoms	1480
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	128	$-0.36 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	124	$0.14 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	127	$0.18 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	112	$0.01 \pm 0.32$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1273 atoms were assigned a chemical shift out of a possible 1550. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	508/512 (99%)	201/204 (99%)	212/212 (100%)	95/96 (99%)
Sidechain	709/927 (76%)	458/604 (76%)	251/288 (87%)	0/35 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	56/111 (50%)	28/54 (52%)	27/48 (56%)	1/9 (11%)
Overall	1273/1550 (82%)	687/862 (80%)	490/548 (89%)	96/140 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1480 atoms were assigned a chemical shift out of a possible 1804. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	607/618 (98%)	240/247 (97%)	255/256 (100%)	112/115 (97%)
Sidechain	805/1047 (77%)	520/685 (76%)	285/326 (87%)	0/36 (0%)
Aromatic	68/139 (49%)	34/67 (51%)	33/63 (52%)	1/9 (11%)
Overall	1480/1804 (82%)	794/999 (79%)	573/645 (89%)	113/160 (71%)

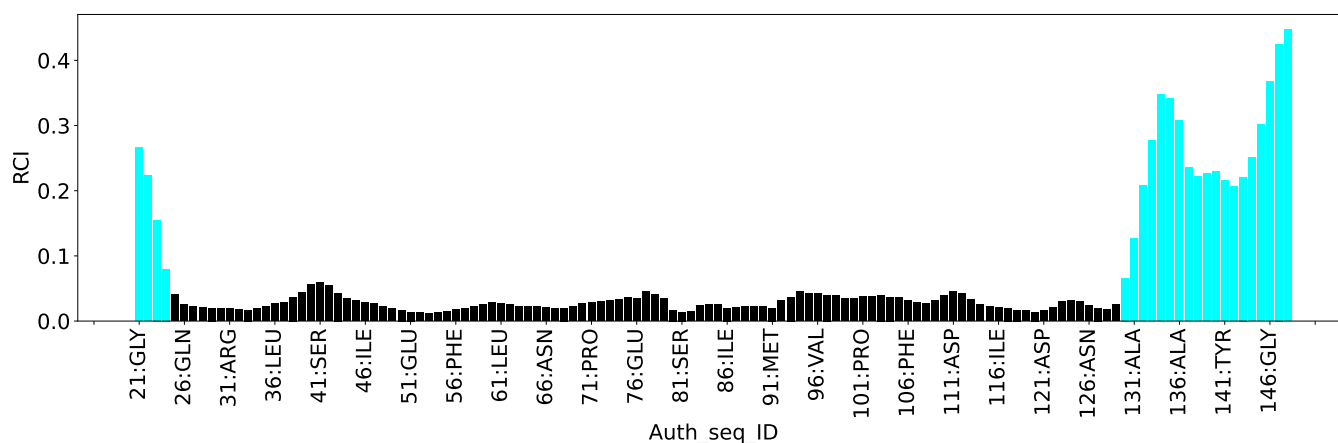
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain X:



## 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	2385
Intra-residue ( $ i-j =0$ )	538
Sequential ( $ i-j =1$ )	666
Medium range ( $ i-j >1$ and $ i-j <5$ )	417
Long range ( $ i-j \geq 5$ )	764
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	194
Number of unmapped restraints	0
Number of restraints per residue	20.1
Number of long range restraints per residue <sup>1</sup>	6.0

<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)	88.8	0.2
0.2-0.5 (Medium)	70.4	0.5
>0.5 (Large)	2.4	0.67

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	9.6	7.69
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None



## 9 Distance violation analysis ⓘ

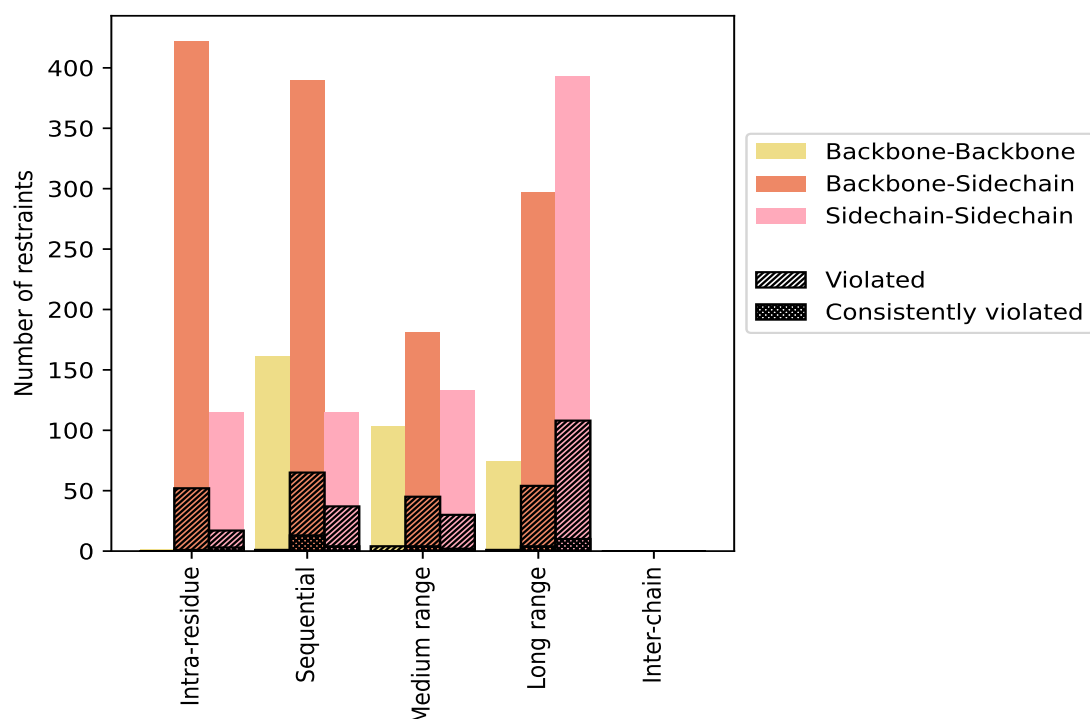
### 9.1 Summary of distance violations ⓘ

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>538</b>	<b>22.6</b>	<b>69</b>	<b>12.8</b>	<b>2.9</b>	<b>4</b>	<b>0.7</b>	<b>0.2</b>
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	422	17.7	52	12.3	2.2	1	0.2	0.0
Sidechain-Sidechain	115	4.8	17	14.8	0.7	3	2.6	0.1
<b>Sequential (<math> i-j =1</math>)</b>	<b>666</b>	<b>27.9</b>	<b>103</b>	<b>15.5</b>	<b>4.3</b>	<b>17</b>	<b>2.6</b>	<b>0.7</b>
Backbone-Backbone	161	6.8	1	0.6	0.0	0	0.0	0.0
Backbone-Sidechain	390	16.4	65	16.7	2.7	13	3.3	0.5
Sidechain-Sidechain	115	4.8	37	32.2	1.6	4	3.5	0.2
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>417</b>	<b>17.5</b>	<b>79</b>	<b>18.9</b>	<b>3.3</b>	<b>6</b>	<b>1.4</b>	<b>0.3</b>
Backbone-Backbone	103	4.3	4	3.9	0.2	0	0.0	0.0
Backbone-Sidechain	181	7.6	45	24.9	1.9	4	2.2	0.2
Sidechain-Sidechain	133	5.6	30	22.6	1.3	2	1.5	0.1
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>764</b>	<b>32.0</b>	<b>163</b>	<b>21.3</b>	<b>6.8</b>	<b>14</b>	<b>1.8</b>	<b>0.6</b>
Backbone-Backbone	74	3.1	1	1.4	0.0	0	0.0	0.0
Backbone-Sidechain	297	12.5	54	18.2	2.3	4	1.3	0.2
Sidechain-Sidechain	393	16.5	108	27.5	4.5	10	2.5	0.4
<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>2385</b>	<b>100.0</b>	<b>414</b>	<b>17.4</b>	<b>17.4</b>	<b>41</b>	<b>1.7</b>	<b>1.7</b>
Backbone-Backbone	339	14.2	6	1.8	0.3	0	0.0	0.0
Backbone-Sidechain	1290	54.1	216	16.7	9.1	22	1.7	0.9
Sidechain-Sidechain	756	31.7	192	25.4	8.1	19	2.5	0.8

<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

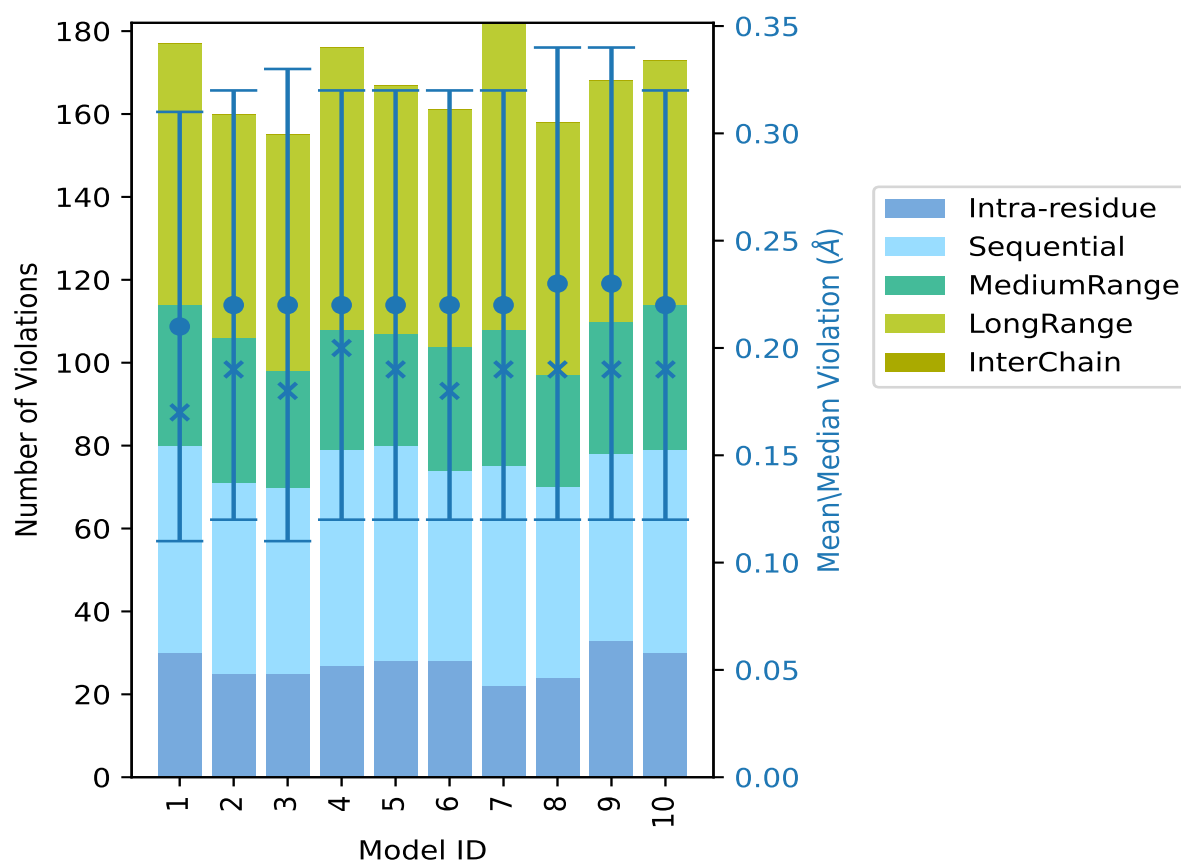
## 9.2 Distance violation statistics for each model [i](#)

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						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>	Total				
1	30	50	34	63	0	177	0.21	0.63	0.1	0.17
2	25	46	35	54	0	160	0.22	0.54	0.1	0.19
3	25	45	28	57	0	155	0.22	0.67	0.11	0.18
4	27	52	29	68	0	176	0.22	0.56	0.1	0.2
5	28	52	27	60	0	167	0.22	0.6	0.1	0.19
6	28	46	30	57	0	161	0.22	0.56	0.1	0.18
7	22	53	33	74	0	182	0.22	0.53	0.1	0.19
8	24	46	27	61	0	158	0.23	0.51	0.11	0.19
9	33	45	32	58	0	168	0.23	0.58	0.11	0.19
10	30	49	35	59	0	173	0.22	0.53	0.1	0.19

<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 [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1971(IR:469, SQ:563, MR:338, LR:601, 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>	%
23	19	24	50	0	116	1	10.0
13	20	6	29	0	68	2	20.0
4	11	12	22	0	49	3	30.0

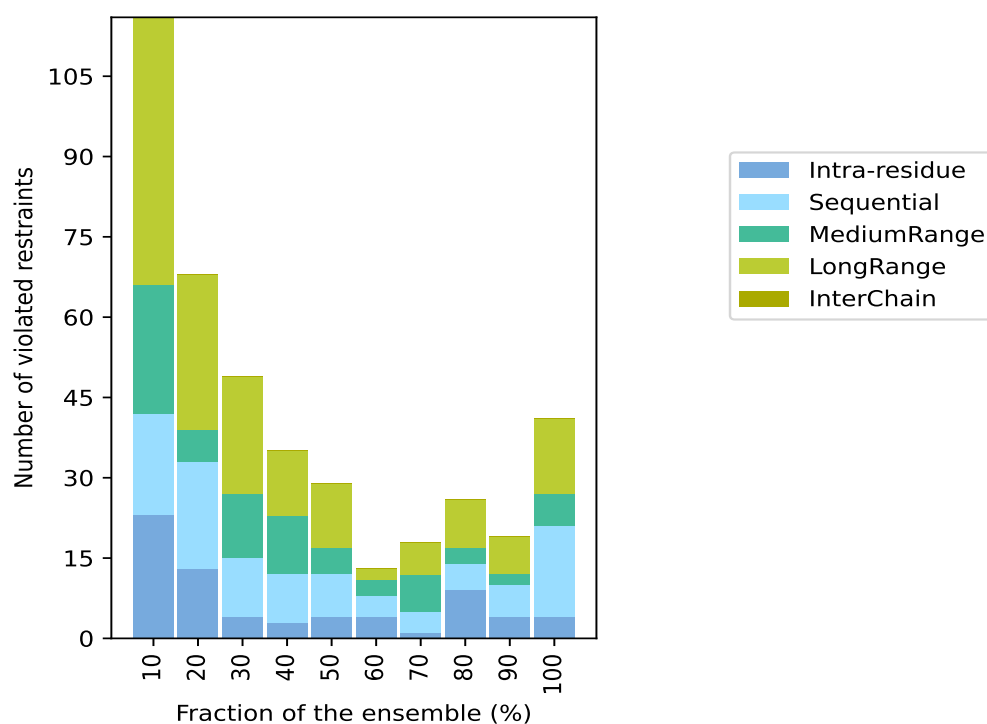
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
3	9	11	12	0	35	4	40.0
4	8	5	12	0	29	5	50.0
4	4	3	2	0	13	6	60.0
1	4	7	6	0	18	7	70.0
9	5	3	9	0	26	8	80.0
4	6	2	7	0	19	9	90.0
4	17	6	14	0	41	10	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 ⓘ

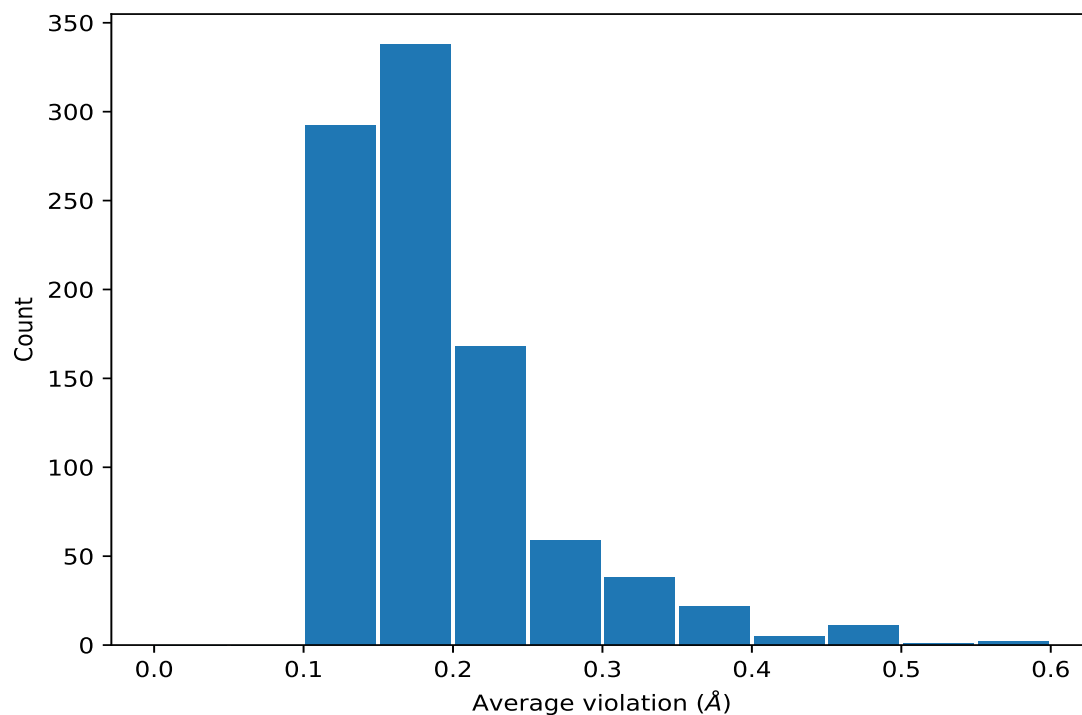


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	10	0.47	0.05	0.46
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	10	0.45	0.03	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	10	0.45	0.03	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	10	0.45	0.03	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	10	0.45	0.03	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	10	0.45	0.03	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	10	0.45	0.03	0.44
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	10	0.43	0.14	0.44
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	10	0.4	0.08	0.42
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	10	0.39	0.07	0.36
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	10	0.37	0.01	0.37
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	10	0.37	0.06	0.34
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	10	0.37	0.03	0.37
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	10	0.36	0.04	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	10	0.36	0.04	0.36

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	10	0.36	0.04	0.36
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	10	0.36	0.04	0.34
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	10	0.34	0.04	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	10	0.34	0.04	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	10	0.34	0.04	0.36
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	10	0.33	0.06	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	10	0.33	0.06	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	10	0.33	0.06	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	10	0.33	0.06	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	10	0.33	0.06	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	10	0.33	0.06	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	10	0.33	0.06	0.34
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	10	0.32	0.11	0.39
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	10	0.32	0.02	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	10	0.32	0.02	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	10	0.32	0.02	0.31
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	10	0.32	0.05	0.32
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	10	0.3	0.03	0.32
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	10	0.29	0.09	0.25
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	10	0.29	0.01	0.29
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	10	0.29	0.09	0.28
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	10	0.29	0.06	0.28
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	10	0.28	0.06	0.26
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	10	0.27	0.08	0.28
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	10	0.27	0.08	0.28
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	10	0.26	0.05	0.26
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	10	0.26	0.05	0.26
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	10	0.26	0.05	0.26
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	10	0.25	0.12	0.2
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	10	0.25	0.12	0.2
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	10	0.25	0.12	0.2
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	10	0.25	0.03	0.25
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	10	0.24	0.08	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	10	0.24	0.04	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	10	0.24	0.04	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	10	0.24	0.04	0.25
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	10	0.24	0.1	0.24
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	10	0.22	0.03	0.22
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	10	0.21	0.06	0.2
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	10	0.21	0.06	0.2
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	10	0.21	0.06	0.2
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	10	0.2	0.04	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	10	0.2	0.02	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	10	0.2	0.02	0.19
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	10	0.19	0.02	0.19
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	10	0.19	0.02	0.19
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	10	0.19	0.02	0.19
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	10	0.19	0.03	0.19
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	10	0.19	0.03	0.19
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	10	0.18	0.04	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	10	0.18	0.02	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	10	0.18	0.02	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	10	0.18	0.02	0.18
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	10	0.18	0.02	0.18
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	10	0.17	0.03	0.18
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	10	0.17	0.01	0.17
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	10	0.17	0.01	0.17
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	10	0.17	0.01	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	10	0.14	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	10	0.14	0.03	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	10	0.14	0.03	0.16
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	9	0.45	0.04	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	9	0.43	0.02	0.44
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	9	0.39	0.02	0.39
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	9	0.28	0.05	0.28
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	9	0.28	0.05	0.28
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	9	0.24	0.04	0.25
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	9	0.24	0.07	0.21
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	9	0.23	0.05	0.25
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	9	0.23	0.1	0.19
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	9	0.23	0.1	0.19
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	9	0.23	0.1	0.19
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	9	0.21	0.09	0.2
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	9	0.18	0.02	0.18
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	9	0.18	0.06	0.19
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	9	0.18	0.06	0.19
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	9	0.17	0.04	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	9	0.17	0.04	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	9	0.17	0.04	0.18
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	9	0.17	0.04	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	9	0.17	0.04	0.16
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	9	0.16	0.02	0.16
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	9	0.15	0.03	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	9	0.15	0.03	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	9	0.15	0.03	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	9	0.15	0.03	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	9	0.15	0.03	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	9	0.15	0.03	0.17
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	9	0.15	0.01	0.15
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	9	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	9	0.13	0.02	0.12
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	9	0.13	0.02	0.12
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	9	0.12	0.02	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	9	0.11	0.0	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	9	0.11	0.0	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	9	0.11	0.0	0.11
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	8	0.46	0.07	0.46
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	8	0.46	0.07	0.46
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	8	0.37	0.08	0.41
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	8	0.37	0.03	0.38
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	8	0.37	0.03	0.38
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	8	0.36	0.05	0.38
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	8	0.35	0.02	0.36
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	8	0.32	0.11	0.3
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	8	0.28	0.13	0.22
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	8	0.28	0.13	0.22
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	8	0.28	0.13	0.22
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	8	0.27	0.07	0.25
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	8	0.25	0.08	0.23
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	8	0.25	0.08	0.23
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	8	0.25	0.08	0.23
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	8	0.23	0.05	0.26
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	8	0.22	0.04	0.23
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	8	0.2	0.08	0.18
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	8	0.2	0.04	0.21
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	8	0.2	0.06	0.18
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	8	0.2	0.06	0.18
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	8	0.2	0.06	0.18
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	8	0.2	0.06	0.18
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	8	0.2	0.06	0.18
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	8	0.2	0.06	0.18
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	8	0.19	0.03	0.2
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	8	0.18	0.05	0.19
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	8	0.18	0.05	0.19
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	8	0.18	0.05	0.19
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	8	0.18	0.05	0.19
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	8	0.18	0.05	0.19
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	8	0.18	0.05	0.19
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	8	0.18	0.03	0.18
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	8	0.18	0.03	0.18
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	8	0.18	0.03	0.18
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	8	0.17	0.06	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	8	0.17	0.06	0.17
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	8	0.17	0.04	0.17
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	8	0.16	0.03	0.16
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	8	0.16	0.03	0.16
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	8	0.16	0.03	0.16
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	8	0.16	0.03	0.16
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	8	0.14	0.02	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	8	0.14	0.02	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	8	0.14	0.02	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	8	0.14	0.02	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	8	0.14	0.02	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	8	0.14	0.02	0.13
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	8	0.14	0.01	0.14
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	8	0.13	0.02	0.14
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	8	0.13	0.02	0.14
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	8	0.13	0.02	0.14
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	8	0.13	0.02	0.14
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	8	0.13	0.02	0.14
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	8	0.13	0.02	0.14
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	8	0.13	0.01	0.12
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	8	0.13	0.03	0.12
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	8	0.13	0.03	0.12
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	7	0.33	0.15	0.25
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	7	0.33	0.15	0.25
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	7	0.32	0.16	0.29
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	7	0.25	0.08	0.26
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	7	0.25	0.0	0.25
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	7	0.24	0.15	0.17
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	7	0.24	0.03	0.26
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	7	0.23	0.04	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	7	0.23	0.04	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	7	0.23	0.04	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	7	0.23	0.04	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	7	0.23	0.04	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	7	0.23	0.04	0.24

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	7	0.21	0.06	0.21
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	7	0.21	0.06	0.21
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	7	0.21	0.06	0.21
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	7	0.21	0.06	0.21
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	7	0.21	0.06	0.21
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	7	0.21	0.06	0.21
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	7	0.21	0.11	0.16
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	7	0.21	0.11	0.16
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	7	0.21	0.11	0.16
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	7	0.19	0.04	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	7	0.19	0.04	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	7	0.19	0.04	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	7	0.19	0.04	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	7	0.19	0.04	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	7	0.19	0.04	0.2
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	7	0.19	0.02	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	7	0.19	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)
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	7	0.19	0.05	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	7	0.19	0.05	0.16
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	7	0.17	0.04	0.17
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	7	0.17	0.04	0.17
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	7	0.17	0.07	0.15
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	7	0.16	0.04	0.16
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	7	0.15	0.03	0.14
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	7	0.15	0.05	0.14
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	7	0.15	0.05	0.14
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	7	0.15	0.05	0.14
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	7	0.15	0.05	0.14
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	7	0.15	0.05	0.14
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	7	0.15	0.05	0.14
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	7	0.1	0.0	0.1
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	7	0.1	0.0	0.1
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	6	0.34	0.06	0.37
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	6	0.34	0.06	0.37
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	6	0.34	0.06	0.37
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	6	0.28	0.01	0.29
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	6	0.28	0.02	0.28
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	6	0.26	0.03	0.28
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	6	0.26	0.03	0.28
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	6	0.26	0.03	0.28
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	6	0.26	0.03	0.28
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	6	0.26	0.03	0.28
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	6	0.26	0.03	0.28
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	6	0.19	0.07	0.2
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	6	0.19	0.07	0.2
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	6	0.19	0.04	0.17
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	6	0.16	0.03	0.16
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	6	0.16	0.03	0.16
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	6	0.16	0.03	0.16
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	6	0.16	0.03	0.16
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	6	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	6	0.16	0.03	0.16
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	6	0.15	0.03	0.16
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	6	0.15	0.03	0.16
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	6	0.15	0.03	0.15
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	6	0.15	0.03	0.15
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	6	0.15	0.03	0.15
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	6	0.14	0.02	0.15
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	6	0.14	0.02	0.15
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	6	0.13	0.02	0.12
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	6	0.13	0.02	0.12
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	6	0.13	0.02	0.12
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	6	0.12	0.01	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	6	0.11	0.01	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	6	0.11	0.01	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	6	0.11	0.01	0.12
(1,105)	1:106:X:PHE:HD1	1:107:X:THR:HA	5	0.35	0.04	0.34
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE1	5	0.33	0.03	0.32
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE2	5	0.33	0.03	0.32
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE3	5	0.33	0.03	0.32
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG2	5	0.31	0.01	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG3	5	0.31	0.01	0.31
(1,883)	1:136:X:ALA:HB1	1:137:X:PHE:HB3	5	0.3	0.08	0.27
(1,883)	1:136:X:ALA:HB2	1:137:X:PHE:HB3	5	0.3	0.08	0.27
(1,883)	1:136:X:ALA:HB3	1:137:X:PHE:HB3	5	0.3	0.08	0.27
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD2	5	0.24	0.01	0.24
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD3	5	0.24	0.01	0.24
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG2	5	0.23	0.07	0.2
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG3	5	0.23	0.07	0.2
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG11	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG12	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG13	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG21	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG22	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG23	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG11	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG12	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG13	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG21	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG22	5	0.23	0.1	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG23	5	0.23	0.1	0.28
(1,1600)	1:46:X:ILE:H	1:47:X:GLN:HB3	5	0.21	0.09	0.15
(1,1595)	1:43:X:ILE:HG13	1:44:X:ALA:H	5	0.21	0.08	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,150)	1:33:X:ILE:HB	1:49:X:ASP:HA	5	0.19	0.06	0.19
(1,788)	1:37:X:ARG:HA	1:43:X:ILE:HG12	5	0.18	0.06	0.17
(1,956)	1:72:X:GLN:H	1:72:X:GLN:HB3	5	0.18	0.03	0.19
(1,1546)	1:69:X:LEU:H	1:78:X:PRO:HB2	5	0.17	0.03	0.19
(1,250)	1:137:X:PHE:HD1	1:138:X:PRO:HD2	5	0.17	0.02	0.17
(1,783)	1:74:X:PRO:HB2	1:106:X:PHE:HE1	5	0.17	0.05	0.17
(1,2258)	1:102:X:LEU:HD11	1:122:X:GLU:HB3	5	0.17	0.02	0.16
(1,2258)	1:102:X:LEU:HD12	1:122:X:GLU:HB3	5	0.17	0.02	0.16
(1,2258)	1:102:X:LEU:HD13	1:122:X:GLU:HB3	5	0.17	0.02	0.16
(1,2258)	1:102:X:LEU:HD21	1:122:X:GLU:HB3	5	0.17	0.02	0.16
(1,2258)	1:102:X:LEU:HD22	1:122:X:GLU:HB3	5	0.17	0.02	0.16
(1,2258)	1:102:X:LEU:HD23	1:122:X:GLU:HB3	5	0.17	0.02	0.16
(1,96)	1:29:X:LYS:HA	1:73:X:PHE:HD1	5	0.16	0.04	0.17
(1,1003)	1:125:X:LYS:HB3	1:126:X:ASN:H	5	0.16	0.02	0.16
(1,742)	1:122:X:GLU:HA	1:125:X:LYS:HB3	5	0.16	0.02	0.14
(1,153)	1:121:X:ASP:HA	1:124:X:TRP:HB3	5	0.16	0.03	0.17
(1,236)	1:58:X:ILE:HD11	1:127:X:PRO:HD2	5	0.15	0.03	0.17
(1,236)	1:58:X:ILE:HD12	1:127:X:PRO:HD2	5	0.15	0.03	0.17
(1,236)	1:58:X:ILE:HD13	1:127:X:PRO:HD2	5	0.15	0.03	0.17
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB2	5	0.15	0.04	0.13
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB3	5	0.15	0.04	0.13
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD11	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD12	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD13	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD11	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD12	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD13	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD11	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD12	5	0.15	0.03	0.13
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD13	5	0.15	0.03	0.13
(1,441)	1:58:X:ILE:HD11	1:126:X:ASN:HA	5	0.14	0.03	0.15
(1,441)	1:58:X:ILE:HD12	1:126:X:ASN:HA	5	0.14	0.03	0.15
(1,441)	1:58:X:ILE:HD13	1:126:X:ASN:HA	5	0.14	0.03	0.15
(1,1989)	1:61:X:LEU:HD11	1:128:X:PRO:HG3	5	0.14	0.02	0.14
(1,1989)	1:61:X:LEU:HD12	1:128:X:PRO:HG3	5	0.14	0.02	0.14
(1,1989)	1:61:X:LEU:HD13	1:128:X:PRO:HG3	5	0.14	0.02	0.14
(1,1989)	1:61:X:LEU:HD21	1:128:X:PRO:HG3	5	0.14	0.02	0.14
(1,1989)	1:61:X:LEU:HD22	1:128:X:PRO:HG3	5	0.14	0.02	0.14
(1,1989)	1:61:X:LEU:HD23	1:128:X:PRO:HG3	5	0.14	0.02	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB2	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB3	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB2	5	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB3	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB2	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB3	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB2	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB3	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB2	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB3	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB2	5	0.14	0.01	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB3	5	0.14	0.01	0.14
(1,912)	1:50:X:VAL:HA	1:68:X:LEU:HG	5	0.13	0.02	0.13
(1,1212)	1:50:X:VAL:HB	1:51:X:GLU:H	5	0.13	0.01	0.12
(1,1573)	1:43:X:ILE:HG13	1:54:X:LEU:H	5	0.12	0.02	0.11
(1,929)	1:94:X:GLN:HG3	1:95:X:GLY:H	4	0.32	0.03	0.32
(1,445)	1:86:X:ILE:HD11	1:91:X:MET:HB2	4	0.32	0.02	0.32
(1,445)	1:86:X:ILE:HD12	1:91:X:MET:HB2	4	0.32	0.02	0.32
(1,445)	1:86:X:ILE:HD13	1:91:X:MET:HB2	4	0.32	0.02	0.32
(1,1745)	1:29:X:LYS:HG2	1:73:X:PHE:HD1	4	0.25	0.06	0.24
(1,1745)	1:29:X:LYS:HG3	1:73:X:PHE:HD1	4	0.25	0.06	0.24
(1,839)	1:102:X:LEU:HD21	1:122:X:GLU:HG3	4	0.24	0.06	0.22
(1,839)	1:102:X:LEU:HD22	1:122:X:GLU:HG3	4	0.24	0.06	0.22
(1,839)	1:102:X:LEU:HD23	1:122:X:GLU:HG3	4	0.24	0.06	0.22
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG2	4	0.24	0.07	0.28
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG3	4	0.24	0.07	0.28
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD2	4	0.24	0.0	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD3	4	0.24	0.0	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD11	4	0.23	0.01	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD12	4	0.23	0.01	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD13	4	0.23	0.01	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD21	4	0.23	0.01	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD22	4	0.23	0.01	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD23	4	0.23	0.01	0.24
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD11	4	0.23	0.03	0.23
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD12	4	0.23	0.03	0.23
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD13	4	0.23	0.03	0.23
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD21	4	0.23	0.03	0.23
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD22	4	0.23	0.03	0.23
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD23	4	0.23	0.03	0.23
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG2	4	0.22	0.11	0.2
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG3	4	0.22	0.11	0.2
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG2	4	0.22	0.11	0.2
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG3	4	0.22	0.11	0.2
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD11	4	0.2	0.07	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD12	4	0.2	0.07	0.2
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD13	4	0.2	0.07	0.2
(1,2156)	1:90:X:LEU:HD11	1:91:X:MET:HG3	4	0.2	0.02	0.2
(1,2156)	1:90:X:LEU:HD12	1:91:X:MET:HG3	4	0.2	0.02	0.2
(1,2156)	1:90:X:LEU:HD13	1:91:X:MET:HG3	4	0.2	0.02	0.2
(1,2156)	1:90:X:LEU:HD21	1:91:X:MET:HG3	4	0.2	0.02	0.2
(1,2156)	1:90:X:LEU:HD22	1:91:X:MET:HG3	4	0.2	0.02	0.2
(1,2156)	1:90:X:LEU:HD23	1:91:X:MET:HG3	4	0.2	0.02	0.2
(1,190)	1:25:X:LEU:HA	1:74:X:PRO:HD3	4	0.18	0.03	0.18
(1,209)	1:77:X:LYS:HD3	1:78:X:PRO:HD3	4	0.18	0.05	0.16
(1,1441)	1:90:X:LEU:H	1:91:X:MET:HB3	4	0.17	0.05	0.16
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE1	4	0.17	0.02	0.18
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE2	4	0.17	0.02	0.18
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE3	4	0.17	0.02	0.18
(1,206)	1:78:X:PRO:HD2	1:106:X:PHE:HE1	4	0.17	0.03	0.17
(1,62)	1:29:X:LYS:HA	1:74:X:PRO:HD2	4	0.16	0.03	0.16
(1,1208)	1:47:X:GLN:HG2	1:51:X:GLU:H	4	0.16	0.04	0.16
(1,1640)	1:138:X:PRO:HB2	1:139:X:TYR:HD1	4	0.16	0.05	0.14
(1,1055)	1:73:X:PHE:HD1	1:76:X:GLU:H	4	0.15	0.08	0.11
(1,808)	1:57:X:THR:HA	1:63:X:ILE:HG13	4	0.15	0.02	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD11	4	0.15	0.02	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD12	4	0.15	0.02	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD13	4	0.15	0.02	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD11	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD12	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD13	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD21	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD22	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD23	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD11	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD12	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD13	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD21	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD22	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD23	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD11	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD12	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD13	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD21	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD22	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD23	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD11	4	0.15	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD12	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD13	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD21	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD22	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD23	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD11	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD12	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD13	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD21	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD22	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD23	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD11	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD12	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD13	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD21	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD22	4	0.15	0.03	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD23	4	0.15	0.03	0.16
(1,2077)	1:79:X:VAL:HG11	1:81:X:SER:H	4	0.15	0.03	0.13
(1,2077)	1:79:X:VAL:HG12	1:81:X:SER:H	4	0.15	0.03	0.13
(1,2077)	1:79:X:VAL:HG13	1:81:X:SER:H	4	0.15	0.03	0.13
(1,2077)	1:79:X:VAL:HG21	1:81:X:SER:H	4	0.15	0.03	0.13
(1,2077)	1:79:X:VAL:HG22	1:81:X:SER:H	4	0.15	0.03	0.13
(1,2077)	1:79:X:VAL:HG23	1:81:X:SER:H	4	0.15	0.03	0.13
(1,2317)	1:117:X:GLN:HG2	1:118:X:SER:H	4	0.14	0.02	0.14
(1,2317)	1:117:X:GLN:HG3	1:118:X:SER:H	4	0.14	0.02	0.14
(1,764)	1:32:X:LEU:HG	1:74:X:PRO:HB2	4	0.14	0.05	0.12
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD11	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD12	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD13	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD11	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD12	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD13	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD11	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD12	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD13	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD11	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD12	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD13	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD11	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD12	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD13	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD11	4	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD12	4	0.14	0.03	0.14
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD13	4	0.14	0.03	0.14
(1,1784)	1:32:X:LEU:HD11	1:111:X:ASP:HA	4	0.14	0.04	0.12
(1,1784)	1:32:X:LEU:HD12	1:111:X:ASP:HA	4	0.14	0.04	0.12
(1,1784)	1:32:X:LEU:HD13	1:111:X:ASP:HA	4	0.14	0.04	0.12
(1,1784)	1:32:X:LEU:HD21	1:111:X:ASP:HA	4	0.14	0.04	0.12
(1,1784)	1:32:X:LEU:HD22	1:111:X:ASP:HA	4	0.14	0.04	0.12
(1,1784)	1:32:X:LEU:HD23	1:111:X:ASP:HA	4	0.14	0.04	0.12
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD11	4	0.14	0.03	0.12
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD12	4	0.14	0.03	0.12
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD13	4	0.14	0.03	0.12
(1,431)	1:86:X:ILE:HD11	1:91:X:MET:HA	4	0.14	0.03	0.12
(1,431)	1:86:X:ILE:HD12	1:91:X:MET:HA	4	0.14	0.03	0.12
(1,431)	1:86:X:ILE:HD13	1:91:X:MET:HA	4	0.14	0.03	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG11	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG12	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG13	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG21	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG22	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG23	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG11	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG12	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG13	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG21	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG22	4	0.13	0.01	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG23	4	0.13	0.01	0.13
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD11	4	0.12	0.02	0.12
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD12	4	0.12	0.02	0.12
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD13	4	0.12	0.02	0.12
(1,574)	1:23:X:THR:HG21	1:26:X:GLN:HB3	4	0.12	0.02	0.12
(1,574)	1:23:X:THR:HG22	1:26:X:GLN:HB3	4	0.12	0.02	0.12
(1,574)	1:23:X:THR:HG23	1:26:X:GLN:HB3	4	0.12	0.02	0.12
(1,1050)	1:73:X:PHE:HB2	1:76:X:GLU:H	4	0.12	0.02	0.12
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD11	4	0.12	0.01	0.12
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD12	4	0.12	0.01	0.12
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD13	4	0.12	0.01	0.12
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD21	4	0.12	0.01	0.12
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD22	4	0.12	0.01	0.12
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD23	4	0.12	0.01	0.12
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD11	3	0.37	0.09	0.42
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD12	3	0.37	0.09	0.42
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD13	3	0.37	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)
(1,996)	1:86:X:ILE:H	1:91:X:MET:HG2	3	0.36	0.11	0.31
(1,818)	1:83:X:TYR:HB3	1:85:X:PRO:HD2	3	0.35	0.04	0.38
(1,973)	1:103:X:VAL:H	1:104:X:ASN:HB3	3	0.32	0.05	0.3
(1,202)	1:36:X:LEU:HB3	1:113:X:GLY:HA3	3	0.3	0.04	0.28
(1,878)	1:33:X:ILE:HB	1:34:X:GLU:HG3	3	0.28	0.08	0.23
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB2	3	0.27	0.09	0.27
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB3	3	0.27	0.09	0.27
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG11	3	0.27	0.03	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG12	3	0.27	0.03	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG13	3	0.27	0.03	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG21	3	0.27	0.03	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG22	3	0.27	0.03	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG23	3	0.27	0.03	0.28
(1,378)	1:33:X:ILE:HD11	1:52:X:TYR:HE1	3	0.27	0.12	0.34
(1,378)	1:33:X:ILE:HD12	1:52:X:TYR:HE1	3	0.27	0.12	0.34
(1,378)	1:33:X:ILE:HD13	1:52:X:TYR:HE1	3	0.27	0.12	0.34
(1,718)	1:33:X:ILE:HB	1:34:X:GLU:HB2	3	0.26	0.02	0.26
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD11	3	0.22	0.07	0.21
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD12	3	0.22	0.07	0.21
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD13	3	0.22	0.07	0.21
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD11	3	0.22	0.02	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD12	3	0.22	0.02	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD13	3	0.22	0.02	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD21	3	0.22	0.02	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD22	3	0.22	0.02	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD23	3	0.22	0.02	0.23
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD11	3	0.21	0.03	0.22
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD12	3	0.21	0.03	0.22
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD13	3	0.21	0.03	0.22
(1,380)	1:43:X:ILE:HD11	1:52:X:TYR:HE1	3	0.21	0.09	0.21
(1,380)	1:43:X:ILE:HD12	1:52:X:TYR:HE1	3	0.21	0.09	0.21
(1,380)	1:43:X:ILE:HD13	1:52:X:TYR:HE1	3	0.21	0.09	0.21
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD11	3	0.21	0.01	0.21
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD12	3	0.21	0.01	0.21
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD13	3	0.21	0.01	0.21
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG11	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG12	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG13	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG21	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG22	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG23	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG11	3	0.21	0.08	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG12	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG13	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG21	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG22	3	0.21	0.08	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG23	3	0.21	0.08	0.16
(1,2294)	1:112:X:LEU:HD11	1:115:X:ILE:HG12	3	0.21	0.03	0.19
(1,2294)	1:112:X:LEU:HD12	1:115:X:ILE:HG12	3	0.21	0.03	0.19
(1,2294)	1:112:X:LEU:HD13	1:115:X:ILE:HG12	3	0.21	0.03	0.19
(1,2294)	1:112:X:LEU:HD21	1:115:X:ILE:HG12	3	0.21	0.03	0.19
(1,2294)	1:112:X:LEU:HD22	1:115:X:ILE:HG12	3	0.21	0.03	0.19
(1,2294)	1:112:X:LEU:HD23	1:115:X:ILE:HG12	3	0.21	0.03	0.19
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD2	3	0.19	0.07	0.24
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD3	3	0.19	0.07	0.24
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD2	3	0.19	0.07	0.24
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD3	3	0.19	0.07	0.24
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD21	3	0.18	0.06	0.16
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD22	3	0.18	0.06	0.16
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD23	3	0.18	0.06	0.16
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE1	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE2	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE3	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE1	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE2	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE3	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE1	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE2	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE3	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE1	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE2	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE3	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE1	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE2	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE3	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE1	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE2	3	0.18	0.05	0.16
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE3	3	0.18	0.05	0.16
(1,1412)	1:57:X:THR:H	1:57:X:THR:HB	3	0.17	0.04	0.15
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE1	3	0.17	0.04	0.17
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE2	3	0.17	0.04	0.17
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE3	3	0.17	0.04	0.17
(1,1614)	1:57:X:THR:HG21	1:60:X:ASN:H	3	0.17	0.07	0.12
(1,1614)	1:57:X:THR:HG22	1:60:X:ASN:H	3	0.17	0.07	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1614)	1:57:X:THR:HG23	1:60:X:ASN:H	3	0.17	0.07	0.12
(1,47)	1:70:X:PRO:HA	1:73:X:PHE:HB2	3	0.16	0.04	0.18
(1,675)	1:77:X:LYS:HG2	1:106:X:PHE:HD1	3	0.16	0.07	0.11
(1,684)	1:106:X:PHE:HE1	1:112:X:LEU:HB3	3	0.16	0.02	0.16
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG11	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG12	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG13	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG21	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG22	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG23	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG11	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG12	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG13	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG21	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG22	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG23	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG11	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG12	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG13	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG21	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG22	3	0.16	0.02	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG23	3	0.16	0.02	0.15
(1,955)	1:71:X:PRO:HG3	1:72:X:GLN:H	3	0.16	0.0	0.16
(1,1260)	1:137:X:PHE:HA	1:139:X:TYR:H	3	0.15	0.02	0.16
(1,1882)	1:45:X:GLU:HG2	1:48:X:LYS:HD2	3	0.15	0.03	0.16
(1,1882)	1:45:X:GLU:HG3	1:48:X:LYS:HD2	3	0.15	0.03	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD11	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD12	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD13	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD21	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD22	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD23	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD11	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD12	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD13	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD21	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD22	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD23	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD11	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD12	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD13	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD21	3	0.14	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD22	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD23	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD11	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD12	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD13	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD21	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD22	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD23	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD11	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD12	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD13	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD21	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD22	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD23	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD11	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD12	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD13	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD21	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD22	3	0.14	0.02	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD23	3	0.14	0.02	0.16
(1,962)	1:91:X:MET:H	1:91:X:MET:HE1	3	0.14	0.02	0.13
(1,962)	1:91:X:MET:H	1:91:X:MET:HE2	3	0.14	0.02	0.13
(1,962)	1:91:X:MET:H	1:91:X:MET:HE3	3	0.14	0.02	0.13
(1,1530)	1:130:X:LEU:HD11	1:131:X:ALA:H	3	0.14	0.02	0.14
(1,1530)	1:130:X:LEU:HD12	1:131:X:ALA:H	3	0.14	0.02	0.14
(1,1530)	1:130:X:LEU:HD13	1:131:X:ALA:H	3	0.14	0.02	0.14
(1,1857)	1:37:X:ARG:HD2	1:52:X:TYR:HE1	3	0.14	0.01	0.14
(1,1857)	1:37:X:ARG:HD3	1:52:X:TYR:HE1	3	0.14	0.01	0.14
(1,835)	1:119:X:LEU:HA	1:122:X:GLU:HG2	3	0.13	0.03	0.13
(1,512)	1:67:X:ILE:HG21	1:78:X:PRO:HD3	3	0.13	0.03	0.12
(1,512)	1:67:X:ILE:HG22	1:78:X:PRO:HD3	3	0.13	0.03	0.12
(1,512)	1:67:X:ILE:HG23	1:78:X:PRO:HD3	3	0.13	0.03	0.12
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG2	3	0.13	0.02	0.13
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG3	3	0.13	0.02	0.13
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG2	3	0.13	0.02	0.13
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG3	3	0.13	0.02	0.13
(1,568)	1:99:X:THR:HG21	1:100:X:SER:HA	3	0.13	0.01	0.12
(1,568)	1:99:X:THR:HG22	1:100:X:SER:HA	3	0.13	0.01	0.12
(1,568)	1:99:X:THR:HG23	1:100:X:SER:HA	3	0.13	0.01	0.12
(1,653)	1:32:X:LEU:HD11	1:74:X:PRO:HB2	3	0.13	0.02	0.12
(1,653)	1:32:X:LEU:HD12	1:74:X:PRO:HB2	3	0.13	0.02	0.12
(1,653)	1:32:X:LEU:HD13	1:74:X:PRO:HB2	3	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,699)	1:52:X:TYR:HB2	1:67:X:ILE:HB	3	0.13	0.03	0.11
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG21	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG22	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG23	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG21	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG22	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG23	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG21	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG22	3	0.12	0.0	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG23	3	0.12	0.0	0.12
(1,359)	1:63:X:ILE:HD11	1:123:X:PHE:HB2	3	0.12	0.02	0.12
(1,359)	1:63:X:ILE:HD12	1:123:X:PHE:HB2	3	0.12	0.02	0.12
(1,359)	1:63:X:ILE:HD13	1:123:X:PHE:HB2	3	0.12	0.02	0.12
(1,894)	1:43:X:ILE:HG13	1:52:X:TYR:HB2	3	0.12	0.02	0.12
(1,1513)	1:73:X:PHE:HD1	1:75:X:GLN:H	3	0.12	0.02	0.12
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD2	3	0.12	0.02	0.11
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD3	3	0.12	0.02	0.11
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD2	3	0.12	0.02	0.11
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD3	3	0.12	0.02	0.11
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD2	3	0.12	0.02	0.11
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD3	3	0.12	0.02	0.11
(1,2105)	1:82:X:VAL:HG11	1:86:X:ILE:HA	3	0.12	0.02	0.11
(1,2105)	1:82:X:VAL:HG12	1:86:X:ILE:HA	3	0.12	0.02	0.11
(1,2105)	1:82:X:VAL:HG13	1:86:X:ILE:HA	3	0.12	0.02	0.11
(1,2105)	1:82:X:VAL:HG21	1:86:X:ILE:HA	3	0.12	0.02	0.11
(1,2105)	1:82:X:VAL:HG22	1:86:X:ILE:HA	3	0.12	0.02	0.11
(1,2105)	1:82:X:VAL:HG23	1:86:X:ILE:HA	3	0.12	0.02	0.11
(1,1027)	1:96:X:VAL:H	1:97:X:TYR:H	3	0.11	0.01	0.11
(1,1578)	1:68:X:LEU:H	1:78:X:PRO:HB3	3	0.11	0.0	0.11
(1,1421)	1:91:X:MET:HE1	1:98:X:VAL:H	3	0.1	0.0	0.1
(1,1421)	1:91:X:MET:HE2	1:98:X:VAL:H	3	0.1	0.0	0.1
(1,1421)	1:91:X:MET:HE3	1:98:X:VAL:H	3	0.1	0.0	0.1
(1,2053)	1:75:X:GLN:HG2	1:76:X:GLU:HG3	2	0.55	0.04	0.55
(1,2053)	1:75:X:GLN:HG3	1:76:X:GLU:HG3	2	0.55	0.04	0.55
(1,1092)	1:30:X:GLN:H	1:30:X:GLN:HB3	2	0.52	0.01	0.52
(1,871)	1:73:X:PHE:HB2	1:76:X:GLU:HB3	2	0.46	0.05	0.46
(1,858)	1:70:X:PRO:HB3	1:76:X:GLU:HB3	2	0.42	0.05	0.42
(1,1608)	1:48:X:LYS:H	1:51:X:GLU:HB3	2	0.4	0.01	0.4
(1,888)	1:121:X:ASP:HB2	1:122:X:GLU:HG3	2	0.39	0.28	0.39
(1,67)	1:67:X:ILE:HA	1:80:X:ILE:HG12	2	0.35	0.02	0.35
(1,1012)	1:96:X:VAL:HB	1:97:X:TYR:H	2	0.3	0.02	0.3
(1,2085)	1:80:X:ILE:HD11	1:106:X:PHE:HB2	2	0.29	0.0	0.29

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2085)	1:80:X:ILE:HD11	1:106:X:PHE:HB3	2	0.29	0.0	0.29
(1,2085)	1:80:X:ILE:HD12	1:106:X:PHE:HB2	2	0.29	0.0	0.29
(1,2085)	1:80:X:ILE:HD12	1:106:X:PHE:HB3	2	0.29	0.0	0.29
(1,2085)	1:80:X:ILE:HD13	1:106:X:PHE:HB2	2	0.29	0.0	0.29
(1,2085)	1:80:X:ILE:HD13	1:106:X:PHE:HB3	2	0.29	0.0	0.29
(1,1076)	1:96:X:VAL:H	1:96:X:VAL:HB	2	0.28	0.01	0.28
(1,1403)	1:36:X:LEU:H	1:37:X:ARG:HB3	2	0.28	0.14	0.28
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE1	2	0.25	0.0	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE2	2	0.25	0.0	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE3	2	0.25	0.0	0.25
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG21	2	0.24	0.0	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG22	2	0.24	0.0	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG23	2	0.24	0.0	0.24
(1,1639)	1:138:X:PRO:HB3	1:139:X:TYR:HD1	2	0.23	0.01	0.23
(1,872)	1:80:X:ILE:HD11	1:103:X:VAL:HB	2	0.22	0.05	0.22
(1,872)	1:80:X:ILE:HD12	1:103:X:VAL:HB	2	0.22	0.05	0.22
(1,872)	1:80:X:ILE:HD13	1:103:X:VAL:HB	2	0.22	0.05	0.22
(1,920)	1:80:X:ILE:HG12	1:81:X:SER:H	2	0.22	0.02	0.22
(1,1094)	1:47:X:GLN:H	1:47:X:GLN:HB3	2	0.22	0.01	0.22
(1,2339)	1:122:X:GLU:HA	1:125:X:LYS:HG2	2	0.22	0.1	0.22
(1,2339)	1:122:X:GLU:HA	1:125:X:LYS:HG3	2	0.22	0.1	0.22
(1,1737)	1:29:X:LYS:HB2	1:73:X:PHE:HD1	2	0.21	0.03	0.21
(1,1737)	1:29:X:LYS:HB3	1:73:X:PHE:HD1	2	0.21	0.03	0.21
(1,2047)	1:72:X:GLN:H	1:72:X:GLN:HG2	2	0.2	0.02	0.2
(1,2047)	1:72:X:GLN:H	1:72:X:GLN:HG3	2	0.2	0.02	0.2
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD11	2	0.2	0.02	0.2
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD12	2	0.2	0.02	0.2
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD13	2	0.2	0.02	0.2
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD21	2	0.2	0.02	0.2
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD22	2	0.2	0.02	0.2
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD23	2	0.2	0.02	0.2
(1,295)	1:90:X:LEU:HB2	1:100:X:SER:HA	2	0.2	0.05	0.2
(1,578)	1:140:X:LEU:HD21	1:141:X:TYR:HE1	2	0.2	0.02	0.2
(1,578)	1:140:X:LEU:HD22	1:141:X:TYR:HE1	2	0.2	0.02	0.2
(1,578)	1:140:X:LEU:HD23	1:141:X:TYR:HE1	2	0.2	0.02	0.2
(1,1277)	1:34:X:GLU:H	1:34:X:GLU:HG2	2	0.2	0.02	0.2
(1,769)	1:33:X:ILE:HD11	1:69:X:LEU:HB2	2	0.18	0.04	0.18
(1,769)	1:33:X:ILE:HD12	1:69:X:LEU:HB2	2	0.18	0.04	0.18
(1,769)	1:33:X:ILE:HD13	1:69:X:LEU:HB2	2	0.18	0.04	0.18
(1,2280)	1:107:X:THR:HG21	1:110:X:SER:HB2	2	0.18	0.04	0.18
(1,2280)	1:107:X:THR:HG21	1:110:X:SER:HB3	2	0.18	0.04	0.18
(1,2280)	1:107:X:THR:HG22	1:110:X:SER:HB2	2	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2280)	1:107:X:THR:HG22	1:110:X:SER:HB3	2	0.18	0.04	0.18
(1,2280)	1:107:X:THR:HG23	1:110:X:SER:HB2	2	0.18	0.04	0.18
(1,2280)	1:107:X:THR:HG23	1:110:X:SER:HB3	2	0.18	0.04	0.18
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG21	2	0.18	0.0	0.18
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG22	2	0.18	0.0	0.18
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG23	2	0.18	0.0	0.18
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG21	2	0.18	0.0	0.18
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG22	2	0.18	0.0	0.18
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG23	2	0.18	0.0	0.18
(1,249)	1:137:X:PHE:HD1	1:138:X:PRO:HD3	2	0.17	0.03	0.17
(1,1248)	1:30:X:GLN:HB3	1:31:X:ARG:H	2	0.17	0.0	0.17
(1,1440)	1:90:X:LEU:H	1:90:X:LEU:HG	2	0.17	0.0	0.17
(1,654)	1:48:X:LYS:HD3	1:49:X:ASP:HA	2	0.16	0.04	0.16
(1,825)	1:137:X:PHE:HB3	1:138:X:PRO:HD3	2	0.16	0.01	0.16
(1,1048)	1:73:X:PHE:HA	1:76:X:GLU:H	2	0.16	0.01	0.16
(1,1554)	1:52:X:TYR:H	1:52:X:TYR:HD1	2	0.16	0.02	0.16
(1,657)	1:86:X:ILE:HG13	1:91:X:MET:HB3	2	0.16	0.04	0.16
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD11	2	0.16	0.01	0.16
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD12	2	0.16	0.01	0.16
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD13	2	0.16	0.01	0.16
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD21	2	0.16	0.01	0.16
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD22	2	0.16	0.01	0.16
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD23	2	0.16	0.01	0.16
(1,2154)	1:90:X:LEU:HG	1:100:X:SER:HB2	2	0.16	0.02	0.16
(1,2154)	1:90:X:LEU:HG	1:100:X:SER:HB3	2	0.16	0.02	0.16
(1,1377)	1:97:X:TYR:HD1	1:98:X:VAL:H	2	0.16	0.02	0.16
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD11	2	0.16	0.02	0.16
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD12	2	0.16	0.02	0.16
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD13	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD11	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD12	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD13	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD11	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD12	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD13	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD11	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD12	2	0.16	0.02	0.16
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD13	2	0.16	0.02	0.16
(1,966)	1:91:X:MET:H	1:91:X:MET:HG2	2	0.16	0.05	0.16
(1,1679)	1:138:X:PRO:HB3	1:139:X:TYR:HE1	2	0.16	0.05	0.16
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD11	2	0.16	0.05	0.16
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD12	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)
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD13	2	0.16	0.05	0.16
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD21	2	0.16	0.05	0.16
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD22	2	0.16	0.05	0.16
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD23	2	0.16	0.05	0.16
(1,1486)	1:73:X:PHE:H	1:76:X:GLU:HG2	2	0.15	0.05	0.15
(1,267)	1:76:X:GLU:HA	1:76:X:GLU:HG3	2	0.15	0.03	0.15
(1,334)	1:93:X:LYS:HA	1:93:X:LYS:HD3	2	0.15	0.03	0.15
(1,987)	1:34:X:GLU:HG3	1:35:X:SER:H	2	0.15	0.02	0.15
(1,1840)	1:36:X:LEU:HD11	1:113:X:GLY:HA2	2	0.15	0.02	0.15
(1,1840)	1:36:X:LEU:HD12	1:113:X:GLY:HA2	2	0.15	0.02	0.15
(1,1840)	1:36:X:LEU:HD13	1:113:X:GLY:HA2	2	0.15	0.02	0.15
(1,1840)	1:36:X:LEU:HD21	1:113:X:GLY:HA2	2	0.15	0.02	0.15
(1,1840)	1:36:X:LEU:HD22	1:113:X:GLY:HA2	2	0.15	0.02	0.15
(1,1840)	1:36:X:LEU:HD23	1:113:X:GLY:HA2	2	0.15	0.02	0.15
(1,1753)	1:29:X:LYS:HE2	1:69:X:LEU:HB2	2	0.14	0.03	0.14
(1,1753)	1:29:X:LYS:HE3	1:69:X:LEU:HB2	2	0.14	0.03	0.14
(1,136)	1:46:X:ILE:HG13	1:52:X:TYR:HA	2	0.14	0.03	0.14
(1,1564)	1:65:X:ILE:HG12	1:66:X:ASN:H	2	0.14	0.03	0.14
(1,1888)	1:45:X:GLU:HG2	1:52:X:TYR:HE1	2	0.14	0.0	0.14
(1,1888)	1:45:X:GLU:HG3	1:52:X:TYR:HE1	2	0.14	0.0	0.14
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD21	2	0.14	0.01	0.14
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD22	2	0.14	0.01	0.14
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD23	2	0.14	0.01	0.14
(1,651)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	2	0.14	0.02	0.14
(1,651)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	2	0.14	0.02	0.14
(1,651)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	2	0.14	0.02	0.14
(1,1654)	1:63:X:ILE:HD11	1:123:X:PHE:HE1	2	0.14	0.02	0.14
(1,1654)	1:63:X:ILE:HD12	1:123:X:PHE:HE1	2	0.14	0.02	0.14
(1,1654)	1:63:X:ILE:HD13	1:123:X:PHE:HE1	2	0.14	0.02	0.14
(1,671)	1:124:X:TRP:HB3	1:125:X:LYS:HB3	2	0.12	0.02	0.12
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD11	2	0.12	0.02	0.12
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD12	2	0.12	0.02	0.12
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD13	2	0.12	0.02	0.12
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD21	2	0.12	0.02	0.12
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD22	2	0.12	0.02	0.12
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD23	2	0.12	0.02	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG11	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG12	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG13	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG21	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG22	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG23	2	0.12	0.01	0.12

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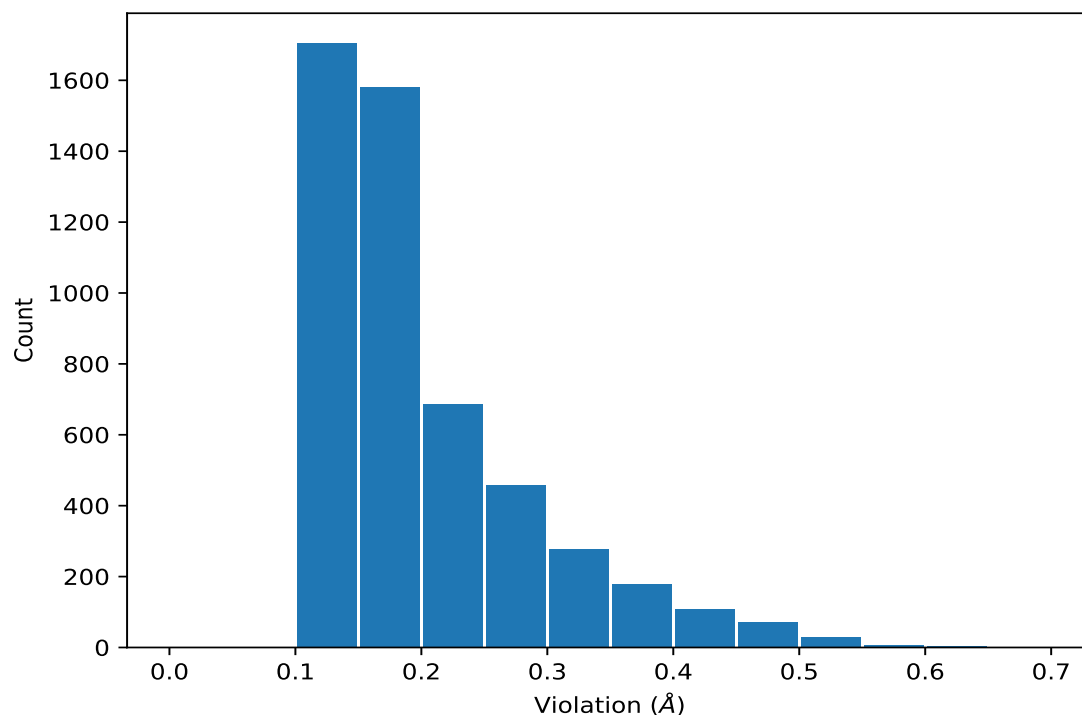
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG11	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG12	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG13	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG21	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG22	2	0.12	0.01	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG23	2	0.12	0.01	0.12
(1,2137)	1:87:X:ARG:HD2	1:131:X:ALA:HA	2	0.12	0.02	0.12
(1,2137)	1:87:X:ARG:HD3	1:131:X:ALA:HA	2	0.12	0.02	0.12
(1,231)	1:43:X:ILE:HG13	1:54:X:LEU:HA	2	0.12	0.01	0.12
(1,264)	1:111:X:ASP:HA	1:112:X:LEU:HB3	2	0.12	0.01	0.12
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG11	2	0.12	0.01	0.12
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG12	2	0.12	0.01	0.12
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG13	2	0.12	0.01	0.12
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG21	2	0.12	0.01	0.12
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG22	2	0.12	0.01	0.12
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG23	2	0.12	0.01	0.12
(1,2260)	1:102:X:LEU:HD11	1:122:X:GLU:HG2	2	0.12	0.01	0.12
(1,2260)	1:102:X:LEU:HD12	1:122:X:GLU:HG2	2	0.12	0.01	0.12
(1,2260)	1:102:X:LEU:HD13	1:122:X:GLU:HG2	2	0.12	0.01	0.12
(1,2260)	1:102:X:LEU:HD21	1:122:X:GLU:HG2	2	0.12	0.01	0.12
(1,2260)	1:102:X:LEU:HD22	1:122:X:GLU:HG2	2	0.12	0.01	0.12
(1,2260)	1:102:X:LEU:HD23	1:122:X:GLU:HG2	2	0.12	0.01	0.12
(1,1728)	1:28:X:GLN:HG2	1:74:X:PRO:HD3	2	0.12	0.02	0.12
(1,1728)	1:28:X:GLN:HG3	1:74:X:PRO:HD3	2	0.12	0.02	0.12
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD11	2	0.12	0.0	0.12
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD12	2	0.12	0.0	0.12
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD13	2	0.12	0.0	0.12
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE1	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE2	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE3	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE1	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE2	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE3	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE1	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE2	2	0.11	0.0	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE3	2	0.11	0.0	0.11
(1,1100)	1:120:X:LEU:H	1:120:X:LEU:HG	2	0.11	0.0	0.11
(1,2151)	1:90:X:LEU:HB3	1:100:X:SER:HB2	2	0.11	0.0	0.11
(1,2151)	1:90:X:LEU:HB3	1:100:X:SER:HB3	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)
(1,888)	1:121:X:ASP:HB2	1:122:X:GLU:HG3	3	0.67
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	1	0.63
(1,2053)	1:75:X:GLN:HG2	1:76:X:GLU:HG3	5	0.6
(1,2053)	1:75:X:GLN:HG3	1:76:X:GLU:HG3	5	0.6
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	9	0.58
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	9	0.57
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	4	0.56
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	4	0.56
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	6	0.56
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	2	0.54
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	2	0.54
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	7	0.53
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	7	0.53
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	2	0.53
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	10	0.53
(1,1092)	1:30:X:GLN:H	1:30:X:GLN:HB3	2	0.52
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	4	0.52
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	7	0.52
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	10	0.51
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	10	0.51
(1,2053)	1:75:X:GLN:HG2	1:76:X:GLU:HG3	8	0.51
(1,2053)	1:75:X:GLN:HG3	1:76:X:GLU:HG3	8	0.51
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	6	0.51
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	6	0.51
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	6	0.51
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	6	0.51
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	6	0.51
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	6	0.51
(1,1092)	1:30:X:GLN:H	1:30:X:GLN:HB3	1	0.51
(1,996)	1:86:X:ILE:H	1:91:X:MET:HG2	10	0.51
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	8	0.51
(1,871)	1:73:X:PHE:HB2	1:76:X:GLU:HB3	8	0.51
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	8	0.51
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	5	0.5
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	5	0.5
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	8	0.5
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	8	0.5
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	9	0.5
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	4	0.5
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	6	0.49
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	6	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	4	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	4	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	4	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	4	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	4	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	4	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	5	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	5	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	5	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	5	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	5	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	7	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	7	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	7	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	7	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	7	0.49
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	7	0.49
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	3	0.49
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	5	0.49
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	6	0.49
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	8	0.49
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	3	0.49
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	6	0.49
(1,1901)	1:48:X:LYS:HG2	1:49:X:ASP:H	5	0.48
(1,1901)	1:48:X:LYS:HG3	1:49:X:ASP:H	5	0.48
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	7	0.48
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	1	0.48
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	1	0.48
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	1	0.48
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	10	0.48
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	10	0.48
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	10	0.48
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	3	0.48
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	9	0.48
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	2	0.47
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	2	0.47
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	2	0.47
(1,858)	1:70:X:PRO:HB3	1:76:X:GLU:HB3	5	0.47
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	3	0.47
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	8	0.47
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	3	0.46
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	3	0.46
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	9	0.46
(1,883)	1:136:X:ALA:HB1	1:137:X:PHE:HB3	8	0.46
(1,883)	1:136:X:ALA:HB2	1:137:X:PHE:HB3	8	0.46
(1,883)	1:136:X:ALA:HB3	1:137:X:PHE:HB3	8	0.46
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	1	0.46
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	1	0.46
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	1	0.46
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	6	0.46
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	2	0.45
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	2	0.45
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	10	0.45
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	10	0.45
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	6	0.45
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	10	0.45
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	10	0.45
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	10	0.45
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD11	10	0.45
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD12	10	0.45
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD13	10	0.45
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	3	0.45
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	9	0.45
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	10	0.45
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	10	0.45
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	10	0.45
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	4	0.45
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	2	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	2	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	2	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	2	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	2	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	2	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	9	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	9	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	9	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	9	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	9	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	9	0.44
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	10	0.44
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	2	0.44
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	6	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	1	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	3	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	4	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	5	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	7	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	8	0.44
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	9	0.44
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	5	0.44
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	5	0.44
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	7	0.44
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	7	0.44
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	7	0.44
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	9	0.44
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	1	0.44
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	2	0.44
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	7	0.44
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	3	0.43
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	3	0.43
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	3	0.43
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	3	0.43
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	3	0.43
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	3	0.43
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	9	0.43
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	2	0.43
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	2	0.43
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	5	0.43
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	9	0.43
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	7	0.43
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	1	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	1	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	1	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	1	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	1	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	1	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	8	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	8	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	8	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	8	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	8	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	8	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG11	10	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG12	10	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG13	10	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG21	10	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG22	10	0.42
(1,2046)	1:70:X:PRO:HD2	1:79:X:VAL:HG23	10	0.42
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	7	0.42
(1,1403)	1:36:X:LEU:H	1:37:X:ARG:HB3	6	0.42
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	6	0.42
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	10	0.42
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD11	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD12	1	0.42
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD13	1	0.42
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	8	0.42
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	1	0.42
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	10	0.42
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	9	0.41
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	9	0.41
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	9	0.41
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	9	0.41
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	9	0.41
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	9	0.41
(1,1608)	1:48:X:LYS:H	1:51:X:GLU:HB3	9	0.41
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	5	0.41
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	9	0.41
(1,871)	1:73:X:PHE:HB2	1:76:X:GLU:HB3	5	0.41
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	3	0.41
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	4	0.41
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	8	0.41
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	6	0.41
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	6	0.41
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	6	0.41
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	5	0.41
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	7	0.41
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	1	0.41
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	6	0.4
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	6	0.4
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	7	0.4
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	7	0.4
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	1	0.4
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	9	0.4
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	10	0.4
(1,878)	1:33:X:ILE:HB	1:34:X:GLU:HG3	9	0.4
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	5	0.4
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	6	0.4
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	4	0.4
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	4	0.4
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	4	0.4
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	6	0.4
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	7	0.4
(1,258)	1:53:X:ARG:HB3	1:66:X:ASN:HA	10	0.4
(1,105)	1:106:X:PHE:HD1	1:107:X:THR:HA	9	0.4
(1,89)	1:61:X:LEU:HB2	1:62:X:THR:HA	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	5	0.39
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	5	0.39
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	8	0.39
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	8	0.39
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	8	0.39
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	7	0.39
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	7	0.39
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	7	0.39
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	1	0.39
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	4	0.39
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	8	0.39
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	4	0.39
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	3	0.39
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	8	0.39
(1,818)	1:83:X:TYR:HB3	1:85:X:PRO:HD2	4	0.39
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	10	0.39
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	7	0.39
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	6	0.39
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	6	0.39
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	6	0.39
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	2	0.39
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	3	0.39
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	10	0.39
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	3	0.39
(1,105)	1:106:X:PHE:HD1	1:107:X:THR:HA	8	0.39
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	10	0.39
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	7	0.39
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	8	0.38
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	8	0.38
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	8	0.38
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	8	0.38
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	8	0.38
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	8	0.38
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	3	0.38
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	3	0.38
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB2	1	0.38
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB3	1	0.38
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	3	0.38
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	3	0.38
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	9	0.38
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	9	0.38
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	10	0.38
(1,1608)	1:48:X:LYS:H	1:51:X:GLU:HB3	1	0.38
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	10	0.38
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	10	0.38
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	10	0.38
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	6	0.38
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	3	0.38
(1,973)	1:103:X:VAL:H	1:104:X:ASN:HB3	8	0.38
(1,818)	1:83:X:TYR:HB3	1:85:X:PRO:HD2	8	0.38
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	7	0.38
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE1	9	0.38
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE2	9	0.38
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE3	9	0.38
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	4	0.38
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	4	0.38
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	4	0.38
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	3	0.38
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	2	0.38
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	1	0.37
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	1	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	5	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	5	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	5	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	5	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	5	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	5	0.37
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	1	0.37
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	1	0.37
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	1	0.37
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	8	0.37
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	8	0.37
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	8	0.37
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	2	0.37
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	5	0.37
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	6	0.37
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	7	0.37
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	8	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	2	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	2	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	2	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	7	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	7	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	9	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	9	0.37
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	9	0.37
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	6	0.37
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	4	0.37
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	5	0.37
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	6	0.37
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	8	0.37
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	9	0.37
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	10	0.37
(1,67)	1:67:X:ILE:HA	1:80:X:ILE:HG12	7	0.37
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	6	0.36
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	6	0.36
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	6	0.36
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	6	0.36
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	6	0.36
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	6	0.36
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	4	0.36
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	4	0.36
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	6	0.36
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	6	0.36
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG2	9	0.36
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG3	9	0.36
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	3	0.36
(1,999)	1:86:X:ILE:H	1:131:X:ALA:HB1	3	0.36
(1,999)	1:86:X:ILE:H	1:131:X:ALA:HB2	3	0.36
(1,999)	1:86:X:ILE:H	1:131:X:ALA:HB3	3	0.36
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	8	0.36
(1,929)	1:94:X:GLN:HG3	1:95:X:GLY:H	1	0.36
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	1	0.36
(1,858)	1:70:X:PRO:HB3	1:76:X:GLU:HB3	8	0.36
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	1	0.36
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	4	0.36
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	5	0.36
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	9	0.36
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	2	0.36
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	1	0.36
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	8	0.36
(1,759)	1:37:X:ARG:HB2	1:38:X:ASN:HA	10	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	1	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	1	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	8	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	8	0.36
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	8	0.36
(1,378)	1:33:X:ILE:HD11	1:52:X:TYR:HE1	10	0.36
(1,378)	1:33:X:ILE:HD12	1:52:X:TYR:HE1	10	0.36
(1,378)	1:33:X:ILE:HD13	1:52:X:TYR:HE1	10	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	7	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	7	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	7	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	8	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	8	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	8	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	9	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	9	0.36
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	9	0.36
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	5	0.36
(1,202)	1:36:X:LEU:HB3	1:113:X:GLY:HA3	7	0.36
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	1	0.36
(1,147)	1:120:X:LEU:HB3	1:121:X:ASP:HA	7	0.36
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	7	0.36
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	6	0.36
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	7	0.36
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	6	0.35
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	6	0.35
(1,1388)	1:33:X:ILE:H	1:34:X:GLU:HG3	4	0.35
(1,1109)	1:120:X:LEU:H	1:121:X:ASP:HB3	10	0.35
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	6	0.35
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	1	0.35
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	3	0.35
(1,839)	1:102:X:LEU:HD21	1:122:X:GLU:HG3	3	0.35
(1,839)	1:102:X:LEU:HD22	1:122:X:GLU:HG3	3	0.35
(1,839)	1:102:X:LEU:HD23	1:122:X:GLU:HG3	3	0.35
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	6	0.35
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	7	0.35
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	10	0.35
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	5	0.35
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	6	0.35
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	4	0.35
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	6	0.35
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	6	0.35
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	4	0.35
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	4	0.35
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	4	0.35
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	6	0.35
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	6	0.35
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	6	0.35
(1,405)	1:115:X:ILE:HA	1:115:X:ILE:HD11	1	0.35
(1,405)	1:115:X:ILE:HA	1:115:X:ILE:HD12	1	0.35
(1,405)	1:115:X:ILE:HA	1:115:X:ILE:HD13	1	0.35
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	2	0.35
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	6	0.35
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG11	7	0.34
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG12	7	0.34
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG13	7	0.34
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG21	7	0.34
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG22	7	0.34
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG23	7	0.34
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG11	7	0.34
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG12	7	0.34
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG13	7	0.34
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG21	7	0.34
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG22	7	0.34
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG23	7	0.34
(1,2052)	1:75:X:GLN:HG2	1:76:X:GLU:HB3	9	0.34
(1,2052)	1:75:X:GLN:HG3	1:76:X:GLU:HB3	9	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	10	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	10	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	10	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	10	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	10	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	10	0.34
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	7	0.34
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	7	0.34
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG2	6	0.34
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG3	6	0.34
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG2	6	0.34
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG3	6	0.34
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	1	0.34
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	5	0.34
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	2	0.34
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	2	0.34
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:86:X:ILE:HD11	1:91:X:MET:HB2	1	0.34
(1,445)	1:86:X:ILE:HD12	1:91:X:MET:HB2	1	0.34
(1,445)	1:86:X:ILE:HD13	1:91:X:MET:HB2	1	0.34
(1,445)	1:86:X:ILE:HD11	1:91:X:MET:HB2	10	0.34
(1,445)	1:86:X:ILE:HD12	1:91:X:MET:HB2	10	0.34
(1,445)	1:86:X:ILE:HD13	1:91:X:MET:HB2	10	0.34
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	3	0.34
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	3	0.34
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	3	0.34
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE1	4	0.34
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE2	4	0.34
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE3	4	0.34
(1,378)	1:33:X:ILE:HD11	1:52:X:TYR:HE1	1	0.34
(1,378)	1:33:X:ILE:HD12	1:52:X:TYR:HE1	1	0.34
(1,378)	1:33:X:ILE:HD13	1:52:X:TYR:HE1	1	0.34
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	3	0.34
(1,105)	1:106:X:PHE:HD1	1:107:X:THR:HA	1	0.34
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	7	0.34
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	1	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	1	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	1	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	1	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	1	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	1	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	3	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	3	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	3	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	3	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	3	0.33
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	3	0.33
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	5	0.33
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	5	0.33
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	5	0.33
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	5	0.33
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	5	0.33
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	5	0.33
(1,1745)	1:29:X:LYS:HG2	1:73:X:PHE:HD1	4	0.33
(1,1745)	1:29:X:LYS:HG3	1:73:X:PHE:HD1	4	0.33
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	3	0.33
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	5	0.33
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	5	0.33
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	2	0.33
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	4	0.33
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	5	0.33
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	10	0.33
(1,929)	1:94:X:GLN:HG3	1:95:X:GLY:H	5	0.33
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	9	0.33
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	9	0.33
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	9	0.33
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	9	0.33
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	3	0.33
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	3	0.33
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	3	0.33
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	7	0.33
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	7	0.33
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	7	0.33
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	1	0.33
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	1	0.33
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	1	0.33
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	5	0.33
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	5	0.33
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	5	0.33
(1,67)	1:67:X:ILE:HA	1:80:X:ILE:HG12	6	0.33
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	8	0.33
(1,2339)	1:122:X:GLU:HA	1:125:X:LYS:HG2	3	0.32
(1,2339)	1:122:X:GLU:HA	1:125:X:LYS:HG3	3	0.32
(1,2177)	1:91:X:MET:HG2	1:95:X:GLY:HA2	10	0.32
(1,2177)	1:91:X:MET:HG2	1:95:X:GLY:HA3	10	0.32
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG11	5	0.32
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG12	5	0.32
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG13	5	0.32
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG21	5	0.32
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG22	5	0.32
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG23	5	0.32
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG11	5	0.32
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG12	5	0.32
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG13	5	0.32
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG21	5	0.32
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG22	5	0.32
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG23	5	0.32
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	2	0.32
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	2	0.32
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG2	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG3	8	0.32
(1,1678)	1:140:X:LEU:HD11	1:141:X:TYR:HE1	2	0.32
(1,1678)	1:140:X:LEU:HD12	1:141:X:TYR:HE1	2	0.32
(1,1678)	1:140:X:LEU:HD13	1:141:X:TYR:HE1	2	0.32
(1,1600)	1:46:X:ILE:H	1:47:X:GLN:HB3	1	0.32
(1,1600)	1:46:X:ILE:H	1:47:X:GLN:HB3	9	0.32
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	2	0.32
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	4	0.32
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	7	0.32
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	1	0.32
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	4	0.32
(1,1012)	1:96:X:VAL:HB	1:97:X:TYR:H	4	0.32
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	8	0.32
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	9	0.32
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	3	0.32
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	3	0.32
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	3	0.32
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE1	8	0.32
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE2	8	0.32
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE3	8	0.32
(1,380)	1:43:X:ILE:HD11	1:52:X:TYR:HE1	10	0.32
(1,380)	1:43:X:ILE:HD12	1:52:X:TYR:HE1	10	0.32
(1,380)	1:43:X:ILE:HD13	1:52:X:TYR:HE1	10	0.32
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	2	0.32
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	2	0.32
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	2	0.32
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	2	0.32
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	7	0.32
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	2	0.32
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	1	0.31
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	1	0.31
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	9	0.31
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	9	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG2	1	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG3	1	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG2	5	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG3	5	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG2	7	0.31
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG3	7	0.31
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD11	10	0.31
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD12	10	0.31
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD13	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	9	0.31
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	9	0.31
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	4	0.31
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	5	0.31
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	8	0.31
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	8	0.31
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	5	0.31
(1,996)	1:86:X:ILE:H	1:91:X:MET:HG2	7	0.31
(1,929)	1:94:X:GLN:HG3	1:95:X:GLY:H	6	0.31
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	7	0.31
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	7	0.31
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	7	0.31
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	9	0.31
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	9	0.31
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	9	0.31
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	9	0.31
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	9	0.31
(1,809)	1:62:X:THR:HA	1:63:X:ILE:HG13	1	0.31
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	3	0.31
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	8	0.31
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	8	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	5	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	5	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	5	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	6	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	6	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	6	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	9	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	9	0.31
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	9	0.31
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	3	0.31
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	3	0.31
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	3	0.31
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	5	0.31
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	5	0.31
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	5	0.31
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	4	0.31
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	2	0.31
(1,105)	1:106:X:PHE:HD1	1:107:X:THR:HA	2	0.31
(1,105)	1:106:X:PHE:HD1	1:107:X:THR:HA	3	0.31
(1,2303)	1:116:X:ILE:H	1:117:X:GLN:HG2	10	0.3
(1,2303)	1:116:X:ILE:H	1:117:X:GLN:HG3	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	2	0.3
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	2	0.3
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG11	4	0.3
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG12	4	0.3
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG13	4	0.3
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG21	4	0.3
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG22	4	0.3
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG23	4	0.3
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	3	0.3
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	3	0.3
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	3	0.3
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	3	0.3
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	3	0.3
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	3	0.3
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	3	0.3
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	3	0.3
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	3	0.3
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	3	0.3
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	3	0.3
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	3	0.3
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	3	0.3
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	3	0.3
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	9	0.3
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	9	0.3
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	3	0.3
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	3	0.3
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	3	0.3
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	3	0.3
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	3	0.3
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	3	0.3
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG2	4	0.3
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG3	4	0.3
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG2	4	0.3
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG3	4	0.3
(1,1595)	1:43:X:ILE:HG13	1:44:X:ALA:H	10	0.3
(1,1533)	1:130:X:LEU:HB2	1:131:X:ALA:H	2	0.3
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	5	0.3
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	2	0.3
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	2	0.3
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	2	0.3
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	9	0.3
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	2	0.3
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	3	0.3
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	6	0.3
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	1	0.3
(1,978)	1:39:X:SER:H	1:40:X:HIS:HB3	7	0.3
(1,973)	1:103:X:VAL:H	1:104:X:ASN:HB3	4	0.3
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	2	0.3
(1,823)	1:137:X:PHE:HB3	1:137:X:PHE:HD1	8	0.3
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	9	0.3
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	9	0.3
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	9	0.3
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD11	5	0.3
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD12	5	0.3
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD13	5	0.3
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	8	0.3
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	8	0.3
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	8	0.3
(1,445)	1:86:X:ILE:HD11	1:91:X:MET:HB2	5	0.3
(1,445)	1:86:X:ILE:HD12	1:91:X:MET:HB2	5	0.3
(1,445)	1:86:X:ILE:HD13	1:91:X:MET:HB2	5	0.3
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE1	2	0.3
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE2	2	0.3
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE3	2	0.3
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE1	6	0.3
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE2	6	0.3
(1,396)	1:91:X:MET:HB3	1:91:X:MET:HE3	6	0.3
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	7	0.3
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	10	0.3
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	5	0.3
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	7	0.3
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	6	0.3
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	9	0.3
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	10	0.3
(1,150)	1:33:X:ILE:HB	1:49:X:ASP:HA	8	0.3
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	10	0.3
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	1	0.3
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG2	2	0.29
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG3	2	0.29
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG2	4	0.29
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG3	4	0.29
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG11	9	0.29
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG12	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG13	9	0.29
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG21	9	0.29
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG22	9	0.29
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG23	9	0.29
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG11	9	0.29
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG12	9	0.29
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG13	9	0.29
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG21	9	0.29
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG22	9	0.29
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG23	9	0.29
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	1	0.29
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	1	0.29
(1,2085)	1:80:X:ILE:HD11	1:106:X:PHE:HB2	7	0.29
(1,2085)	1:80:X:ILE:HD11	1:106:X:PHE:HB3	7	0.29
(1,2085)	1:80:X:ILE:HD12	1:106:X:PHE:HB2	7	0.29
(1,2085)	1:80:X:ILE:HD12	1:106:X:PHE:HB3	7	0.29
(1,2085)	1:80:X:ILE:HD13	1:106:X:PHE:HB2	7	0.29
(1,2085)	1:80:X:ILE:HD13	1:106:X:PHE:HB3	7	0.29
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	7	0.29
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	7	0.29
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	7	0.29
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	7	0.29
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	7	0.29
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	7	0.29
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	4	0.29
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	4	0.29
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	4	0.29
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	4	0.29
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	4	0.29
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	4	0.29
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	5	0.29
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	5	0.29
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	5	0.29
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	5	0.29
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	5	0.29
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	5	0.29
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	7	0.29
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	7	0.29
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	7	0.29
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	7	0.29
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	7	0.29
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	7	0.29
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	7	0.29
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	7	0.29
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	7	0.29
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	7	0.29
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	7	0.29
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	7	0.29
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	7	0.29
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	7	0.29
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	7	0.29
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	7	0.29
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	7	0.29
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	7	0.29
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	7	0.29
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	7	0.29
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	7	0.29
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	7	0.29
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	7	0.29
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	7	0.29
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	7	0.29
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	7	0.29
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	7	0.29
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	7	0.29
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	7	0.29
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	7	0.29
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	7	0.29
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	7	0.29
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	7	0.29
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	7	0.29
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	7	0.29
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG2	7	0.29
(1,1755)	1:30:X:GLN:H	1:30:X:GLN:HG3	7	0.29
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	6	0.29
(1,1595)	1:43:X:ILE:HG13	1:44:X:ALA:H	2	0.29
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	1	0.29
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	10	0.29
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	2	0.29
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	4	0.29
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	6	0.29
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	7	0.29
(1,1076)	1:96:X:VAL:H	1:96:X:VAL:HB	8	0.29
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	5	0.29
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	7	0.29
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	9	0.29
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	10	0.29
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	7	0.29
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	10	0.29
(1,929)	1:94:X:GLN:HG3	1:95:X:GLY:H	3	0.29
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	6	0.29
(1,899)	1:52:X:TYR:HB3	1:67:X:ILE:HG12	4	0.29
(1,883)	1:136:X:ALA:HB1	1:137:X:PHE:HB3	2	0.29
(1,883)	1:136:X:ALA:HB2	1:137:X:PHE:HB3	2	0.29
(1,883)	1:136:X:ALA:HB3	1:137:X:PHE:HB3	2	0.29
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	2	0.29
(1,818)	1:83:X:TYR:HB3	1:85:X:PRO:HD2	1	0.29
(1,788)	1:37:X:ARG:HA	1:43:X:ILE:HG12	10	0.29
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	5	0.29
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	1	0.29
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	4	0.29
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	4	0.29
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	4	0.29
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	1	0.29
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	1	0.29
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	1	0.29
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG21	10	0.29
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG22	10	0.29
(1,516)	1:56:X:PHE:HB2	1:63:X:ILE:HG23	10	0.29
(1,445)	1:86:X:ILE:HD11	1:91:X:MET:HB2	7	0.29
(1,445)	1:86:X:ILE:HD12	1:91:X:MET:HB2	7	0.29
(1,445)	1:86:X:ILE:HD13	1:91:X:MET:HB2	7	0.29
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	5	0.29
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	5	0.29
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	5	0.29
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	7	0.29
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	7	0.29
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	7	0.29
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	8	0.29
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD11	3	0.29
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD12	3	0.29
(1,255)	1:66:X:ASN:HA	1:67:X:ILE:HD13	3	0.29
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	4	0.29
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	10	0.29
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG11	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG12	2	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG13	2	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG21	2	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG22	2	0.28
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG23	2	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG11	2	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG12	2	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG13	2	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG21	2	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG22	2	0.28
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG23	2	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG11	8	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG12	8	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG13	8	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG21	8	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG22	8	0.28
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG23	8	0.28
(1,2085)	1:80:X:ILE:HD11	1:106:X:PHE:HB2	6	0.28
(1,2085)	1:80:X:ILE:HD11	1:106:X:PHE:HB3	6	0.28
(1,2085)	1:80:X:ILE:HD12	1:106:X:PHE:HB2	6	0.28
(1,2085)	1:80:X:ILE:HD12	1:106:X:PHE:HB3	6	0.28
(1,2085)	1:80:X:ILE:HD13	1:106:X:PHE:HB2	6	0.28
(1,2085)	1:80:X:ILE:HD13	1:106:X:PHE:HB3	6	0.28
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	1	0.28
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	1	0.28
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	5	0.28
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	5	0.28
(1,1810)	1:36:X:LEU:H	1:112:X:LEU:HD11	1	0.28
(1,1810)	1:36:X:LEU:H	1:112:X:LEU:HD12	1	0.28
(1,1810)	1:36:X:LEU:H	1:112:X:LEU:HD13	1	0.28
(1,1810)	1:36:X:LEU:H	1:112:X:LEU:HD21	1	0.28
(1,1810)	1:36:X:LEU:H	1:112:X:LEU:HD22	1	0.28
(1,1810)	1:36:X:LEU:H	1:112:X:LEU:HD23	1	0.28
(1,1745)	1:29:X:LYS:HG2	1:73:X:PHE:HD1	3	0.28
(1,1745)	1:29:X:LYS:HG3	1:73:X:PHE:HD1	3	0.28
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG2	9	0.28
(1,1719)	1:26:X:GLN:HA	1:26:X:GLN:HG3	9	0.28
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	2	0.28
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	4	0.28
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	3	0.28
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	7	0.28
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	2	0.28
(1,1058)	1:124:X:TRP:H	1:124:X:TRP:HB3	8	0.28
(1,1055)	1:73:X:PHE:HD1	1:76:X:GLU:H	2	0.28
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	10	0.28
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	4	0.28
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	10	0.28
(1,718)	1:33:X:ILE:HB	1:34:X:GLU:HB2	7	0.28
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	9	0.28
(1,202)	1:36:X:LEU:HB3	1:113:X:GLY:HA3	6	0.28
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	10	0.28
(1,69)	1:57:X:THR:HA	1:61:X:LEU:HB2	5	0.28
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	9	0.28
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	6	0.28
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD11	5	0.27
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD12	5	0.27
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD13	5	0.27
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD21	5	0.27
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD22	5	0.27
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD23	5	0.27
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	9	0.27
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	9	0.27
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	4	0.27
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	4	0.27
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB2	4	0.27
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB3	4	0.27
(1,1614)	1:57:X:THR:HG21	1:60:X:ASN:H	9	0.27
(1,1614)	1:57:X:THR:HG22	1:60:X:ASN:H	9	0.27
(1,1614)	1:57:X:THR:HG23	1:60:X:ASN:H	9	0.27
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	6	0.27
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	8	0.27
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	1	0.27
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	7	0.27
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	10	0.27
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	6	0.27
(1,1089)	1:125:X:LYS:H	1:125:X:LYS:HB3	9	0.27
(1,1076)	1:96:X:VAL:H	1:96:X:VAL:HB	4	0.27
(1,1012)	1:96:X:VAL:HB	1:97:X:TYR:H	8	0.27
(1,973)	1:103:X:VAL:H	1:104:X:ASN:HB3	5	0.27
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	6	0.27
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	6	0.27
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	6	0.27
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	9	0.27
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	10	0.27
(1,883)	1:136:X:ALA:HB1	1:137:X:PHE:HB3	1	0.27
(1,883)	1:136:X:ALA:HB2	1:137:X:PHE:HB3	1	0.27
(1,883)	1:136:X:ALA:HB3	1:137:X:PHE:HB3	1	0.27
(1,872)	1:80:X:ILE:HD11	1:103:X:VAL:HB	7	0.27
(1,872)	1:80:X:ILE:HD12	1:103:X:VAL:HB	7	0.27
(1,872)	1:80:X:ILE:HD13	1:103:X:VAL:HB	7	0.27
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	8	0.27
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	8	0.27
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	8	0.27
(1,831)	1:34:X:GLU:HG3	1:35:X:SER:HA	4	0.27
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	3	0.27
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	9	0.27
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	10	0.27
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	10	0.27
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	10	0.27
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	10	0.27
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	1	0.27
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	1	0.27
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	1	0.27
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	5	0.27
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	6	0.27
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	3	0.27
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	9	0.27
(1,180)	1:48:X:LYS:HA	1:48:X:LYS:HD2	5	0.27
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	10	0.27
(1,2375)	1:137:X:PHE:HD1	1:140:X:LEU:HD11	10	0.26
(1,2375)	1:137:X:PHE:HD1	1:140:X:LEU:HD12	10	0.26
(1,2375)	1:137:X:PHE:HD1	1:140:X:LEU:HD13	10	0.26
(1,2375)	1:137:X:PHE:HD1	1:140:X:LEU:HD21	10	0.26
(1,2375)	1:137:X:PHE:HD1	1:140:X:LEU:HD22	10	0.26
(1,2375)	1:137:X:PHE:HD1	1:140:X:LEU:HD23	10	0.26
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG2	10	0.26
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG3	10	0.26
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD11	6	0.26
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD12	6	0.26
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD13	6	0.26
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD21	6	0.26
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD22	6	0.26
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD23	6	0.26
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	5	0.26
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	5	0.26
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	5	0.26
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	5	0.26
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	5	0.26
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	9	0.26
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	9	0.26
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	9	0.26
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	9	0.26
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	9	0.26
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	9	0.26
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	6	0.26
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	5	0.26
(1,1581)	1:66:X:ASN:H	1:67:X:ILE:HG12	10	0.26
(1,1441)	1:90:X:LEU:H	1:91:X:MET:HB3	10	0.26
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	9	0.26
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	1	0.26
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	5	0.26
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	10	0.26
(1,996)	1:86:X:ILE:H	1:91:X:MET:HG2	1	0.26
(1,883)	1:136:X:ALA:HB1	1:137:X:PHE:HB3	4	0.26
(1,883)	1:136:X:ALA:HB2	1:137:X:PHE:HB3	4	0.26
(1,883)	1:136:X:ALA:HB3	1:137:X:PHE:HB3	4	0.26
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	3	0.26
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	3	0.26
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	3	0.26
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	4	0.26
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	4	0.26
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	4	0.26
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	2	0.26
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	6	0.26
(1,718)	1:33:X:ILE:HB	1:34:X:GLU:HB2	10	0.26
(1,675)	1:77:X:LYS:HG2	1:106:X:PHE:HD1	6	0.26
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	5	0.26
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	5	0.26
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	5	0.26
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	4	0.26
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	4	0.26
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	4	0.26
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	5	0.26
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD21	10	0.26
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD22	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD23	10	0.26
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	1	0.26
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	8	0.26
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	4	0.26
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	10	0.26
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	7	0.26
(1,202)	1:36:X:LEU:HB3	1:113:X:GLY:HA3	9	0.26
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	4	0.26
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	5	0.26
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	5	0.26
(1,11)	1:115:X:ILE:HA	1:116:X:ILE:HD11	10	0.26
(1,11)	1:115:X:ILE:HA	1:116:X:ILE:HD12	10	0.26
(1,11)	1:115:X:ILE:HA	1:116:X:ILE:HD13	10	0.26
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	2	0.25
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	2	0.25
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD2	4	0.25
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD3	4	0.25
(1,2294)	1:112:X:LEU:HD11	1:115:X:ILE:HG12	1	0.25
(1,2294)	1:112:X:LEU:HD12	1:115:X:ILE:HG12	1	0.25
(1,2294)	1:112:X:LEU:HD13	1:115:X:ILE:HG12	1	0.25
(1,2294)	1:112:X:LEU:HD21	1:115:X:ILE:HG12	1	0.25
(1,2294)	1:112:X:LEU:HD22	1:115:X:ILE:HG12	1	0.25
(1,2294)	1:112:X:LEU:HD23	1:115:X:ILE:HG12	1	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	7	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	7	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	7	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	7	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	7	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	7	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	8	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	8	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	8	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	8	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	8	0.25
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	8	0.25
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE1	3	0.25
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE2	3	0.25
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE3	3	0.25
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE1	3	0.25
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE2	3	0.25
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE3	3	0.25
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE1	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE2	3	0.25
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE3	3	0.25
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE1	3	0.25
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE2	3	0.25
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE3	3	0.25
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE1	3	0.25
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE2	3	0.25
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE3	3	0.25
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE1	3	0.25
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE2	3	0.25
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE3	3	0.25
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	4	0.25
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	4	0.25
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	4	0.25
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	4	0.25
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	4	0.25
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	4	0.25
(1,1979)	1:61:X:LEU:HA	1:61:X:LEU:HD11	9	0.25
(1,1979)	1:61:X:LEU:HA	1:61:X:LEU:HD12	9	0.25
(1,1979)	1:61:X:LEU:HA	1:61:X:LEU:HD13	9	0.25
(1,1979)	1:61:X:LEU:HA	1:61:X:LEU:HD21	9	0.25
(1,1979)	1:61:X:LEU:HA	1:61:X:LEU:HD22	9	0.25
(1,1979)	1:61:X:LEU:HA	1:61:X:LEU:HD23	9	0.25
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	4	0.25
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	4	0.25
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	2	0.25
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	2	0.25
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	2	0.25
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	2	0.25
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	2	0.25
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	2	0.25
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	6	0.25
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	6	0.25
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	6	0.25
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	6	0.25
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	6	0.25
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	6	0.25
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	2	0.25
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	2	0.25
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	2	0.25
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	2	0.25
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	2	0.25
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	4	0.25
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	4	0.25
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	4	0.25
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	4	0.25
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	4	0.25
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	4	0.25
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	4	0.25
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	4	0.25
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	4	0.25
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	4	0.25
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	4	0.25
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	4	0.25
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	8	0.25
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	1	0.25
(1,1350)	1:43:X:ILE:H	1:54:X:LEU:HB3	3	0.25
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	7	0.25
(1,1051)	1:76:X:GLU:H	1:76:X:GLU:HG3	2	0.25
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	4	0.25
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	6	0.25
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	10	0.25
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	10	0.25
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	10	0.25
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	3	0.25
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	5	0.25
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	7	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	1	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	1	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	1	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	6	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	6	0.25
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	6	0.25
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	5	0.25
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	2	0.25
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	6	0.25
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	7	0.25
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	8	0.25
(1,783)	1:74:X:PRO:HB2	1:106:X:PHE:HE1	10	0.25
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	9	0.25
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	1	0.25
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	3	0.25
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	10	0.25
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	2	0.25
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	8	0.25
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	8	0.25
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	8	0.25
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	6	0.25
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	6	0.25
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	6	0.25
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD11	10	0.25
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD12	10	0.25
(1,433)	1:85:X:PRO:HA	1:86:X:ILE:HD13	10	0.25
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	9	0.25
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	9	0.25
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	9	0.25
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD11	6	0.25
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD12	6	0.25
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD13	6	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE1	2	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE2	2	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE3	2	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE1	4	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE2	4	0.25
(1,327)	1:107:X:THR:HA	1:108:X:MET:HE3	4	0.25
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	4	0.25
(1,295)	1:90:X:LEU:HB2	1:100:X:SER:HA	10	0.25
(1,277)	1:77:X:LYS:HA	1:77:X:LYS:HD3	4	0.25
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	10	0.25
(1,234)	1:143:X:ASN:HA	1:144:X:PRO:HB2	8	0.25
(1,209)	1:77:X:LYS:HD3	1:78:X:PRO:HD3	3	0.25
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	5	0.25
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	8	0.25
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	1	0.25
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD2	8	0.24
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD3	8	0.24
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD2	8	0.24
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD3	8	0.24
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD2	10	0.24
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD3	10	0.24
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD2	10	0.24
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD3	10	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD2	7	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD3	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD2	9	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD3	9	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD2	10	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD3	10	0.24
(1,2344)	1:124:X:TRP:HA	1:125:X:LYS:HG2	3	0.24
(1,2344)	1:124:X:TRP:HA	1:125:X:LYS:HG3	3	0.24
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD2	8	0.24
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD3	8	0.24
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD2	9	0.24
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD3	9	0.24
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	10	0.24
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	10	0.24
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	10	0.24
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	10	0.24
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	10	0.24
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	10	0.24
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	10	0.24
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	10	0.24
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	10	0.24
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	10	0.24
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	10	0.24
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	10	0.24
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	8	0.24
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	8	0.24
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	6	0.24
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	6	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	4	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	4	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	4	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	4	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	4	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	4	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	6	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	6	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	6	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	6	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	6	0.24
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	6	0.24
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	2	0.24
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	2	0.24
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	2	0.24
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	2	0.24
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	2	0.24
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	2	0.24
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	2	0.24
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	2	0.24
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	2	0.24
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	2	0.24
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	2	0.24
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	2	0.24
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	2	0.24
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	2	0.24
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	2	0.24
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	2	0.24
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	2	0.24
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	2	0.24
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	2	0.24
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	2	0.24
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	2	0.24
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	2	0.24
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	2	0.24
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	2	0.24
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	2	0.24
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	2	0.24
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	2	0.24
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	2	0.24
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	2	0.24
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	2	0.24
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	2	0.24
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	2	0.24
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	2	0.24
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	2	0.24
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	2	0.24
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	10	0.24
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	10	0.24
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	10	0.24
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	10	0.24
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	10	0.24
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	10	0.24
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	1	0.24
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	1	0.24
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	1	0.24
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	1	0.24
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	1	0.24
(1,1737)	1:29:X:LYS:HB2	1:73:X:PHE:HD1	8	0.24
(1,1737)	1:29:X:LYS:HB3	1:73:X:PHE:HD1	8	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD11	3	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD12	3	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD13	3	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD21	3	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD22	3	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD23	3	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD11	4	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD12	4	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD13	4	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD21	4	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD22	4	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD23	4	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD11	6	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD12	6	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD13	6	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD21	6	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD22	6	0.24
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD23	6	0.24
(1,1639)	1:138:X:PRO:HB3	1:139:X:TYR:HD1	9	0.24
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	8	0.24
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	8	0.24
(1,920)	1:80:X:ILE:HG12	1:81:X:SER:H	7	0.24
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	4	0.24
(1,883)	1:136:X:ALA:HB1	1:137:X:PHE:HB3	3	0.24
(1,883)	1:136:X:ALA:HB2	1:137:X:PHE:HB3	3	0.24
(1,883)	1:136:X:ALA:HB3	1:137:X:PHE:HB3	3	0.24
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	5	0.24
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	5	0.24
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	5	0.24
(1,839)	1:102:X:LEU:HD21	1:122:X:GLU:HG3	8	0.24
(1,839)	1:102:X:LEU:HD22	1:122:X:GLU:HG3	8	0.24
(1,839)	1:102:X:LEU:HD23	1:122:X:GLU:HG3	8	0.24
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	3	0.24
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	4	0.24
(1,786)	1:100:X:SER:HA	1:101:X:PRO:HB2	9	0.24
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	7	0.24
(1,718)	1:33:X:ILE:HB	1:34:X:GLU:HB2	1	0.24
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	8	0.24
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	8	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG21	2	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG22	2	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG23	2	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG21	4	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG22	4	0.24
(1,559)	1:92:X:ASP:HA	1:99:X:THR:HG23	4	0.24
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD11	7	0.24
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD12	7	0.24
(1,426)	1:32:X:LEU:HA	1:33:X:ILE:HD13	7	0.24
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	2	0.24
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	2	0.24
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	2	0.24
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	2	0.24
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	2	0.24
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	2	0.24
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	2	0.24
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	2	0.24
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	2	0.24
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	4	0.24
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	4	0.24
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	4	0.24
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	1	0.24
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	4	0.24
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	8	0.24
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	10	0.24
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	10	0.24
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD2	6	0.23
(1,2369)	1:131:X:ALA:HA	1:132:X:PRO:HD3	6	0.23
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD2	1	0.23
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD3	1	0.23
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD2	10	0.23
(1,2301)	1:114:X:LYS:HA	1:114:X:LYS:HD3	10	0.23
(1,2222)	1:98:X:VAL:HG11	1:119:X:LEU:HD11	9	0.23
(1,2222)	1:98:X:VAL:HG11	1:119:X:LEU:HD12	9	0.23
(1,2222)	1:98:X:VAL:HG11	1:119:X:LEU:HD13	9	0.23
(1,2222)	1:98:X:VAL:HG11	1:119:X:LEU:HD21	9	0.23
(1,2222)	1:98:X:VAL:HG11	1:119:X:LEU:HD22	9	0.23
(1,2222)	1:98:X:VAL:HG11	1:119:X:LEU:HD23	9	0.23
(1,2222)	1:98:X:VAL:HG12	1:119:X:LEU:HD11	9	0.23
(1,2222)	1:98:X:VAL:HG12	1:119:X:LEU:HD12	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2222)	1:98:X:VAL:HG12	1:119:X:LEU:HD13	9	0.23
(1,2222)	1:98:X:VAL:HG12	1:119:X:LEU:HD21	9	0.23
(1,2222)	1:98:X:VAL:HG12	1:119:X:LEU:HD22	9	0.23
(1,2222)	1:98:X:VAL:HG12	1:119:X:LEU:HD23	9	0.23
(1,2222)	1:98:X:VAL:HG13	1:119:X:LEU:HD11	9	0.23
(1,2222)	1:98:X:VAL:HG13	1:119:X:LEU:HD12	9	0.23
(1,2222)	1:98:X:VAL:HG13	1:119:X:LEU:HD13	9	0.23
(1,2222)	1:98:X:VAL:HG13	1:119:X:LEU:HD21	9	0.23
(1,2222)	1:98:X:VAL:HG13	1:119:X:LEU:HD22	9	0.23
(1,2222)	1:98:X:VAL:HG13	1:119:X:LEU:HD23	9	0.23
(1,2222)	1:98:X:VAL:HG21	1:119:X:LEU:HD11	9	0.23
(1,2222)	1:98:X:VAL:HG21	1:119:X:LEU:HD12	9	0.23
(1,2222)	1:98:X:VAL:HG21	1:119:X:LEU:HD13	9	0.23
(1,2222)	1:98:X:VAL:HG21	1:119:X:LEU:HD21	9	0.23
(1,2222)	1:98:X:VAL:HG21	1:119:X:LEU:HD22	9	0.23
(1,2222)	1:98:X:VAL:HG21	1:119:X:LEU:HD23	9	0.23
(1,2222)	1:98:X:VAL:HG22	1:119:X:LEU:HD11	9	0.23
(1,2222)	1:98:X:VAL:HG22	1:119:X:LEU:HD12	9	0.23
(1,2222)	1:98:X:VAL:HG22	1:119:X:LEU:HD13	9	0.23
(1,2222)	1:98:X:VAL:HG22	1:119:X:LEU:HD21	9	0.23
(1,2222)	1:98:X:VAL:HG22	1:119:X:LEU:HD22	9	0.23
(1,2222)	1:98:X:VAL:HG22	1:119:X:LEU:HD23	9	0.23
(1,2222)	1:98:X:VAL:HG23	1:119:X:LEU:HD11	9	0.23
(1,2222)	1:98:X:VAL:HG23	1:119:X:LEU:HD12	9	0.23
(1,2222)	1:98:X:VAL:HG23	1:119:X:LEU:HD13	9	0.23
(1,2222)	1:98:X:VAL:HG23	1:119:X:LEU:HD21	9	0.23
(1,2222)	1:98:X:VAL:HG23	1:119:X:LEU:HD22	9	0.23
(1,2222)	1:98:X:VAL:HG23	1:119:X:LEU:HD23	9	0.23
(1,2202)	1:94:X:GLN:HG2	1:96:X:VAL:H	10	0.23
(1,2202)	1:94:X:GLN:HG3	1:96:X:VAL:H	10	0.23
(1,2156)	1:90:X:LEU:HD11	1:91:X:MET:HG3	4	0.23
(1,2156)	1:90:X:LEU:HD12	1:91:X:MET:HG3	4	0.23
(1,2156)	1:90:X:LEU:HD13	1:91:X:MET:HG3	4	0.23
(1,2156)	1:90:X:LEU:HD21	1:91:X:MET:HG3	4	0.23
(1,2156)	1:90:X:LEU:HD22	1:91:X:MET:HG3	4	0.23
(1,2156)	1:90:X:LEU:HD23	1:91:X:MET:HG3	4	0.23
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	1	0.23
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	1	0.23
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	1	0.23
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	1	0.23
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	1	0.23
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG11	7	0.23
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG12	7	0.23
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG13	7	0.23
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG21	7	0.23
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG22	7	0.23
(1,2087)	1:81:X:SER:HA	1:96:X:VAL:HG23	7	0.23
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	7	0.23
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	7	0.23
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	7	0.23
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	7	0.23
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	7	0.23
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	7	0.23
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB2	9	0.23
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB3	9	0.23
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	4	0.23
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	4	0.23
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	4	0.23
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	4	0.23
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	4	0.23
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	4	0.23
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	2	0.23
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	2	0.23
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	2	0.23
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	2	0.23
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	2	0.23
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	2	0.23
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	2	0.23
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	2	0.23
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	2	0.23
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	2	0.23
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	2	0.23
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	2	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD11	4	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD12	4	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD13	4	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD21	4	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD22	4	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD23	4	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD11	7	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD12	7	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD13	7	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD21	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD22	7	0.23
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD23	7	0.23
(1,1640)	1:138:X:PRO:HB2	1:139:X:TYR:HD1	7	0.23
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	4	0.23
(1,1412)	1:57:X:THR:H	1:57:X:THR:HB	9	0.23
(1,1241)	1:25:X:LEU:HD11	1:29:X:LYS:H	9	0.23
(1,1241)	1:25:X:LEU:HD12	1:29:X:LYS:H	9	0.23
(1,1241)	1:25:X:LEU:HD13	1:29:X:LYS:H	9	0.23
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	3	0.23
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	4	0.23
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	6	0.23
(1,878)	1:33:X:ILE:HB	1:34:X:GLU:HG3	4	0.23
(1,806)	1:63:X:ILE:HG12	1:64:X:ASN:HA	4	0.23
(1,769)	1:33:X:ILE:HD11	1:69:X:LEU:HB2	4	0.23
(1,769)	1:33:X:ILE:HD12	1:69:X:LEU:HB2	4	0.23
(1,769)	1:33:X:ILE:HD13	1:69:X:LEU:HB2	4	0.23
(1,764)	1:32:X:LEU:HG	1:74:X:PRO:HB2	5	0.23
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD11	4	0.23
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD12	4	0.23
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD13	4	0.23
(1,465)	1:58:X:ILE:HG21	1:61:X:LEU:HB2	9	0.23
(1,465)	1:58:X:ILE:HG22	1:61:X:LEU:HB2	9	0.23
(1,465)	1:58:X:ILE:HG23	1:61:X:LEU:HB2	9	0.23
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	3	0.23
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	3	0.23
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	3	0.23
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	9	0.23
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	9	0.23
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	9	0.23
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	10	0.23
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	10	0.23
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	10	0.23
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	10	0.23
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	10	0.23
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	10	0.23
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	10	0.23
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	10	0.23
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	10	0.23
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	6	0.23
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	6	0.23
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	6	0.23
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	3	0.23
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	3	0.23
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	4	0.23
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	4	0.23
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	4	0.23
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	3	0.23
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	9	0.23
(1,190)	1:25:X:LEU:HA	1:74:X:PRO:HD3	6	0.23
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	1	0.23
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	2	0.23
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	9	0.23
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	4	0.23
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	1	0.22
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	1	0.22
(1,2280)	1:107:X:THR:HG21	1:110:X:SER:HB2	2	0.22
(1,2280)	1:107:X:THR:HG21	1:110:X:SER:HB3	2	0.22
(1,2280)	1:107:X:THR:HG22	1:110:X:SER:HB2	2	0.22
(1,2280)	1:107:X:THR:HG22	1:110:X:SER:HB3	2	0.22
(1,2280)	1:107:X:THR:HG23	1:110:X:SER:HB2	2	0.22
(1,2280)	1:107:X:THR:HG23	1:110:X:SER:HB3	2	0.22
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	2	0.22
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	2	0.22
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	5	0.22
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	5	0.22
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	8	0.22
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	8	0.22
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	8	0.22
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	8	0.22
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	8	0.22
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	8	0.22
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	8	0.22
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	8	0.22
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	8	0.22
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	8	0.22
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	8	0.22
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	8	0.22
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD11	9	0.22
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD12	9	0.22
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD13	9	0.22
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD21	9	0.22
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD22	9	0.22
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD23	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	4	0.22
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	4	0.22
(1,2047)	1:72:X:GLN:H	1:72:X:GLN:HG2	7	0.22
(1,2047)	1:72:X:GLN:H	1:72:X:GLN:HG3	7	0.22
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	2	0.22
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	2	0.22
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	7	0.22
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	7	0.22
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	7	0.22
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	7	0.22
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	7	0.22
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	7	0.22
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	6	0.22
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	6	0.22
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	6	0.22
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	6	0.22
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	6	0.22
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	6	0.22
(1,1639)	1:138:X:PRO:HB3	1:139:X:TYR:HD1	4	0.22
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	9	0.22
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	10	0.22
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	3	0.22
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	8	0.22
(1,1277)	1:34:X:GLU:H	1:34:X:GLU:HG2	4	0.22
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	2	0.22
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	7	0.22
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	5	0.22
(1,1094)	1:47:X:GLN:H	1:47:X:GLN:HB3	1	0.22
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	3	0.22
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	8	0.22
(1,878)	1:33:X:ILE:HB	1:34:X:GLU:HG3	5	0.22
(1,868)	1:90:X:LEU:HG	1:122:X:GLU:HB3	1	0.22
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	4	0.22
(1,830)	1:76:X:GLU:HA	1:76:X:GLU:HG2	5	0.22
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	4	0.22
(1,822)	1:121:X:ASP:HB2	1:122:X:GLU:HA	3	0.22
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	1	0.22
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	7	0.22
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	7	0.22
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	7	0.22
(1,578)	1:140:X:LEU:HD21	1:141:X:TYR:HE1	2	0.22
(1,578)	1:140:X:LEU:HD22	1:141:X:TYR:HE1	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:140:X:LEU:HD23	1:141:X:TYR:HE1	2	0.22
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	9	0.22
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	9	0.22
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	9	0.22
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD11	2	0.22
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD12	2	0.22
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD13	2	0.22
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD11	10	0.22
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD12	10	0.22
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD13	10	0.22
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	5	0.22
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	8	0.22
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	7	0.22
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	2	0.22
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	4	0.22
(1,243)	1:54:X:LEU:HG	1:55:X:PRO:HD3	5	0.22
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	2	0.22
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	1	0.22
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	6	0.21
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	6	0.21
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	4	0.21
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	4	0.21
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	4	0.21
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	4	0.21
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	4	0.21
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	4	0.21
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	2	0.21
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	2	0.21
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	8	0.21
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	8	0.21
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	8	0.21
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	8	0.21
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	8	0.21
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	8	0.21
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	8	0.21
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	8	0.21
(1,1784)	1:32:X:LEU:HD11	1:111:X:ASP:HA	3	0.21
(1,1784)	1:32:X:LEU:HD12	1:111:X:ASP:HA	3	0.21
(1,1784)	1:32:X:LEU:HD13	1:111:X:ASP:HA	3	0.21
(1,1784)	1:32:X:LEU:HD21	1:111:X:ASP:HA	3	0.21
(1,1784)	1:32:X:LEU:HD22	1:111:X:ASP:HA	3	0.21
(1,1784)	1:32:X:LEU:HD23	1:111:X:ASP:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	6	0.21
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	6	0.21
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	6	0.21
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	6	0.21
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	6	0.21
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	6	0.21
(1,1745)	1:29:X:LYS:HG2	1:73:X:PHE:HD1	7	0.21
(1,1745)	1:29:X:LYS:HG3	1:73:X:PHE:HD1	7	0.21
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG2	8	0.21
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG3	8	0.21
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD11	5	0.21
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD12	5	0.21
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD13	5	0.21
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD21	5	0.21
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD22	5	0.21
(1,1702)	1:25:X:LEU:HA	1:25:X:LEU:HD23	5	0.21
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD11	5	0.21
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD12	5	0.21
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD13	5	0.21
(1,1595)	1:43:X:ILE:HG13	1:44:X:ALA:H	7	0.21
(1,1546)	1:69:X:LEU:H	1:78:X:PRO:HB2	9	0.21
(1,1490)	1:88:X:HIS:H	1:91:X:MET:HB3	10	0.21
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	6	0.21
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	1	0.21
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	9	0.21
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	7	0.21
(1,1208)	1:47:X:GLN:HG2	1:51:X:GLU:H	10	0.21
(1,1094)	1:47:X:GLN:H	1:47:X:GLN:HB3	9	0.21
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	2	0.21
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	2	0.21
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	2	0.21
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	10	0.21
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	10	0.21
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	10	0.21
(1,776)	1:89:X:HIS:HE1	1:122:X:GLU:HG2	5	0.21
(1,754)	1:77:X:LYS:HB2	1:78:X:PRO:HD3	6	0.21
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	2	0.21
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	7	0.21
(1,657)	1:86:X:ILE:HG13	1:91:X:MET:HB3	6	0.21
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	10	0.21
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	10	0.21
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD11	2	0.21
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD12	2	0.21
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD13	2	0.21
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD11	2	0.21
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD12	2	0.21
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD13	2	0.21
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD11	2	0.21
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD12	2	0.21
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD13	2	0.21
(1,582)	1:22:X:LEU:HA	1:22:X:LEU:HD21	2	0.21
(1,582)	1:22:X:LEU:HA	1:22:X:LEU:HD22	2	0.21
(1,582)	1:22:X:LEU:HA	1:22:X:LEU:HD23	2	0.21
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	10	0.21
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	10	0.21
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	10	0.21
(1,484)	1:74:X:PRO:HD3	1:108:X:MET:HE1	3	0.21
(1,484)	1:74:X:PRO:HD3	1:108:X:MET:HE2	3	0.21
(1,484)	1:74:X:PRO:HD3	1:108:X:MET:HE3	3	0.21
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	3	0.21
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	3	0.21
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	3	0.21
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	1	0.21
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	1	0.21
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	1	0.21
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD11	8	0.21
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD12	8	0.21
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD13	8	0.21
(1,380)	1:43:X:ILE:HD11	1:52:X:TYR:HE1	2	0.21
(1,380)	1:43:X:ILE:HD12	1:52:X:TYR:HE1	2	0.21
(1,380)	1:43:X:ILE:HD13	1:52:X:TYR:HE1	2	0.21
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE1	7	0.21
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE2	7	0.21
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE3	7	0.21
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	1	0.21
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	1	0.21
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	1	0.21
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	7	0.21
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	7	0.21
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	7	0.21
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	5	0.21
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	8	0.21
(1,96)	1:29:X:LYS:HA	1:73:X:PHE:HD1	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2258)	1:102:X:LEU:HD11	1:122:X:GLU:HB3	9	0.2
(1,2258)	1:102:X:LEU:HD12	1:122:X:GLU:HB3	9	0.2
(1,2258)	1:102:X:LEU:HD13	1:122:X:GLU:HB3	9	0.2
(1,2258)	1:102:X:LEU:HD21	1:122:X:GLU:HB3	9	0.2
(1,2258)	1:102:X:LEU:HD22	1:122:X:GLU:HB3	9	0.2
(1,2258)	1:102:X:LEU:HD23	1:122:X:GLU:HB3	9	0.2
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	9	0.2
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	9	0.2
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	9	0.2
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	9	0.2
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	9	0.2
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	9	0.2
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	9	0.2
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	9	0.2
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	9	0.2
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	9	0.2
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	9	0.2
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	9	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD11	4	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD12	4	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD13	4	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD21	4	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD22	4	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD23	4	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD11	7	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD12	7	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD13	7	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD21	7	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD22	7	0.2
(1,2227)	1:100:X:SER:HA	1:102:X:LEU:HD23	7	0.2
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	3	0.2
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	3	0.2
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD11	5	0.2
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD12	5	0.2
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD13	5	0.2
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD21	5	0.2
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD22	5	0.2
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD23	5	0.2
(1,2156)	1:90:X:LEU:HD11	1:91:X:MET:HG3	6	0.2
(1,2156)	1:90:X:LEU:HD12	1:91:X:MET:HG3	6	0.2
(1,2156)	1:90:X:LEU:HD13	1:91:X:MET:HG3	6	0.2
(1,2156)	1:90:X:LEU:HD21	1:91:X:MET:HG3	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2156)	1:90:X:LEU:HD22	1:91:X:MET:HG3	6	0.2
(1,2156)	1:90:X:LEU:HD23	1:91:X:MET:HG3	6	0.2
(1,2077)	1:79:X:VAL:HG11	1:81:X:SER:H	4	0.2
(1,2077)	1:79:X:VAL:HG12	1:81:X:SER:H	4	0.2
(1,2077)	1:79:X:VAL:HG13	1:81:X:SER:H	4	0.2
(1,2077)	1:79:X:VAL:HG21	1:81:X:SER:H	4	0.2
(1,2077)	1:79:X:VAL:HG22	1:81:X:SER:H	4	0.2
(1,2077)	1:79:X:VAL:HG23	1:81:X:SER:H	4	0.2
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD11	2	0.2
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD12	2	0.2
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD13	2	0.2
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD21	2	0.2
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD22	2	0.2
(1,2005)	1:65:X:ILE:HG13	1:119:X:LEU:HD23	2	0.2
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	3	0.2
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	3	0.2
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	7	0.2
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	7	0.2
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	7	0.2
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	7	0.2
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	7	0.2
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	7	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	3	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	3	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	3	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	3	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	3	0.2
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	3	0.2
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG2	1	0.2
(1,1871)	1:43:X:ILE:HD11	1:45:X:GLU:HG3	1	0.2
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG2	1	0.2
(1,1871)	1:43:X:ILE:HD12	1:45:X:GLU:HG3	1	0.2
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG2	1	0.2
(1,1871)	1:43:X:ILE:HD13	1:45:X:GLU:HG3	1	0.2
(1,1831)	1:36:X:LEU:HD11	1:52:X:TYR:HE1	7	0.2
(1,1831)	1:36:X:LEU:HD12	1:52:X:TYR:HE1	7	0.2
(1,1831)	1:36:X:LEU:HD13	1:52:X:TYR:HE1	7	0.2
(1,1831)	1:36:X:LEU:HD21	1:52:X:TYR:HE1	7	0.2
(1,1831)	1:36:X:LEU:HD22	1:52:X:TYR:HE1	7	0.2
(1,1831)	1:36:X:LEU:HD23	1:52:X:TYR:HE1	7	0.2
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG2	7	0.2
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG3	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1679)	1:138:X:PRO:HB3	1:139:X:TYR:HE1	7	0.2
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	1	0.2
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	3	0.2
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	10	0.2
(1,1546)	1:69:X:LEU:H	1:78:X:PRO:HB2	2	0.2
(1,1486)	1:73:X:PHE:H	1:76:X:GLU:HG2	7	0.2
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	1	0.2
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	2	0.2
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	4	0.2
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	4	0.2
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	4	0.2
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	5	0.2
(1,1003)	1:125:X:LYS:HB3	1:126:X:ASN:H	5	0.2
(1,966)	1:91:X:MET:H	1:91:X:MET:HG2	3	0.2
(1,956)	1:72:X:GLN:H	1:72:X:GLN:HB3	1	0.2
(1,956)	1:72:X:GLN:H	1:72:X:GLN:HB3	10	0.2
(1,920)	1:80:X:ILE:HG12	1:81:X:SER:H	6	0.2
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	7	0.2
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	3	0.2
(1,839)	1:102:X:LEU:HD21	1:122:X:GLU:HG3	2	0.2
(1,839)	1:102:X:LEU:HD22	1:122:X:GLU:HG3	2	0.2
(1,839)	1:102:X:LEU:HD23	1:122:X:GLU:HG3	2	0.2
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	7	0.2
(1,742)	1:122:X:GLU:HA	1:125:X:LYS:HB3	4	0.2
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	4	0.2
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	7	0.2
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	10	0.2
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	1	0.2
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	1	0.2
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	1	0.2
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	5	0.2
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	5	0.2
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	5	0.2
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	6	0.2
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	6	0.2
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	6	0.2
(1,654)	1:48:X:LYS:HD3	1:49:X:ASP:HA	5	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	1	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	1	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	1	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	1	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	1	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	1	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	1	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	1	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	8	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	8	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	8	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	8	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	8	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	8	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	8	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	8	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	8	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	9	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	9	0.2
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	9	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	9	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	9	0.2
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	9	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	9	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	9	0.2
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	9	0.2
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	5	0.2
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	5	0.2
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	5	0.2
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	7	0.2
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	7	0.2
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	7	0.2
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	7	0.2
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	9	0.2
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	2	0.2
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	2	0.2
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	2	0.2
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	1	0.2
(1,250)	1:137:X:PHE:HD1	1:138:X:PRO:HD2	4	0.2
(1,249)	1:137:X:PHE:HD1	1:138:X:PRO:HD3	7	0.2
(1,209)	1:77:X:LYS:HD3	1:78:X:PRO:HD3	8	0.2
(1,206)	1:78:X:PRO:HD2	1:106:X:PHE:HE1	1	0.2
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	2	0.2
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	7	0.2
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	4	0.2
(1,150)	1:33:X:ILE:HB	1:49:X:ASP:HA	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	3	0.2
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	9	0.2
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	4	0.2
(1,62)	1:29:X:LYS:HA	1:74:X:PRO:HD2	3	0.2
(1,47)	1:70:X:PRO:HA	1:73:X:PHE:HB2	2	0.2
(1,2294)	1:112:X:LEU:HD11	1:115:X:ILE:HG12	7	0.19
(1,2294)	1:112:X:LEU:HD12	1:115:X:ILE:HG12	7	0.19
(1,2294)	1:112:X:LEU:HD13	1:115:X:ILE:HG12	7	0.19
(1,2294)	1:112:X:LEU:HD21	1:115:X:ILE:HG12	7	0.19
(1,2294)	1:112:X:LEU:HD22	1:115:X:ILE:HG12	7	0.19
(1,2294)	1:112:X:LEU:HD23	1:115:X:ILE:HG12	7	0.19
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	10	0.19
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	10	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	2	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	2	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	2	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	2	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	2	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	2	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	2	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	2	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	2	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	2	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	2	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	2	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	3	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	3	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	3	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	3	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	3	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	3	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	3	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	3	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	3	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	3	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	3	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	3	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	4	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	4	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	4	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	4	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	4	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	4	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	4	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	4	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	4	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	4	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	4	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	5	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	5	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	5	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	5	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	5	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	5	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	5	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	5	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	5	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	5	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	5	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	5	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	6	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	6	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	6	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	6	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	6	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	6	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	6	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	6	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	6	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	6	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	6	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	6	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	7	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	7	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	7	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	7	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	7	0.19
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	7	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	7	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	7	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	7	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	7	0.19
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	7	0.19
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	9	0.19
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	9	0.19
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG11	4	0.19
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG12	4	0.19
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG13	4	0.19
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG21	4	0.19
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG22	4	0.19
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG23	4	0.19
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG11	4	0.19
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG12	4	0.19
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG13	4	0.19
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG21	4	0.19
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG22	4	0.19
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG23	4	0.19
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG11	4	0.19
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG12	4	0.19
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG13	4	0.19
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG21	4	0.19
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG22	4	0.19
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG23	4	0.19
(1,2156)	1:90:X:LEU:HD11	1:91:X:MET:HG3	8	0.19
(1,2156)	1:90:X:LEU:HD12	1:91:X:MET:HG3	8	0.19
(1,2156)	1:90:X:LEU:HD13	1:91:X:MET:HG3	8	0.19
(1,2156)	1:90:X:LEU:HD21	1:91:X:MET:HG3	8	0.19
(1,2156)	1:90:X:LEU:HD22	1:91:X:MET:HG3	8	0.19
(1,2156)	1:90:X:LEU:HD23	1:91:X:MET:HG3	8	0.19
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	10	0.19
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	10	0.19
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	5	0.19
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	5	0.19
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	5	0.19
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	5	0.19
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	5	0.19
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	5	0.19
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	10	0.19
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	10	0.19
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	10	0.19
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	10	0.19
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	10	0.19
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	10	0.19
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	1	0.19
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	10	0.19
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	10	0.19
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	9	0.19
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	9	0.19
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	9	0.19
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	9	0.19
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	9	0.19
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	9	0.19
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD2	7	0.19
(1,1849)	1:37:X:ARG:HA	1:37:X:ARG:HD3	7	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	4	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	4	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	4	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	4	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	4	0.19
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	4	0.19
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	4	0.19
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	4	0.19
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	4	0.19
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	4	0.19
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	4	0.19
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	4	0.19
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	4	0.19
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	4	0.19
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	4	0.19
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	4	0.19
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	4	0.19
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	4	0.19
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	4	0.19
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	4	0.19
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	4	0.19
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	4	0.19
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	4	0.19
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	4	0.19
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	4	0.19
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	4	0.19
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	4	0.19
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	4	0.19
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	4	0.19
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	4	0.19
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	4	0.19
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	4	0.19
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	4	0.19
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	4	0.19
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	4	0.19
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	9	0.19
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	9	0.19
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	9	0.19
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	9	0.19
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	9	0.19
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	9	0.19
(1,1811)	1:36:X:LEU:HA	1:36:X:LEU:HD11	7	0.19
(1,1811)	1:36:X:LEU:HA	1:36:X:LEU:HD12	7	0.19
(1,1811)	1:36:X:LEU:HA	1:36:X:LEU:HD13	7	0.19
(1,1811)	1:36:X:LEU:HA	1:36:X:LEU:HD21	7	0.19
(1,1811)	1:36:X:LEU:HA	1:36:X:LEU:HD22	7	0.19
(1,1811)	1:36:X:LEU:HA	1:36:X:LEU:HD23	7	0.19
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	9	0.19
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	9	0.19
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	9	0.19
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	9	0.19
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	9	0.19
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	9	0.19
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	7	0.19
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	7	0.19
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	7	0.19
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	7	0.19
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	7	0.19
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	7	0.19
(1,1745)	1:29:X:LYS:HG2	1:73:X:PHE:HD1	8	0.19
(1,1745)	1:29:X:LYS:HG3	1:73:X:PHE:HD1	8	0.19
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG2	1	0.19
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG3	1	0.19
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG2	5	0.19
(1,1708)	1:25:X:LEU:HB2	1:26:X:GLN:HG3	5	0.19
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD11	2	0.19
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD12	2	0.19
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD13	2	0.19
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD21	2	0.19
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD22	2	0.19
(1,1686)	1:22:X:LEU:HA	1:22:X:LEU:HD23	2	0.19
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1554)	1:52:X:TYR:H	1:52:X:TYR:HD1	7	0.19
(1,1546)	1:69:X:LEU:H	1:78:X:PRO:HB2	10	0.19
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	9	0.19
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	6	0.19
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	9	0.19
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	10	0.19
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	6	0.19
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	3	0.19
(1,1208)	1:47:X:GLN:HG2	1:51:X:GLU:H	8	0.19
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	8	0.19
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	9	0.19
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	1	0.19
(1,956)	1:72:X:GLN:H	1:72:X:GLN:HB3	9	0.19
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	5	0.19
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	5	0.19
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	5	0.19
(1,905)	1:56:X:PHE:HB2	1:63:X:ILE:HB	2	0.19
(1,839)	1:102:X:LEU:HD21	1:122:X:GLU:HG3	9	0.19
(1,839)	1:102:X:LEU:HD22	1:122:X:GLU:HG3	9	0.19
(1,839)	1:102:X:LEU:HD23	1:122:X:GLU:HG3	9	0.19
(1,783)	1:74:X:PRO:HB2	1:106:X:PHE:HE1	5	0.19
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	9	0.19
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	9	0.19
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	9	0.19
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	1	0.19
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	1	0.19
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	1	0.19
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	2	0.19
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	2	0.19
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	2	0.19
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	4	0.19
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	4	0.19
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	4	0.19
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	8	0.19
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	8	0.19
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	8	0.19
(1,431)	1:86:X:ILE:HD11	1:91:X:MET:HA	8	0.19
(1,431)	1:86:X:ILE:HD12	1:91:X:MET:HA	8	0.19
(1,431)	1:86:X:ILE:HD13	1:91:X:MET:HA	8	0.19
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD11	3	0.19
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD12	3	0.19
(1,411)	1:30:X:GLN:HA	1:33:X:ILE:HD13	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	4	0.19
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	4	0.19
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	4	0.19
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	7	0.19
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	7	0.19
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	7	0.19
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD11	10	0.19
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD12	10	0.19
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD13	10	0.19
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE1	2	0.19
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE2	2	0.19
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE3	2	0.19
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE1	8	0.19
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE2	8	0.19
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE3	8	0.19
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	2	0.19
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	2	0.19
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	2	0.19
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	6	0.19
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	6	0.19
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	6	0.19
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	6	0.19
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	6	0.19
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	6	0.19
(1,190)	1:25:X:LEU:HA	1:74:X:PRO:HD3	2	0.19
(1,153)	1:121:X:ASP:HA	1:124:X:TRP:HB3	4	0.19
(1,150)	1:33:X:ILE:HB	1:49:X:ASP:HA	3	0.19
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	1	0.19
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	2	0.19
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	6	0.19
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	2	0.19
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	5	0.19
(1,96)	1:29:X:LYS:HA	1:73:X:PHE:HD1	7	0.19
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	6	0.19
(1,62)	1:29:X:LYS:HA	1:74:X:PRO:HD2	5	0.19
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	9	0.19
(1,2317)	1:117:X:GLN:HG2	1:118:X:SER:H	5	0.18
(1,2317)	1:117:X:GLN:HG3	1:118:X:SER:H	5	0.18
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD11	6	0.18
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD12	6	0.18
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD13	6	0.18
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD11	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD12	6	0.18
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD13	6	0.18
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD11	6	0.18
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD12	6	0.18
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD13	6	0.18
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD11	6	0.18
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD12	6	0.18
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD13	6	0.18
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD11	6	0.18
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD12	6	0.18
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD13	6	0.18
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD11	6	0.18
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD12	6	0.18
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD13	6	0.18
(1,2294)	1:112:X:LEU:HD11	1:115:X:ILE:HG12	6	0.18
(1,2294)	1:112:X:LEU:HD12	1:115:X:ILE:HG12	6	0.18
(1,2294)	1:112:X:LEU:HD13	1:115:X:ILE:HG12	6	0.18
(1,2294)	1:112:X:LEU:HD21	1:115:X:ILE:HG12	6	0.18
(1,2294)	1:112:X:LEU:HD22	1:115:X:ILE:HG12	6	0.18
(1,2294)	1:112:X:LEU:HD23	1:115:X:ILE:HG12	6	0.18
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	4	0.18
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	4	0.18
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG21	2	0.18
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG22	2	0.18
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG23	2	0.18
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG21	2	0.18
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG22	2	0.18
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG23	2	0.18
(1,2154)	1:90:X:LEU:HG	1:100:X:SER:HB2	9	0.18
(1,2154)	1:90:X:LEU:HG	1:100:X:SER:HB3	9	0.18
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD11	3	0.18
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD12	3	0.18
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD13	3	0.18
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD21	3	0.18
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD22	3	0.18
(1,2148)	1:90:X:LEU:HA	1:119:X:LEU:HD23	3	0.18
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	7	0.18
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	7	0.18
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	9	0.18
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	9	0.18
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	9	0.18
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	9	0.18
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	9	0.18
(1,2047)	1:72:X:GLN:H	1:72:X:GLN:HG2	3	0.18
(1,2047)	1:72:X:GLN:H	1:72:X:GLN:HG3	3	0.18
(1,1999)	1:64:X:ASN:HB2	1:83:X:TYR:H	4	0.18
(1,1999)	1:64:X:ASN:HB3	1:83:X:TYR:H	4	0.18
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	2	0.18
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	2	0.18
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	2	0.18
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	2	0.18
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	2	0.18
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	2	0.18
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	8	0.18
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	8	0.18
(1,1882)	1:45:X:GLU:HG2	1:48:X:LYS:HD2	5	0.18
(1,1882)	1:45:X:GLU:HG3	1:48:X:LYS:HD2	5	0.18
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	3	0.18
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	3	0.18
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	3	0.18
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	3	0.18
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	3	0.18
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	3	0.18
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	8	0.18
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	8	0.18
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	8	0.18
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	8	0.18
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	8	0.18
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	8	0.18
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	8	0.18
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	8	0.18
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	8	0.18
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	8	0.18
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	8	0.18
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	8	0.18
(1,1753)	1:29:X:LYS:HE2	1:69:X:LEU:HB2	8	0.18
(1,1753)	1:29:X:LYS:HE3	1:69:X:LEU:HB2	8	0.18
(1,1737)	1:29:X:LYS:HB2	1:73:X:PHE:HD1	7	0.18
(1,1737)	1:29:X:LYS:HB3	1:73:X:PHE:HD1	7	0.18
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	10	0.18
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	7	0.18
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD11	8	0.18
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD12	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD13	8	0.18
(1,1427)	1:83:X:TYR:H	1:84:X:PRO:HD3	5	0.18
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	1	0.18
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	5	0.18
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	7	0.18
(1,1260)	1:137:X:PHE:HA	1:139:X:TYR:H	8	0.18
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	10	0.18
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	6	0.18
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	9	0.18
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	10	0.18
(1,1014)	1:36:X:LEU:HB2	1:38:X:ASN:H	2	0.18
(1,1000)	1:86:X:ILE:H	1:128:X:PRO:HB3	3	0.18
(1,956)	1:72:X:GLN:H	1:72:X:GLN:HB3	5	0.18
(1,872)	1:80:X:ILE:HD11	1:103:X:VAL:HB	6	0.18
(1,872)	1:80:X:ILE:HD12	1:103:X:VAL:HB	6	0.18
(1,872)	1:80:X:ILE:HD13	1:103:X:VAL:HB	6	0.18
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	8	0.18
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	9	0.18
(1,838)	1:105:X:ASN:HB2	1:115:X:ILE:HD11	6	0.18
(1,838)	1:105:X:ASN:HB2	1:115:X:ILE:HD12	6	0.18
(1,838)	1:105:X:ASN:HB2	1:115:X:ILE:HD13	6	0.18
(1,758)	1:43:X:ILE:HG12	1:52:X:TYR:HB2	2	0.18
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	3	0.18
(1,708)	1:117:X:GLN:HA	1:120:X:LEU:HB2	10	0.18
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	2	0.18
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	2	0.18
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	2	0.18
(1,684)	1:106:X:PHE:HE1	1:112:X:LEU:HB3	5	0.18
(1,656)	1:77:X:LYS:HD3	1:106:X:PHE:HB3	7	0.18
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	6	0.18
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	6	0.18
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	6	0.18
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	6	0.18
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	6	0.18
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	6	0.18
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD11	10	0.18
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD12	10	0.18
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD13	10	0.18
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD11	10	0.18
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD12	10	0.18
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD13	10	0.18
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD11	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD12	10	0.18
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD13	10	0.18
(1,441)	1:58:X:ILE:HD11	1:126:X:ASN:HA	6	0.18
(1,441)	1:58:X:ILE:HD12	1:126:X:ASN:HA	6	0.18
(1,441)	1:58:X:ILE:HD13	1:126:X:ASN:HA	6	0.18
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	7	0.18
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	7	0.18
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	7	0.18
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	7	0.18
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	7	0.18
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	7	0.18
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	7	0.18
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	7	0.18
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	7	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	1	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	1	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	1	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	3	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	3	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	3	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	8	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	8	0.18
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	8	0.18
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	9	0.18
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	9	0.18
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	9	0.18
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	8	0.18
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	8	0.18
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	8	0.18
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	6	0.18
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	6	0.18
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	6	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	5	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	5	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	5	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	8	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	8	0.18
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	8	0.18
(1,334)	1:93:X:LYS:HA	1:93:X:LYS:HD3	5	0.18
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	10	0.18
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	10	0.18
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:76:X:GLU:HA	1:76:X:GLU:HG3	8	0.18
(1,250)	1:137:X:PHE:HD1	1:138:X:PRO:HD2	6	0.18
(1,236)	1:58:X:ILE:HD11	1:127:X:PRO:HD2	10	0.18
(1,236)	1:58:X:ILE:HD12	1:127:X:PRO:HD2	10	0.18
(1,236)	1:58:X:ILE:HD13	1:127:X:PRO:HD2	10	0.18
(1,206)	1:78:X:PRO:HD2	1:106:X:PHE:HE1	8	0.18
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	3	0.18
(1,199)	1:113:X:GLY:HA2	1:114:X:LYS:HB3	6	0.18
(1,153)	1:121:X:ASP:HA	1:124:X:TRP:HB3	9	0.18
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	10	0.18
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	8	0.18
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	2	0.18
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	2	0.18
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	2	0.18
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	7	0.18
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	7	0.18
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	7	0.18
(1,47)	1:70:X:PRO:HA	1:73:X:PHE:HB2	3	0.18
(1,3)	1:23:X:THR:HB	1:26:X:GLN:HA	9	0.18
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	9	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	9	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	9	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	9	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	9	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	9	0.17
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	9	0.17
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	9	0.17
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	9	0.17
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	9	0.17
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	9	0.17
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	9	0.17
(1,2312)	1:117:X:GLN:H	1:117:X:GLN:HG2	10	0.17
(1,2312)	1:117:X:GLN:H	1:117:X:GLN:HG3	10	0.17
(1,2306)	1:116:X:ILE:HA	1:119:X:LEU:HD11	3	0.17
(1,2306)	1:116:X:ILE:HA	1:119:X:LEU:HD12	3	0.17
(1,2306)	1:116:X:ILE:HA	1:119:X:LEU:HD13	3	0.17
(1,2306)	1:116:X:ILE:HA	1:119:X:LEU:HD21	3	0.17
(1,2306)	1:116:X:ILE:HA	1:119:X:LEU:HD22	3	0.17
(1,2306)	1:116:X:ILE:HA	1:119:X:LEU:HD23	3	0.17
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	8	0.17
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	8	0.17
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	9	0.17
(1,2258)	1:102:X:LEU:HD11	1:122:X:GLU:HB3	3	0.17
(1,2258)	1:102:X:LEU:HD12	1:122:X:GLU:HB3	3	0.17
(1,2258)	1:102:X:LEU:HD13	1:122:X:GLU:HB3	3	0.17
(1,2258)	1:102:X:LEU:HD21	1:122:X:GLU:HB3	3	0.17
(1,2258)	1:102:X:LEU:HD22	1:122:X:GLU:HB3	3	0.17
(1,2258)	1:102:X:LEU:HD23	1:122:X:GLU:HB3	3	0.17
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG21	4	0.17
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG22	4	0.17
(1,2187)	1:92:X:ASP:HB2	1:99:X:THR:HG23	4	0.17
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG21	4	0.17
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG22	4	0.17
(1,2187)	1:92:X:ASP:HB3	1:99:X:THR:HG23	4	0.17
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	10	0.17
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	10	0.17
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	10	0.17
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	10	0.17
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	10	0.17
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	10	0.17
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	3	0.17
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	3	0.17
(1,2091)	1:81:X:SER:HB2	1:96:X:VAL:HB	6	0.17
(1,2091)	1:81:X:SER:HB3	1:96:X:VAL:HB	6	0.17
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD11	7	0.17
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD12	7	0.17
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD13	7	0.17
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD21	7	0.17
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD22	7	0.17
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD23	7	0.17
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD11	7	0.17
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD12	7	0.17
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD13	7	0.17
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD21	7	0.17
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD22	7	0.17
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD23	7	0.17
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD11	7	0.17
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD12	7	0.17
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD13	7	0.17
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD21	7	0.17
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD22	7	0.17
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD23	7	0.17
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD11	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD12	7	0.17
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD13	7	0.17
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD21	7	0.17
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD22	7	0.17
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD23	7	0.17
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD11	7	0.17
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD12	7	0.17
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD13	7	0.17
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD21	7	0.17
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD22	7	0.17
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD23	7	0.17
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD11	7	0.17
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD12	7	0.17
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD13	7	0.17
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD21	7	0.17
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD22	7	0.17
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD23	7	0.17
(1,2034)	1:69:X:LEU:HD11	1:70:X:PRO:HD3	1	0.17
(1,2034)	1:69:X:LEU:HD12	1:70:X:PRO:HD3	1	0.17
(1,2034)	1:69:X:LEU:HD13	1:70:X:PRO:HD3	1	0.17
(1,2034)	1:69:X:LEU:HD21	1:70:X:PRO:HD3	1	0.17
(1,2034)	1:69:X:LEU:HD22	1:70:X:PRO:HD3	1	0.17
(1,2034)	1:69:X:LEU:HD23	1:70:X:PRO:HD3	1	0.17
(1,1989)	1:61:X:LEU:HD11	1:128:X:PRO:HG3	2	0.17
(1,1989)	1:61:X:LEU:HD12	1:128:X:PRO:HG3	2	0.17
(1,1989)	1:61:X:LEU:HD13	1:128:X:PRO:HG3	2	0.17
(1,1989)	1:61:X:LEU:HD21	1:128:X:PRO:HG3	2	0.17
(1,1989)	1:61:X:LEU:HD22	1:128:X:PRO:HG3	2	0.17
(1,1989)	1:61:X:LEU:HD23	1:128:X:PRO:HG3	2	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	1	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	1	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	1	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	1	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	1	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	1	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	4	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	4	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	4	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	4	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	4	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	4	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	6	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	6	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	6	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	6	0.17
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	6	0.17
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	8	0.17
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	8	0.17
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD11	2	0.17
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD12	2	0.17
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD13	2	0.17
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD21	2	0.17
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD22	2	0.17
(1,1924)	1:52:X:TYR:HE1	1:69:X:LEU:HD23	2	0.17
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	5	0.17
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	5	0.17
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	5	0.17
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	5	0.17
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	5	0.17
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	5	0.17
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	10	0.17
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	10	0.17
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	10	0.17
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	10	0.17
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	10	0.17
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	10	0.17
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD11	6	0.17
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD12	6	0.17
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD13	6	0.17
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD21	6	0.17
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD22	6	0.17
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD23	6	0.17
(1,1754)	1:29:X:LYS:HE2	1:69:X:LEU:HD11	2	0.17
(1,1754)	1:29:X:LYS:HE2	1:69:X:LEU:HD12	2	0.17
(1,1754)	1:29:X:LYS:HE2	1:69:X:LEU:HD13	2	0.17
(1,1754)	1:29:X:LYS:HE2	1:69:X:LEU:HD21	2	0.17
(1,1754)	1:29:X:LYS:HE2	1:69:X:LEU:HD22	2	0.17
(1,1754)	1:29:X:LYS:HE2	1:69:X:LEU:HD23	2	0.17
(1,1754)	1:29:X:LYS:HE3	1:69:X:LEU:HD11	2	0.17
(1,1754)	1:29:X:LYS:HE3	1:69:X:LEU:HD12	2	0.17
(1,1754)	1:29:X:LYS:HE3	1:69:X:LEU:HD13	2	0.17
(1,1754)	1:29:X:LYS:HE3	1:69:X:LEU:HD21	2	0.17
(1,1754)	1:29:X:LYS:HE3	1:69:X:LEU:HD22	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1754)	1:29:X:LYS:HE3	1:69:X:LEU:HD23	2	0.17
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	5	0.17
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	5	0.17
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	5	0.17
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	1	0.17
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	9	0.17
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	3	0.17
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD11	3	0.17
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD12	3	0.17
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD13	3	0.17
(1,1564)	1:65:X:ILE:HG12	1:66:X:ASN:H	9	0.17
(1,1441)	1:90:X:LEU:H	1:91:X:MET:HB3	8	0.17
(1,1440)	1:90:X:LEU:H	1:90:X:LEU:HG	3	0.17
(1,1440)	1:90:X:LEU:H	1:90:X:LEU:HG	9	0.17
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	8	0.17
(1,1377)	1:97:X:TYR:HD1	1:98:X:VAL:H	8	0.17
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	3	0.17
(1,1277)	1:34:X:GLU:H	1:34:X:GLU:HG2	9	0.17
(1,1248)	1:30:X:GLN:HB3	1:31:X:ARG:H	1	0.17
(1,1248)	1:30:X:GLN:HB3	1:31:X:ARG:H	2	0.17
(1,1236)	1:90:X:LEU:HD21	1:122:X:GLU:H	7	0.17
(1,1236)	1:90:X:LEU:HD22	1:122:X:GLU:H	7	0.17
(1,1236)	1:90:X:LEU:HD23	1:122:X:GLU:H	7	0.17
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	4	0.17
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	6	0.17
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	5	0.17
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	6	0.17
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	8	0.17
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	2	0.17
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	10	0.17
(1,1048)	1:73:X:PHE:HA	1:76:X:GLU:H	2	0.17
(1,1003)	1:125:X:LYS:HB3	1:126:X:ASN:H	10	0.17
(1,962)	1:91:X:MET:H	1:91:X:MET:HE1	9	0.17
(1,962)	1:91:X:MET:H	1:91:X:MET:HE2	9	0.17
(1,962)	1:91:X:MET:H	1:91:X:MET:HE3	9	0.17
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	1	0.17
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	1	0.17
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	1	0.17
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	4	0.17
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	1	0.17
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	3	0.17
(1,835)	1:119:X:LEU:HA	1:122:X:GLU:HG2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,825)	1:137:X:PHE:HB3	1:138:X:PRO:HD3	9	0.17
(1,808)	1:57:X:THR:HA	1:63:X:ILE:HG13	1	0.17
(1,808)	1:57:X:THR:HA	1:63:X:ILE:HG13	2	0.17
(1,788)	1:37:X:ARG:HA	1:43:X:ILE:HG12	6	0.17
(1,788)	1:37:X:ARG:HA	1:43:X:ILE:HG12	7	0.17
(1,783)	1:74:X:PRO:HB2	1:106:X:PHE:HE1	6	0.17
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	4	0.17
(1,742)	1:122:X:GLU:HA	1:125:X:LYS:HB3	1	0.17
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	8	0.17
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	4	0.17
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	4	0.17
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	4	0.17
(1,699)	1:52:X:TYR:HB2	1:67:X:ILE:HB	2	0.17
(1,646)	1:54:X:LEU:HD21	1:56:X:PHE:HB3	2	0.17
(1,646)	1:54:X:LEU:HD22	1:56:X:PHE:HB3	2	0.17
(1,646)	1:54:X:LEU:HD23	1:56:X:PHE:HB3	2	0.17
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD11	1	0.17
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD12	1	0.17
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD13	1	0.17
(1,578)	1:140:X:LEU:HD21	1:141:X:TYR:HE1	10	0.17
(1,578)	1:140:X:LEU:HD22	1:141:X:TYR:HE1	10	0.17
(1,578)	1:140:X:LEU:HD23	1:141:X:TYR:HE1	10	0.17
(1,512)	1:67:X:ILE:HG21	1:78:X:PRO:HD3	10	0.17
(1,512)	1:67:X:ILE:HG22	1:78:X:PRO:HD3	10	0.17
(1,512)	1:67:X:ILE:HG23	1:78:X:PRO:HD3	10	0.17
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	1	0.17
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	1	0.17
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	1	0.17
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	7	0.17
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	7	0.17
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	7	0.17
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	10	0.17
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	10	0.17
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	10	0.17
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	5	0.17
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	5	0.17
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	5	0.17
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	7	0.17
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	7	0.17
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	7	0.17
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	3	0.17
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	3	0.17
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	3	0.17
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	3	0.17
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	3	0.17
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	3	0.17
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	3	0.17
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	3	0.17
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	4	0.17
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	4	0.17
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	4	0.17
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	4	0.17
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	4	0.17
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	4	0.17
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	4	0.17
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	4	0.17
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	4	0.17
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	6	0.17
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	6	0.17
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	6	0.17
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	10	0.17
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	10	0.17
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	10	0.17
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	10	0.17
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	10	0.17
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	10	0.17
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	10	0.17
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	10	0.17
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	10	0.17
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE1	5	0.17
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE2	5	0.17
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE3	5	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	1	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	1	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	1	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	3	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	3	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	3	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	7	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	7	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	7	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	9	0.17
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	9	0.17
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD11	7	0.17
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD12	7	0.17
(1,344)	1:79:X:VAL:HA	1:80:X:ILE:HD13	7	0.17
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	2	0.17
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	6	0.17
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	10	0.17
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	4	0.17
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	8	0.17
(1,250)	1:137:X:PHE:HD1	1:138:X:PRO:HD2	7	0.17
(1,236)	1:58:X:ILE:HD11	1:127:X:PRO:HD2	1	0.17
(1,236)	1:58:X:ILE:HD12	1:127:X:PRO:HD2	1	0.17
(1,236)	1:58:X:ILE:HD13	1:127:X:PRO:HD2	1	0.17
(1,236)	1:58:X:ILE:HD11	1:127:X:PRO:HD2	5	0.17
(1,236)	1:58:X:ILE:HD12	1:127:X:PRO:HD2	5	0.17
(1,236)	1:58:X:ILE:HD13	1:127:X:PRO:HD2	5	0.17
(1,221)	1:70:X:PRO:HD3	1:73:X:PHE:HD1	8	0.17
(1,190)	1:25:X:LEU:HA	1:74:X:PRO:HD3	3	0.17
(1,153)	1:121:X:ASP:HA	1:124:X:TRP:HB3	2	0.17
(1,136)	1:46:X:ILE:HG13	1:52:X:TYR:HA	1	0.17
(1,96)	1:29:X:LYS:HA	1:73:X:PHE:HD1	2	0.17
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	3	0.17
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	3	0.17
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	3	0.17
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	4	0.17
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	4	0.17
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	4	0.17
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	6	0.17
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	6	0.17
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	6	0.17
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	8	0.17
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	8	0.17
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	8	0.17
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	9	0.17
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	9	0.17
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	9	0.17
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	3	0.17
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	5	0.17
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	7	0.17
(1,16)	1:90:X:LEU:HB2	1:100:X:SER:HB2	2	0.17
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	1	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	1	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	1	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	1	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	1	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	1	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	1	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	1	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	1	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	1	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	1	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	2	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	2	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	2	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	2	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	2	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	2	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	2	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	2	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	2	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	2	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	2	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	2	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	4	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	4	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	4	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	4	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	4	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	4	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	4	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	4	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	4	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	4	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	4	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	4	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	6	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	6	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	6	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	6	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	6	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	6	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	6	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	6	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	6	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	6	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	6	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	8	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	8	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	8	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	8	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	8	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	8	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	8	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	8	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	8	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	8	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	8	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	8	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	10	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	10	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	10	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	10	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	10	0.16
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	10	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	10	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	10	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	10	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	10	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	10	0.16
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	10	0.16
(1,2258)	1:102:X:LEU:HD11	1:122:X:GLU:HB3	1	0.16
(1,2258)	1:102:X:LEU:HD12	1:122:X:GLU:HB3	1	0.16
(1,2258)	1:102:X:LEU:HD13	1:122:X:GLU:HB3	1	0.16
(1,2258)	1:102:X:LEU:HD21	1:122:X:GLU:HB3	1	0.16
(1,2258)	1:102:X:LEU:HD22	1:122:X:GLU:HB3	1	0.16
(1,2258)	1:102:X:LEU:HD23	1:122:X:GLU:HB3	1	0.16
(1,2258)	1:102:X:LEU:HD11	1:122:X:GLU:HB3	8	0.16
(1,2258)	1:102:X:LEU:HD12	1:122:X:GLU:HB3	8	0.16
(1,2258)	1:102:X:LEU:HD13	1:122:X:GLU:HB3	8	0.16
(1,2258)	1:102:X:LEU:HD21	1:122:X:GLU:HB3	8	0.16
(1,2258)	1:102:X:LEU:HD22	1:122:X:GLU:HB3	8	0.16
(1,2258)	1:102:X:LEU:HD23	1:122:X:GLU:HB3	8	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD11	5	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD13	5	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD21	5	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD22	5	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD23	5	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD11	5	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD12	5	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD13	5	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD21	5	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD22	5	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD23	5	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD11	5	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD12	5	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD13	5	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD21	5	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD22	5	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD23	5	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD11	5	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD12	5	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD13	5	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD21	5	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD22	5	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD23	5	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD11	5	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD12	5	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD13	5	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD21	5	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD22	5	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD23	5	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD11	5	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD12	5	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD13	5	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD21	5	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD22	5	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD23	5	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD11	8	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD12	8	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD13	8	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD21	8	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD22	8	0.16
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD23	8	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD11	8	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD12	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD13	8	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD21	8	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD22	8	0.16
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD23	8	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD11	8	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD12	8	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD13	8	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD21	8	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD22	8	0.16
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD23	8	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD11	8	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD12	8	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD13	8	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD21	8	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD22	8	0.16
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD23	8	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD11	8	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD12	8	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD13	8	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD21	8	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD22	8	0.16
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD23	8	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD11	8	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD12	8	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD13	8	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD21	8	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD22	8	0.16
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD23	8	0.16
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	5	0.16
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	5	0.16
(1,2156)	1:90:X:LEU:HD11	1:91:X:MET:HG3	7	0.16
(1,2156)	1:90:X:LEU:HD12	1:91:X:MET:HG3	7	0.16
(1,2156)	1:90:X:LEU:HD13	1:91:X:MET:HG3	7	0.16
(1,2156)	1:90:X:LEU:HD21	1:91:X:MET:HG3	7	0.16
(1,2156)	1:90:X:LEU:HD22	1:91:X:MET:HG3	7	0.16
(1,2156)	1:90:X:LEU:HD23	1:91:X:MET:HG3	7	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG11	10	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG12	10	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG13	10	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG21	10	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG22	10	0.16
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG23	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG11	10	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG12	10	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG13	10	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG21	10	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG22	10	0.16
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG23	10	0.16
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	9	0.16
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	9	0.16
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE1	8	0.16
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE2	8	0.16
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE3	8	0.16
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE1	8	0.16
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE2	8	0.16
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE3	8	0.16
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE1	8	0.16
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE2	8	0.16
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE3	8	0.16
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE1	8	0.16
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE2	8	0.16
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE3	8	0.16
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE1	8	0.16
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE2	8	0.16
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE3	8	0.16
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE1	8	0.16
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE2	8	0.16
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE3	8	0.16
(1,2054)	1:75:X:GLN:HG2	1:76:X:GLU:HG2	5	0.16
(1,2054)	1:75:X:GLN:HG3	1:76:X:GLU:HG2	5	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD11	5	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD12	5	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD13	5	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD21	5	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD22	5	0.16
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD23	5	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD11	5	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD12	5	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD13	5	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD21	5	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD22	5	0.16
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD23	5	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD11	5	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD12	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD13	5	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD21	5	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD22	5	0.16
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD23	5	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD11	5	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD12	5	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD13	5	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD21	5	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD22	5	0.16
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD23	5	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD11	5	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD12	5	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD13	5	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD21	5	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD22	5	0.16
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD23	5	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD11	5	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD12	5	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD13	5	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD21	5	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD22	5	0.16
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD23	5	0.16
(1,2015)	1:67:X:ILE:HG21	1:69:X:LEU:HD11	2	0.16
(1,2015)	1:67:X:ILE:HG21	1:69:X:LEU:HD12	2	0.16
(1,2015)	1:67:X:ILE:HG21	1:69:X:LEU:HD13	2	0.16
(1,2015)	1:67:X:ILE:HG21	1:69:X:LEU:HD21	2	0.16
(1,2015)	1:67:X:ILE:HG21	1:69:X:LEU:HD22	2	0.16
(1,2015)	1:67:X:ILE:HG21	1:69:X:LEU:HD23	2	0.16
(1,2015)	1:67:X:ILE:HG22	1:69:X:LEU:HD11	2	0.16
(1,2015)	1:67:X:ILE:HG22	1:69:X:LEU:HD12	2	0.16
(1,2015)	1:67:X:ILE:HG22	1:69:X:LEU:HD13	2	0.16
(1,2015)	1:67:X:ILE:HG22	1:69:X:LEU:HD21	2	0.16
(1,2015)	1:67:X:ILE:HG22	1:69:X:LEU:HD22	2	0.16
(1,2015)	1:67:X:ILE:HG22	1:69:X:LEU:HD23	2	0.16
(1,2015)	1:67:X:ILE:HG23	1:69:X:LEU:HD11	2	0.16
(1,2015)	1:67:X:ILE:HG23	1:69:X:LEU:HD12	2	0.16
(1,2015)	1:67:X:ILE:HG23	1:69:X:LEU:HD13	2	0.16
(1,2015)	1:67:X:ILE:HG23	1:69:X:LEU:HD21	2	0.16
(1,2015)	1:67:X:ILE:HG23	1:69:X:LEU:HD22	2	0.16
(1,2015)	1:67:X:ILE:HG23	1:69:X:LEU:HD23	2	0.16
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	10	0.16
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1929)	1:53:X:ARG:HD2	1:54:X:LEU:HA	5	0.16
(1,1929)	1:53:X:ARG:HD3	1:54:X:LEU:HA	5	0.16
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	3	0.16
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	3	0.16
(1,1882)	1:45:X:GLU:HG2	1:48:X:LYS:HD2	3	0.16
(1,1882)	1:45:X:GLU:HG3	1:48:X:LYS:HD2	3	0.16
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	7	0.16
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	7	0.16
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	7	0.16
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	7	0.16
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	7	0.16
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	7	0.16
(1,1840)	1:36:X:LEU:HD11	1:113:X:GLY:HA2	7	0.16
(1,1840)	1:36:X:LEU:HD12	1:113:X:GLY:HA2	7	0.16
(1,1840)	1:36:X:LEU:HD13	1:113:X:GLY:HA2	7	0.16
(1,1840)	1:36:X:LEU:HD21	1:113:X:GLY:HA2	7	0.16
(1,1840)	1:36:X:LEU:HD22	1:113:X:GLY:HA2	7	0.16
(1,1840)	1:36:X:LEU:HD23	1:113:X:GLY:HA2	7	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	8	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	8	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	8	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	8	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	8	0.16
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	8	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	8	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	8	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	8	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	8	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	8	0.16
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	8	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	8	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	8	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	8	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	8	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	8	0.16
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	8	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	8	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	8	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	8	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	8	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	8	0.16
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	8	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	8	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	8	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	8	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	8	0.16
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	8	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	8	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	8	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	8	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	8	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	8	0.16
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	8	0.16
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	3	0.16
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	3	0.16
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	3	0.16
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	3	0.16
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	3	0.16
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	3	0.16
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB2	9	0.16
(1,1804)	1:34:X:GLU:HG2	1:35:X:SER:HB3	9	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	1	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	1	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	1	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	1	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	1	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	1	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	1	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	1	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	1	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	1	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	1	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	1	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	5	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	5	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	5	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	5	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	5	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	5	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	5	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	5	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	5	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	5	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	5	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	6	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	6	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	6	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	6	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	6	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	6	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	6	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	6	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	6	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	6	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	6	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	6	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	9	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	9	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	9	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	9	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	9	0.16
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	9	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	9	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	9	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	9	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	9	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	9	0.16
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	9	0.16
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	5	0.16
(1,1643)	1:73:X:PHE:HB2	1:73:X:PHE:HD1	6	0.16
(1,1640)	1:138:X:PRO:HB2	1:139:X:TYR:HD1	10	0.16
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	10	0.16
(1,1573)	1:43:X:ILE:HG13	1:54:X:LEU:H	10	0.16
(1,1530)	1:130:X:LEU:HD11	1:131:X:ALA:H	2	0.16
(1,1530)	1:130:X:LEU:HD12	1:131:X:ALA:H	2	0.16
(1,1530)	1:130:X:LEU:HD13	1:131:X:ALA:H	2	0.16
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	2	0.16
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	6	0.16
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	8	0.16
(1,1260)	1:137:X:PHE:HA	1:139:X:TYR:H	7	0.16
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	1	0.16
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	1	0.16
(1,1153)	1:121:X:ASP:H	1:122:X:GLU:HB3	2	0.16
(1,1048)	1:73:X:PHE:HA	1:76:X:GLU:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:125:X:LYS:HB3	1:126:X:ASN:H	8	0.16
(1,987)	1:34:X:GLU:HG3	1:35:X:SER:H	1	0.16
(1,955)	1:71:X:PRO:HG3	1:72:X:GLN:H	1	0.16
(1,955)	1:71:X:PRO:HG3	1:72:X:GLN:H	10	0.16
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	3	0.16
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	4	0.16
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	6	0.16
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	7	0.16
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	1	0.16
(1,825)	1:137:X:PHE:HB3	1:138:X:PRO:HD3	10	0.16
(1,788)	1:37:X:ARG:HA	1:43:X:ILE:HG12	2	0.16
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	5	0.16
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	2	0.16
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	3	0.16
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	3	0.16
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	3	0.16
(1,684)	1:106:X:PHE:HE1	1:112:X:LEU:HB3	10	0.16
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	2	0.16
(1,651)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	6	0.16
(1,651)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	6	0.16
(1,651)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	6	0.16
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD11	4	0.16
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD12	4	0.16
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD13	4	0.16
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD11	4	0.16
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD12	4	0.16
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD13	4	0.16
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD11	4	0.16
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD12	4	0.16
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD13	4	0.16
(1,528)	1:96:X:VAL:HG11	1:137:X:PHE:HD1	4	0.16
(1,528)	1:96:X:VAL:HG12	1:137:X:PHE:HD1	4	0.16
(1,528)	1:96:X:VAL:HG13	1:137:X:PHE:HD1	4	0.16
(1,487)	1:43:X:ILE:HG21	1:52:X:TYR:HE1	1	0.16
(1,487)	1:43:X:ILE:HG22	1:52:X:TYR:HE1	1	0.16
(1,487)	1:43:X:ILE:HG23	1:52:X:TYR:HE1	1	0.16
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	8	0.16
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	8	0.16
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	8	0.16
(1,441)	1:58:X:ILE:HD11	1:126:X:ASN:HA	8	0.16
(1,441)	1:58:X:ILE:HD12	1:126:X:ASN:HA	8	0.16
(1,441)	1:58:X:ILE:HD13	1:126:X:ASN:HA	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	5	0.16
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	5	0.16
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	5	0.16
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	5	0.16
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	5	0.16
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	5	0.16
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	5	0.16
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	5	0.16
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	5	0.16
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	10	0.16
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	10	0.16
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	10	0.16
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	8	0.16
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	8	0.16
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	8	0.16
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	5	0.16
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	5	0.16
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	5	0.16
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	8	0.16
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	8	0.16
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	8	0.16
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	5	0.16
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	5	0.16
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	5	0.16
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	5	0.16
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	5	0.16
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	5	0.16
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	5	0.16
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	5	0.16
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	5	0.16
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE1	6	0.16
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE2	6	0.16
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE3	6	0.16
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD11	10	0.16
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD12	10	0.16
(1,350)	1:56:X:PHE:HD2	1:63:X:ILE:HD13	10	0.16
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	9	0.16
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	9	0.16
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	9	0.16
(1,298)	1:83:X:TYR:HA	1:85:X:PRO:HD2	1	0.16
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD21	1	0.16
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD22	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD23	1	0.16
(1,262)	1:64:X:ASN:HA	1:65:X:ILE:HG12	10	0.16
(1,250)	1:137:X:PHE:HD1	1:138:X:PRO:HD2	1	0.16
(1,206)	1:78:X:PRO:HD2	1:106:X:PHE:HE1	9	0.16
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	8	0.16
(1,142)	1:73:X:PHE:HA	1:76:X:GLU:HB3	6	0.16
(1,121)	1:141:X:TYR:HA	1:141:X:TYR:HD1	10	0.16
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	1	0.16
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	1	0.16
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	1	0.16
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	10	0.16
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	10	0.16
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	10	0.16
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD11	9	0.15
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD12	9	0.15
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD13	9	0.15
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD11	9	0.15
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD12	9	0.15
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD13	9	0.15
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD11	9	0.15
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD12	9	0.15
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD13	9	0.15
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD11	9	0.15
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD12	9	0.15
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD13	9	0.15
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD11	9	0.15
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD12	9	0.15
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD13	9	0.15
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD11	9	0.15
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD12	9	0.15
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD13	9	0.15
(1,2280)	1:107:X:THR:HG21	1:110:X:SER:HB2	4	0.15
(1,2280)	1:107:X:THR:HG21	1:110:X:SER:HB3	4	0.15
(1,2280)	1:107:X:THR:HG22	1:110:X:SER:HB2	4	0.15
(1,2280)	1:107:X:THR:HG22	1:110:X:SER:HB3	4	0.15
(1,2280)	1:107:X:THR:HG23	1:110:X:SER:HB2	4	0.15
(1,2280)	1:107:X:THR:HG23	1:110:X:SER:HB3	4	0.15
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD11	1	0.15
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD12	1	0.15
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD13	1	0.15
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD21	1	0.15
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD22	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2245)	1:102:X:LEU:HB2	1:102:X:LEU:HD23	1	0.15
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD11	1	0.15
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD12	1	0.15
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD13	1	0.15
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD21	1	0.15
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD22	1	0.15
(1,2245)	1:102:X:LEU:HB3	1:102:X:LEU:HD23	1	0.15
(1,2225)	1:100:X:SER:H	1:103:X:VAL:HG11	10	0.15
(1,2225)	1:100:X:SER:H	1:103:X:VAL:HG12	10	0.15
(1,2225)	1:100:X:SER:H	1:103:X:VAL:HG13	10	0.15
(1,2225)	1:100:X:SER:H	1:103:X:VAL:HG21	10	0.15
(1,2225)	1:100:X:SER:H	1:103:X:VAL:HG22	10	0.15
(1,2225)	1:100:X:SER:H	1:103:X:VAL:HG23	10	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG11	8	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG12	8	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG13	8	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG21	8	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG22	8	0.15
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG23	8	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG11	8	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG12	8	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG13	8	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG21	8	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG22	8	0.15
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG23	8	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG11	8	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG12	8	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG13	8	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG21	8	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG22	8	0.15
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG23	8	0.15
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB2	6	0.15
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB3	6	0.15
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB2	6	0.15
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB3	6	0.15
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB2	6	0.15
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB3	6	0.15
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB2	6	0.15
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB3	6	0.15
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB2	6	0.15
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB3	6	0.15
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB2	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB3	6	0.15
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	5	0.15
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	5	0.15
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	5	0.15
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	5	0.15
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	5	0.15
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	5	0.15
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	2	0.15
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	2	0.15
(1,2105)	1:82:X:VAL:HG11	1:86:X:ILE:HA	5	0.15
(1,2105)	1:82:X:VAL:HG12	1:86:X:ILE:HA	5	0.15
(1,2105)	1:82:X:VAL:HG13	1:86:X:ILE:HA	5	0.15
(1,2105)	1:82:X:VAL:HG21	1:86:X:ILE:HA	5	0.15
(1,2105)	1:82:X:VAL:HG22	1:86:X:ILE:HA	5	0.15
(1,2105)	1:82:X:VAL:HG23	1:86:X:ILE:HA	5	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD11	6	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD12	6	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD13	6	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD21	6	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD22	6	0.15
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD23	6	0.15
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD11	6	0.15
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD12	6	0.15
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD13	6	0.15
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD21	6	0.15
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD22	6	0.15
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD23	6	0.15
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD11	6	0.15
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD12	6	0.15
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD13	6	0.15
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD21	6	0.15
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD22	6	0.15
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD23	6	0.15
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD11	6	0.15
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD12	6	0.15
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD13	6	0.15
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD21	6	0.15
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD22	6	0.15
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD23	6	0.15
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD11	6	0.15
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD12	6	0.15
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD13	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD21	6	0.15
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD22	6	0.15
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD23	6	0.15
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD11	6	0.15
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD12	6	0.15
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD13	6	0.15
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD21	6	0.15
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD22	6	0.15
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD23	6	0.15
(1,1989)	1:61:X:LEU:HD11	1:128:X:PRO:HG3	8	0.15
(1,1989)	1:61:X:LEU:HD12	1:128:X:PRO:HG3	8	0.15
(1,1989)	1:61:X:LEU:HD13	1:128:X:PRO:HG3	8	0.15
(1,1989)	1:61:X:LEU:HD21	1:128:X:PRO:HG3	8	0.15
(1,1989)	1:61:X:LEU:HD22	1:128:X:PRO:HG3	8	0.15
(1,1989)	1:61:X:LEU:HD23	1:128:X:PRO:HG3	8	0.15
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	2	0.15
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	2	0.15
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	2	0.15
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	2	0.15
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	2	0.15
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	2	0.15
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	5	0.15
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	5	0.15
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	5	0.15
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	5	0.15
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	5	0.15
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	5	0.15
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	9	0.15
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	9	0.15
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	9	0.15
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	9	0.15
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	9	0.15
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	9	0.15
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG2	4	0.15
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG3	4	0.15
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG2	4	0.15
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG3	4	0.15
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	5	0.15
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	5	0.15
(1,1857)	1:37:X:ARG:HD2	1:52:X:TYR:HE1	3	0.15
(1,1857)	1:37:X:ARG:HD3	1:52:X:TYR:HE1	3	0.15
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	5	0.15
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	5	0.15
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	5	0.15
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	5	0.15
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	5	0.15
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	5	0.15
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	5	0.15
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	5	0.15
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	5	0.15
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	5	0.15
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	5	0.15
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	5	0.15
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	5	0.15
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	5	0.15
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	5	0.15
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	5	0.15
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	5	0.15
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	5	0.15
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	5	0.15
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	5	0.15
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	5	0.15
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	5	0.15
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	5	0.15
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	5	0.15
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	5	0.15
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	5	0.15
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	5	0.15
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	5	0.15
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	5	0.15
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	5	0.15
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	5	0.15
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	5	0.15
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	5	0.15
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	5	0.15
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	5	0.15
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD2	10	0.15
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD3	10	0.15
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD2	10	0.15
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD3	10	0.15
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD2	10	0.15
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD3	10	0.15
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	3	0.15
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	3	0.15
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	3	0.15
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	3	0.15
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	3	0.15
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD11	2	0.15
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD12	2	0.15
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD13	2	0.15
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD21	2	0.15
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD22	2	0.15
(1,1770)	1:32:X:LEU:HA	1:32:X:LEU:HD23	2	0.15
(1,1769)	1:32:X:LEU:H	1:33:X:ILE:HG12	7	0.15
(1,1769)	1:32:X:LEU:H	1:33:X:ILE:HG13	7	0.15
(1,1712)	1:25:X:LEU:HD11	1:74:X:PRO:HD3	5	0.15
(1,1712)	1:25:X:LEU:HD12	1:74:X:PRO:HD3	5	0.15
(1,1712)	1:25:X:LEU:HD13	1:74:X:PRO:HD3	5	0.15
(1,1712)	1:25:X:LEU:HD21	1:74:X:PRO:HD3	5	0.15
(1,1712)	1:25:X:LEU:HD22	1:74:X:PRO:HD3	5	0.15
(1,1712)	1:25:X:LEU:HD23	1:74:X:PRO:HD3	5	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	3	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	3	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	3	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	3	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	3	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	3	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	3	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	3	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	3	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	3	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	3	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	3	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	8	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	8	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	8	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	8	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	8	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	8	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	8	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	8	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	8	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	8	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	8	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD11	10	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD12	10	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD13	10	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD21	10	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD22	10	0.15
(1,1687)	1:22:X:LEU:HB2	1:22:X:LEU:HD23	10	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD11	10	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD12	10	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD13	10	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD21	10	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD22	10	0.15
(1,1687)	1:22:X:LEU:HB3	1:22:X:LEU:HD23	10	0.15
(1,1654)	1:63:X:ILE:HD11	1:123:X:PHE:HE1	9	0.15
(1,1654)	1:63:X:ILE:HD12	1:123:X:PHE:HE1	9	0.15
(1,1654)	1:63:X:ILE:HD13	1:123:X:PHE:HE1	9	0.15
(1,1600)	1:46:X:ILE:H	1:47:X:GLN:HB3	4	0.15
(1,1600)	1:46:X:ILE:H	1:47:X:GLN:HB3	5	0.15
(1,1483)	1:70:X:PRO:HD3	1:73:X:PHE:H	4	0.15
(1,1441)	1:90:X:LEU:H	1:91:X:MET:HB3	4	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD11	1	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD12	1	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD13	1	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD11	4	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD12	4	0.15
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD13	4	0.15
(1,1412)	1:57:X:THR:H	1:57:X:THR:HB	1	0.15
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	5	0.15
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	10	0.15
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	2	0.15
(1,1212)	1:50:X:VAL:HB	1:51:X:GLU:H	5	0.15
(1,1197)	1:92:X:ASP:H	1:99:X:THR:HB	2	0.15
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	6	0.15
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	3	0.15
(1,1050)	1:73:X:PHE:HB2	1:76:X:GLU:H	6	0.15
(1,1003)	1:125:X:LYS:HB3	1:126:X:ASN:H	7	0.15
(1,955)	1:71:X:PRO:HG3	1:72:X:GLN:H	2	0.15
(1,912)	1:50:X:VAL:HA	1:68:X:LEU:HG	8	0.15
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	8	0.15
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	8	0.15
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	8	0.15
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	9	0.15
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	9	0.15
(1,879)	1:102:X:LEU:HA	1:105:X:ASN:HB3	7	0.15
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	8	0.15
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	6	0.15
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	9	0.15
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	6	0.15
(1,671)	1:124:X:TRP:HB3	1:125:X:LYS:HB3	9	0.15
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	4	0.15
(1,653)	1:32:X:LEU:HD11	1:74:X:PRO:HB2	8	0.15
(1,653)	1:32:X:LEU:HD12	1:74:X:PRO:HB2	8	0.15
(1,653)	1:32:X:LEU:HD13	1:74:X:PRO:HB2	8	0.15
(1,594)	1:48:X:LYS:HA	1:48:X:LYS:HD3	5	0.15
(1,574)	1:23:X:THR:HG21	1:26:X:GLN:HB3	10	0.15
(1,574)	1:23:X:THR:HG22	1:26:X:GLN:HB3	10	0.15
(1,574)	1:23:X:THR:HG23	1:26:X:GLN:HB3	10	0.15
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	8	0.15
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	8	0.15
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	8	0.15
(1,452)	1:58:X:ILE:HD11	1:128:X:PRO:HB2	5	0.15
(1,452)	1:58:X:ILE:HD12	1:128:X:PRO:HB2	5	0.15
(1,452)	1:58:X:ILE:HD13	1:128:X:PRO:HB2	5	0.15
(1,441)	1:58:X:ILE:HD11	1:126:X:ASN:HA	7	0.15
(1,441)	1:58:X:ILE:HD12	1:126:X:ASN:HA	7	0.15
(1,441)	1:58:X:ILE:HD13	1:126:X:ASN:HA	7	0.15
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	5	0.15
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	5	0.15
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	5	0.15
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	5	0.15
(1,150)	1:33:X:ILE:HB	1:49:X:ASP:HA	2	0.15
(1,78)	1:58:X:ILE:HD11	1:127:X:PRO:HA	5	0.15
(1,78)	1:58:X:ILE:HD12	1:127:X:PRO:HA	5	0.15
(1,78)	1:58:X:ILE:HD13	1:127:X:PRO:HA	5	0.15
(1,2317)	1:117:X:GLN:HG2	1:118:X:SER:H	6	0.14
(1,2317)	1:117:X:GLN:HG3	1:118:X:SER:H	6	0.14
(1,2258)	1:102:X:LEU:HD11	1:122:X:GLU:HB3	4	0.14
(1,2258)	1:102:X:LEU:HD12	1:122:X:GLU:HB3	4	0.14
(1,2258)	1:102:X:LEU:HD13	1:122:X:GLU:HB3	4	0.14
(1,2258)	1:102:X:LEU:HD21	1:122:X:GLU:HB3	4	0.14
(1,2258)	1:102:X:LEU:HD22	1:122:X:GLU:HB3	4	0.14
(1,2258)	1:102:X:LEU:HD23	1:122:X:GLU:HB3	4	0.14
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG11	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG12	4	0.14
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG13	4	0.14
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG21	4	0.14
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG22	4	0.14
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG23	4	0.14
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG11	4	0.14
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG12	4	0.14
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG13	4	0.14
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG21	4	0.14
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG22	4	0.14
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG23	4	0.14
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG11	6	0.14
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG12	6	0.14
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG13	6	0.14
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG21	6	0.14
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG22	6	0.14
(1,2180)	1:91:X:MET:HE1	1:98:X:VAL:HG23	6	0.14
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG11	6	0.14
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG12	6	0.14
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG13	6	0.14
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG21	6	0.14
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG22	6	0.14
(1,2180)	1:91:X:MET:HE2	1:98:X:VAL:HG23	6	0.14
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG11	6	0.14
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG12	6	0.14
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG13	6	0.14
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG21	6	0.14
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG22	6	0.14
(1,2180)	1:91:X:MET:HE3	1:98:X:VAL:HG23	6	0.14
(1,2163)	1:90:X:LEU:HD11	1:119:X:LEU:HD11	9	0.14
(1,2163)	1:90:X:LEU:HD11	1:119:X:LEU:HD12	9	0.14
(1,2163)	1:90:X:LEU:HD11	1:119:X:LEU:HD13	9	0.14
(1,2163)	1:90:X:LEU:HD11	1:119:X:LEU:HD21	9	0.14
(1,2163)	1:90:X:LEU:HD11	1:119:X:LEU:HD22	9	0.14
(1,2163)	1:90:X:LEU:HD11	1:119:X:LEU:HD23	9	0.14
(1,2163)	1:90:X:LEU:HD12	1:119:X:LEU:HD11	9	0.14
(1,2163)	1:90:X:LEU:HD12	1:119:X:LEU:HD12	9	0.14
(1,2163)	1:90:X:LEU:HD12	1:119:X:LEU:HD13	9	0.14
(1,2163)	1:90:X:LEU:HD12	1:119:X:LEU:HD21	9	0.14
(1,2163)	1:90:X:LEU:HD12	1:119:X:LEU:HD22	9	0.14
(1,2163)	1:90:X:LEU:HD12	1:119:X:LEU:HD23	9	0.14
(1,2163)	1:90:X:LEU:HD13	1:119:X:LEU:HD11	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2163)	1:90:X:LEU:HD13	1:119:X:LEU:HD12	9	0.14
(1,2163)	1:90:X:LEU:HD13	1:119:X:LEU:HD13	9	0.14
(1,2163)	1:90:X:LEU:HD13	1:119:X:LEU:HD21	9	0.14
(1,2163)	1:90:X:LEU:HD13	1:119:X:LEU:HD22	9	0.14
(1,2163)	1:90:X:LEU:HD13	1:119:X:LEU:HD23	9	0.14
(1,2163)	1:90:X:LEU:HD21	1:119:X:LEU:HD11	9	0.14
(1,2163)	1:90:X:LEU:HD21	1:119:X:LEU:HD12	9	0.14
(1,2163)	1:90:X:LEU:HD21	1:119:X:LEU:HD13	9	0.14
(1,2163)	1:90:X:LEU:HD21	1:119:X:LEU:HD21	9	0.14
(1,2163)	1:90:X:LEU:HD21	1:119:X:LEU:HD22	9	0.14
(1,2163)	1:90:X:LEU:HD21	1:119:X:LEU:HD23	9	0.14
(1,2163)	1:90:X:LEU:HD22	1:119:X:LEU:HD11	9	0.14
(1,2163)	1:90:X:LEU:HD22	1:119:X:LEU:HD12	9	0.14
(1,2163)	1:90:X:LEU:HD22	1:119:X:LEU:HD13	9	0.14
(1,2163)	1:90:X:LEU:HD22	1:119:X:LEU:HD21	9	0.14
(1,2163)	1:90:X:LEU:HD22	1:119:X:LEU:HD22	9	0.14
(1,2163)	1:90:X:LEU:HD22	1:119:X:LEU:HD23	9	0.14
(1,2163)	1:90:X:LEU:HD23	1:119:X:LEU:HD11	9	0.14
(1,2163)	1:90:X:LEU:HD23	1:119:X:LEU:HD12	9	0.14
(1,2163)	1:90:X:LEU:HD23	1:119:X:LEU:HD13	9	0.14
(1,2163)	1:90:X:LEU:HD23	1:119:X:LEU:HD21	9	0.14
(1,2163)	1:90:X:LEU:HD23	1:119:X:LEU:HD22	9	0.14
(1,2163)	1:90:X:LEU:HD23	1:119:X:LEU:HD23	9	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB2	1	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB3	1	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB2	1	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB3	1	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB2	1	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB3	1	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB2	1	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB3	1	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB2	1	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB3	1	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB2	1	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB3	1	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB2	7	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB3	7	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB2	7	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB3	7	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB2	7	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB3	7	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB3	7	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB2	7	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB3	7	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB2	7	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB3	7	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB2	8	0.14
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB3	8	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB2	8	0.14
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB3	8	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB2	8	0.14
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB3	8	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB2	8	0.14
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB3	8	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB2	8	0.14
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB3	8	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB2	8	0.14
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB3	8	0.14
(1,2154)	1:90:X:LEU:HG	1:100:X:SER:HB2	3	0.14
(1,2154)	1:90:X:LEU:HG	1:100:X:SER:HB3	3	0.14
(1,2137)	1:87:X:ARG:HD2	1:131:X:ALA:HA	4	0.14
(1,2137)	1:87:X:ARG:HD3	1:131:X:ALA:HA	4	0.14
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG11	9	0.14
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG12	9	0.14
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG13	9	0.14
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG21	9	0.14
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG22	9	0.14
(1,2131)	1:87:X:ARG:HB2	1:129:X:VAL:HG23	9	0.14
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG11	9	0.14
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG12	9	0.14
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG13	9	0.14
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG21	9	0.14
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG22	9	0.14
(1,2131)	1:87:X:ARG:HB3	1:129:X:VAL:HG23	9	0.14
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE1	4	0.14
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE2	4	0.14
(1,2108)	1:82:X:VAL:HG11	1:91:X:MET:HE3	4	0.14
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE1	4	0.14
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE2	4	0.14
(1,2108)	1:82:X:VAL:HG12	1:91:X:MET:HE3	4	0.14
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE1	4	0.14
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE2	4	0.14
(1,2108)	1:82:X:VAL:HG13	1:91:X:MET:HE3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE1	4	0.14
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE2	4	0.14
(1,2108)	1:82:X:VAL:HG21	1:91:X:MET:HE3	4	0.14
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE1	4	0.14
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE2	4	0.14
(1,2108)	1:82:X:VAL:HG22	1:91:X:MET:HE3	4	0.14
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE1	4	0.14
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE2	4	0.14
(1,2108)	1:82:X:VAL:HG23	1:91:X:MET:HE3	4	0.14
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	7	0.14
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	7	0.14
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	7	0.14
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	7	0.14
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	7	0.14
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	7	0.14
(1,2060)	1:77:X:LYS:HG2	1:103:X:VAL:HG11	7	0.14
(1,2060)	1:77:X:LYS:HG2	1:103:X:VAL:HG12	7	0.14
(1,2060)	1:77:X:LYS:HG2	1:103:X:VAL:HG13	7	0.14
(1,2060)	1:77:X:LYS:HG2	1:103:X:VAL:HG21	7	0.14
(1,2060)	1:77:X:LYS:HG2	1:103:X:VAL:HG22	7	0.14
(1,2060)	1:77:X:LYS:HG2	1:103:X:VAL:HG23	7	0.14
(1,1989)	1:61:X:LEU:HD11	1:128:X:PRO:HG3	7	0.14
(1,1989)	1:61:X:LEU:HD12	1:128:X:PRO:HG3	7	0.14
(1,1989)	1:61:X:LEU:HD13	1:128:X:PRO:HG3	7	0.14
(1,1989)	1:61:X:LEU:HD21	1:128:X:PRO:HG3	7	0.14
(1,1989)	1:61:X:LEU:HD22	1:128:X:PRO:HG3	7	0.14
(1,1989)	1:61:X:LEU:HD23	1:128:X:PRO:HG3	7	0.14
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	8	0.14
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	8	0.14
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	8	0.14
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	8	0.14
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	8	0.14
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	8	0.14
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	10	0.14
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	10	0.14
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	10	0.14
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	10	0.14
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	10	0.14
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	10	0.14
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD11	3	0.14
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD12	3	0.14
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD13	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD21	3	0.14
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD22	3	0.14
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD23	3	0.14
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	10	0.14
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	10	0.14
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	10	0.14
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	10	0.14
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	10	0.14
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	10	0.14
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	1	0.14
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	1	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	4	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	4	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	4	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	4	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	4	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	4	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG11	6	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG12	6	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG13	6	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG21	6	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG22	6	0.14
(1,1894)	1:47:X:GLN:HB3	1:50:X:VAL:HG23	6	0.14
(1,1888)	1:45:X:GLU:HG2	1:52:X:TYR:HE1	8	0.14
(1,1888)	1:45:X:GLU:HG3	1:52:X:TYR:HE1	8	0.14
(1,1888)	1:45:X:GLU:HG2	1:52:X:TYR:HE1	10	0.14
(1,1888)	1:45:X:GLU:HG3	1:52:X:TYR:HE1	10	0.14
(1,1857)	1:37:X:ARG:HD2	1:52:X:TYR:HE1	4	0.14
(1,1857)	1:37:X:ARG:HD3	1:52:X:TYR:HE1	4	0.14
(1,1848)	1:37:X:ARG:HA	1:37:X:ARG:HG2	6	0.14
(1,1848)	1:37:X:ARG:HA	1:37:X:ARG:HG3	6	0.14
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	3	0.14
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	3	0.14
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	3	0.14
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	3	0.14
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	3	0.14
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	3	0.14
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	3	0.14
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	3	0.14
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	3	0.14
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	3	0.14
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	3	0.14
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	3	0.14
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	3	0.14
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	3	0.14
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	3	0.14
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	3	0.14
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	3	0.14
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	3	0.14
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	3	0.14
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	3	0.14
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	3	0.14
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	3	0.14
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	3	0.14
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	3	0.14
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	3	0.14
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	3	0.14
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	3	0.14
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	3	0.14
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	3	0.14
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	3	0.14
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	3	0.14
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	3	0.14
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	3	0.14
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	3	0.14
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	3	0.14
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB2	7	0.14
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB3	7	0.14
(1,1795)	1:33:X:ILE:HA	1:112:X:LEU:HD11	2	0.14
(1,1795)	1:33:X:ILE:HA	1:112:X:LEU:HD12	2	0.14
(1,1795)	1:33:X:ILE:HA	1:112:X:LEU:HD13	2	0.14
(1,1795)	1:33:X:ILE:HA	1:112:X:LEU:HD21	2	0.14
(1,1795)	1:33:X:ILE:HA	1:112:X:LEU:HD22	2	0.14
(1,1795)	1:33:X:ILE:HA	1:112:X:LEU:HD23	2	0.14
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	2	0.14
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	2	0.14
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	2	0.14
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	2	0.14
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	2	0.14
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	2	0.14
(1,1718)	1:26:X:GLN:H	1:26:X:GLN:HG2	1	0.14
(1,1718)	1:26:X:GLN:H	1:26:X:GLN:HG3	1	0.14
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	1	0.14
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	1	0.14
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD11	4	0.14
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD12	4	0.14
(1,1644)	1:106:X:PHE:HD1	1:115:X:ILE:HD13	4	0.14
(1,1633)	1:89:X:HIS:HE1	1:122:X:GLU:HG3	7	0.14
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD11	9	0.14
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD12	9	0.14
(1,1632)	1:89:X:HIS:HE1	1:90:X:LEU:HD13	9	0.14
(1,1607)	1:47:X:GLN:HB3	1:48:X:LYS:H	5	0.14
(1,1554)	1:52:X:TYR:H	1:52:X:TYR:HD1	2	0.14
(1,1546)	1:69:X:LEU:H	1:78:X:PRO:HB2	5	0.14
(1,1530)	1:130:X:LEU:HD11	1:131:X:ALA:H	5	0.14
(1,1530)	1:130:X:LEU:HD12	1:131:X:ALA:H	5	0.14
(1,1530)	1:130:X:LEU:HD13	1:131:X:ALA:H	5	0.14
(1,1513)	1:73:X:PHE:HD1	1:75:X:GLN:H	6	0.14
(1,1420)	1:98:X:VAL:H	1:98:X:VAL:HB	8	0.14
(1,1417)	1:86:X:ILE:HG21	1:130:X:LEU:H	10	0.14
(1,1417)	1:86:X:ILE:HG22	1:130:X:LEU:H	10	0.14
(1,1417)	1:86:X:ILE:HG23	1:130:X:LEU:H	10	0.14
(1,1403)	1:36:X:LEU:H	1:37:X:ARG:HB3	10	0.14
(1,1377)	1:97:X:TYR:HD1	1:98:X:VAL:H	4	0.14
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	7	0.14
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	9	0.14
(1,1230)	1:76:X:GLU:HB2	1:77:X:LYS:H	3	0.14
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	1	0.14
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD11	3	0.14
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD12	3	0.14
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD13	3	0.14
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD11	7	0.14
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD12	7	0.14
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD13	7	0.14
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	8	0.14
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	10	0.14
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	4	0.14
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	7	0.14
(1,1003)	1:125:X:LYS:HB3	1:126:X:ASN:H	4	0.14
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	6	0.14
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	9	0.14
(1,912)	1:50:X:VAL:HA	1:68:X:LEU:HG	4	0.14
(1,894)	1:43:X:ILE:HG13	1:52:X:TYR:HB2	7	0.14
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD22	7	0.14
(1,870)	1:43:X:ILE:HG13	1:54:X:LEU:HD23	7	0.14
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	1	0.14
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	7	0.14
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	5	0.14
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	4	0.14
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	5	0.14
(1,769)	1:33:X:ILE:HD11	1:69:X:LEU:HB2	10	0.14
(1,769)	1:33:X:ILE:HD12	1:69:X:LEU:HB2	10	0.14
(1,769)	1:33:X:ILE:HD13	1:69:X:LEU:HB2	10	0.14
(1,745)	1:72:X:GLN:HB3	1:76:X:GLU:HB3	3	0.14
(1,742)	1:122:X:GLU:HA	1:125:X:LYS:HB3	2	0.14
(1,742)	1:122:X:GLU:HA	1:125:X:LYS:HB3	7	0.14
(1,742)	1:122:X:GLU:HA	1:125:X:LYS:HB3	9	0.14
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	3	0.14
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	9	0.14
(1,684)	1:106:X:PHE:HE1	1:112:X:LEU:HB3	9	0.14
(1,568)	1:99:X:THR:HG21	1:100:X:SER:HA	7	0.14
(1,568)	1:99:X:THR:HG22	1:100:X:SER:HA	7	0.14
(1,568)	1:99:X:THR:HG23	1:100:X:SER:HA	7	0.14
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD21	1	0.14
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD22	1	0.14
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD23	1	0.14
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	4	0.14
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	4	0.14
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	4	0.14
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	4	0.14
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	4	0.14
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	4	0.14
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	9	0.14
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	9	0.14
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	9	0.14
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	6	0.14
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	6	0.14
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	6	0.14
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	6	0.14
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	6	0.14
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	6	0.14
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	6	0.14
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	6	0.14
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	6	0.14
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	2	0.14
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	2	0.14
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE1	6	0.14
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE2	6	0.14
(1,395)	1:91:X:MET:HB2	1:91:X:MET:HE3	6	0.14
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	3	0.14
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	3	0.14
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	3	0.14
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE1	4	0.14
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE2	4	0.14
(1,372)	1:91:X:MET:HA	1:91:X:MET:HE3	4	0.14
(1,359)	1:63:X:ILE:HD11	1:123:X:PHE:HB2	8	0.14
(1,359)	1:63:X:ILE:HD12	1:123:X:PHE:HB2	8	0.14
(1,359)	1:63:X:ILE:HD13	1:123:X:PHE:HB2	8	0.14
(1,295)	1:90:X:LEU:HB2	1:100:X:SER:HA	5	0.14
(1,250)	1:137:X:PHE:HD1	1:138:X:PRO:HD2	5	0.14
(1,249)	1:137:X:PHE:HD1	1:138:X:PRO:HD3	6	0.14
(1,190)	1:25:X:LEU:HA	1:74:X:PRO:HD3	4	0.14
(1,188)	1:119:X:LEU:HA	1:122:X:GLU:HB3	5	0.14
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	1	0.14
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	6	0.14
(1,96)	1:29:X:LYS:HA	1:73:X:PHE:HD1	4	0.14
(1,2317)	1:117:X:GLN:HG2	1:118:X:SER:H	1	0.13
(1,2317)	1:117:X:GLN:HG3	1:118:X:SER:H	1	0.13
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD11	7	0.13
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD12	7	0.13
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD13	7	0.13
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD11	7	0.13
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD12	7	0.13
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD13	7	0.13
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD11	7	0.13
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD12	7	0.13
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD13	7	0.13
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD11	7	0.13
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD12	7	0.13
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD13	7	0.13
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD11	7	0.13
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD12	7	0.13
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD13	7	0.13
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD11	7	0.13
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD12	7	0.13
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD13	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2284)	1:110:X:SER:HB2	1:115:X:ILE:HG21	2	0.13
(1,2284)	1:110:X:SER:HB2	1:115:X:ILE:HG22	2	0.13
(1,2284)	1:110:X:SER:HB2	1:115:X:ILE:HG23	2	0.13
(1,2284)	1:110:X:SER:HB3	1:115:X:ILE:HG21	2	0.13
(1,2284)	1:110:X:SER:HB3	1:115:X:ILE:HG22	2	0.13
(1,2284)	1:110:X:SER:HB3	1:115:X:ILE:HG23	2	0.13
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	1	0.13
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	1	0.13
(1,2260)	1:102:X:LEU:HD11	1:122:X:GLU:HG2	1	0.13
(1,2260)	1:102:X:LEU:HD12	1:122:X:GLU:HG2	1	0.13
(1,2260)	1:102:X:LEU:HD13	1:122:X:GLU:HG2	1	0.13
(1,2260)	1:102:X:LEU:HD21	1:122:X:GLU:HG2	1	0.13
(1,2260)	1:102:X:LEU:HD22	1:122:X:GLU:HG2	1	0.13
(1,2260)	1:102:X:LEU:HD23	1:122:X:GLU:HG2	1	0.13
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	7	0.13
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	7	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG11	1	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG12	1	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG13	1	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG21	1	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG22	1	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG23	1	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG11	1	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG12	1	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG13	1	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG21	1	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG22	1	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG23	1	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG11	3	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG12	3	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG13	3	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG21	3	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG22	3	0.13
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG23	3	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG11	3	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG12	3	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG13	3	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG21	3	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG22	3	0.13
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG23	3	0.13
(1,2178)	1:91:X:MET:HE1	1:95:X:GLY:HA2	6	0.13
(1,2178)	1:91:X:MET:HE1	1:95:X:GLY:HA3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2178)	1:91:X:MET:HE2	1:95:X:GLY:HA2	6	0.13
(1,2178)	1:91:X:MET:HE2	1:95:X:GLY:HA3	6	0.13
(1,2178)	1:91:X:MET:HE3	1:95:X:GLY:HA2	6	0.13
(1,2178)	1:91:X:MET:HE3	1:95:X:GLY:HA3	6	0.13
(1,2145)	1:90:X:LEU:H	1:90:X:LEU:HD11	5	0.13
(1,2145)	1:90:X:LEU:H	1:90:X:LEU:HD12	5	0.13
(1,2145)	1:90:X:LEU:H	1:90:X:LEU:HD13	5	0.13
(1,2145)	1:90:X:LEU:H	1:90:X:LEU:HD21	5	0.13
(1,2145)	1:90:X:LEU:H	1:90:X:LEU:HD22	5	0.13
(1,2145)	1:90:X:LEU:H	1:90:X:LEU:HD23	5	0.13
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	7	0.13
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	7	0.13
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	6	0.13
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	6	0.13
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	6	0.13
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	6	0.13
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	6	0.13
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	6	0.13
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG11	4	0.13
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG12	4	0.13
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG13	4	0.13
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG21	4	0.13
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG22	4	0.13
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG23	4	0.13
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG11	4	0.13
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG12	4	0.13
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG13	4	0.13
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG21	4	0.13
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG22	4	0.13
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG23	4	0.13
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG11	5	0.13
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG12	5	0.13
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG13	5	0.13
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG21	5	0.13
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG22	5	0.13
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG23	5	0.13
(1,2077)	1:79:X:VAL:HG11	1:81:X:SER:H	7	0.13
(1,2077)	1:79:X:VAL:HG12	1:81:X:SER:H	7	0.13
(1,2077)	1:79:X:VAL:HG13	1:81:X:SER:H	7	0.13
(1,2077)	1:79:X:VAL:HG21	1:81:X:SER:H	7	0.13
(1,2077)	1:79:X:VAL:HG22	1:81:X:SER:H	7	0.13
(1,2077)	1:79:X:VAL:HG23	1:81:X:SER:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2077)	1:79:X:VAL:HG11	1:81:X:SER:H	8	0.13
(1,2077)	1:79:X:VAL:HG12	1:81:X:SER:H	8	0.13
(1,2077)	1:79:X:VAL:HG13	1:81:X:SER:H	8	0.13
(1,2077)	1:79:X:VAL:HG21	1:81:X:SER:H	8	0.13
(1,2077)	1:79:X:VAL:HG22	1:81:X:SER:H	8	0.13
(1,2077)	1:79:X:VAL:HG23	1:81:X:SER:H	8	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD11	2	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD12	2	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD13	2	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD21	2	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD22	2	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD23	2	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD11	4	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD12	4	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD13	4	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD21	4	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD22	4	0.13
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD23	4	0.13
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG2	9	0.13
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG3	9	0.13
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG2	9	0.13
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG3	9	0.13
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	7	0.13
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	7	0.13
(1,1873)	1:44:X:ALA:HB1	1:53:X:ARG:HD2	6	0.13
(1,1873)	1:44:X:ALA:HB1	1:53:X:ARG:HD3	6	0.13
(1,1873)	1:44:X:ALA:HB2	1:53:X:ARG:HD2	6	0.13
(1,1873)	1:44:X:ALA:HB2	1:53:X:ARG:HD3	6	0.13
(1,1873)	1:44:X:ALA:HB3	1:53:X:ARG:HD2	6	0.13
(1,1873)	1:44:X:ALA:HB3	1:53:X:ARG:HD3	6	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	5	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	5	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	5	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	5	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	5	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	5	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	8	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	8	0.13
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	8	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	8	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	8	0.13
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1857)	1:37:X:ARG:HD2	1:52:X:TYR:HE1	8	0.13
(1,1857)	1:37:X:ARG:HD3	1:52:X:TYR:HE1	8	0.13
(1,1840)	1:36:X:LEU:HD11	1:113:X:GLY:HA2	9	0.13
(1,1840)	1:36:X:LEU:HD12	1:113:X:GLY:HA2	9	0.13
(1,1840)	1:36:X:LEU:HD13	1:113:X:GLY:HA2	9	0.13
(1,1840)	1:36:X:LEU:HD21	1:113:X:GLY:HA2	9	0.13
(1,1840)	1:36:X:LEU:HD22	1:113:X:GLY:HA2	9	0.13
(1,1840)	1:36:X:LEU:HD23	1:113:X:GLY:HA2	9	0.13
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD11	10	0.13
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD12	10	0.13
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD13	10	0.13
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD21	10	0.13
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD22	10	0.13
(1,1837)	1:36:X:LEU:HD11	1:112:X:LEU:HD23	10	0.13
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD11	10	0.13
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD12	10	0.13
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD13	10	0.13
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD21	10	0.13
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD22	10	0.13
(1,1837)	1:36:X:LEU:HD12	1:112:X:LEU:HD23	10	0.13
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD11	10	0.13
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD12	10	0.13
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD13	10	0.13
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD21	10	0.13
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD22	10	0.13
(1,1837)	1:36:X:LEU:HD13	1:112:X:LEU:HD23	10	0.13
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD11	10	0.13
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD12	10	0.13
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD13	10	0.13
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD21	10	0.13
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD22	10	0.13
(1,1837)	1:36:X:LEU:HD21	1:112:X:LEU:HD23	10	0.13
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD11	10	0.13
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD12	10	0.13
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD13	10	0.13
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD21	10	0.13
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD22	10	0.13
(1,1837)	1:36:X:LEU:HD22	1:112:X:LEU:HD23	10	0.13
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD11	10	0.13
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD12	10	0.13
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD13	10	0.13
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD21	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD22	10	0.13
(1,1837)	1:36:X:LEU:HD23	1:112:X:LEU:HD23	10	0.13
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	1	0.13
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	1	0.13
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	1	0.13
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	1	0.13
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	1	0.13
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	1	0.13
(1,1836)	1:36:X:LEU:HD11	1:112:X:LEU:HB2	2	0.13
(1,1836)	1:36:X:LEU:HD12	1:112:X:LEU:HB2	2	0.13
(1,1836)	1:36:X:LEU:HD13	1:112:X:LEU:HB2	2	0.13
(1,1836)	1:36:X:LEU:HD21	1:112:X:LEU:HB2	2	0.13
(1,1836)	1:36:X:LEU:HD22	1:112:X:LEU:HB2	2	0.13
(1,1836)	1:36:X:LEU:HD23	1:112:X:LEU:HB2	2	0.13
(1,1826)	1:36:X:LEU:HD11	1:43:X:ILE:HG13	6	0.13
(1,1826)	1:36:X:LEU:HD12	1:43:X:ILE:HG13	6	0.13
(1,1826)	1:36:X:LEU:HD13	1:43:X:ILE:HG13	6	0.13
(1,1826)	1:36:X:LEU:HD21	1:43:X:ILE:HG13	6	0.13
(1,1826)	1:36:X:LEU:HD22	1:43:X:ILE:HG13	6	0.13
(1,1826)	1:36:X:LEU:HD23	1:43:X:ILE:HG13	6	0.13
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB2	4	0.13
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB3	4	0.13
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB2	6	0.13
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB3	6	0.13
(1,1728)	1:28:X:GLN:HG2	1:74:X:PRO:HD3	8	0.13
(1,1728)	1:28:X:GLN:HG3	1:74:X:PRO:HD3	8	0.13
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	10	0.13
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	10	0.13
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	10	0.13
(1,1596)	1:44:X:ALA:H	1:53:X:ARG:HB2	7	0.13
(1,1573)	1:43:X:ILE:HG13	1:54:X:LEU:H	6	0.13
(1,1561)	1:120:X:LEU:HB3	1:124:X:TRP:HE1	2	0.13
(1,1546)	1:69:X:LEU:H	1:78:X:PRO:HB2	1	0.13
(1,1437)	1:90:X:LEU:H	1:90:X:LEU:HD11	5	0.13
(1,1437)	1:90:X:LEU:H	1:90:X:LEU:HD12	5	0.13
(1,1437)	1:90:X:LEU:H	1:90:X:LEU:HD13	5	0.13
(1,1426)	1:123:X:PHE:H	1:124:X:TRP:HB3	3	0.13
(1,1412)	1:57:X:THR:H	1:57:X:THR:HB	2	0.13
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	10	0.13
(1,1278)	1:34:X:GLU:H	1:34:X:GLU:HB2	1	0.13
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	9	0.13
(1,1212)	1:50:X:VAL:HB	1:51:X:GLU:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1103)	1:46:X:ILE:HG13	1:47:X:GLN:H	6	0.13
(1,987)	1:34:X:GLU:HG3	1:35:X:SER:H	5	0.13
(1,962)	1:91:X:MET:H	1:91:X:MET:HE1	1	0.13
(1,962)	1:91:X:MET:H	1:91:X:MET:HE2	1	0.13
(1,962)	1:91:X:MET:H	1:91:X:MET:HE3	1	0.13
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	4	0.13
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	5	0.13
(1,912)	1:50:X:VAL:HA	1:68:X:LEU:HG	3	0.13
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG21	4	0.13
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG22	4	0.13
(1,906)	1:52:X:TYR:HB3	1:67:X:ILE:HG23	4	0.13
(1,850)	1:78:X:PRO:HB3	1:79:X:VAL:HA	10	0.13
(1,835)	1:119:X:LEU:HA	1:122:X:GLU:HG2	3	0.13
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	1	0.13
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	3	0.13
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	8	0.13
(1,816)	1:52:X:TYR:HB2	1:52:X:TYR:HD1	10	0.13
(1,808)	1:57:X:THR:HA	1:63:X:ILE:HG13	7	0.13
(1,797)	1:56:X:PHE:HD2	1:65:X:ILE:HG12	9	0.13
(1,783)	1:74:X:PRO:HB2	1:106:X:PHE:HE1	4	0.13
(1,764)	1:32:X:LEU:HG	1:74:X:PRO:HB2	9	0.13
(1,753)	1:78:X:PRO:HB3	1:80:X:ILE:HD11	10	0.13
(1,753)	1:78:X:PRO:HB3	1:80:X:ILE:HD12	10	0.13
(1,753)	1:78:X:PRO:HB3	1:80:X:ILE:HD13	10	0.13
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	6	0.13
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	9	0.13
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	1	0.13
(1,707)	1:65:X:ILE:HD11	1:120:X:LEU:HB2	7	0.13
(1,707)	1:65:X:ILE:HD12	1:120:X:LEU:HB2	7	0.13
(1,707)	1:65:X:ILE:HD13	1:120:X:LEU:HB2	7	0.13
(1,654)	1:48:X:LYS:HD3	1:49:X:ASP:HA	6	0.13
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD11	9	0.13
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD12	9	0.13
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD13	9	0.13
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD11	9	0.13
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD12	9	0.13
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD13	9	0.13
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD11	9	0.13
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD12	9	0.13
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD13	9	0.13
(1,574)	1:23:X:THR:HG21	1:26:X:GLN:HB3	3	0.13
(1,574)	1:23:X:THR:HG22	1:26:X:GLN:HB3	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,574)	1:23:X:THR:HG23	1:26:X:GLN:HB3	3	0.13
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD21	2	0.13
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD22	2	0.13
(1,538)	1:68:X:LEU:HA	1:69:X:LEU:HD23	2	0.13
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	5	0.13
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	5	0.13
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	5	0.13
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG21	6	0.13
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG22	6	0.13
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG23	6	0.13
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG21	6	0.13
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG22	6	0.13
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG23	6	0.13
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG21	6	0.13
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG22	6	0.13
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG23	6	0.13
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	7	0.13
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	7	0.13
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	7	0.13
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD11	5	0.13
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD12	5	0.13
(1,451)	1:86:X:ILE:HG21	1:86:X:ILE:HD13	5	0.13
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD11	5	0.13
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD12	5	0.13
(1,451)	1:86:X:ILE:HG22	1:86:X:ILE:HD13	5	0.13
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD11	5	0.13
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD12	5	0.13
(1,451)	1:86:X:ILE:HG23	1:86:X:ILE:HD13	5	0.13
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	6	0.13
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	6	0.13
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	6	0.13
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	8	0.13
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	8	0.13
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	8	0.13
(1,431)	1:86:X:ILE:HD11	1:91:X:MET:HA	4	0.13
(1,431)	1:86:X:ILE:HD12	1:91:X:MET:HA	4	0.13
(1,431)	1:86:X:ILE:HD13	1:91:X:MET:HA	4	0.13
(1,419)	1:43:X:ILE:HD11	1:54:X:LEU:HB3	7	0.13
(1,419)	1:43:X:ILE:HD12	1:54:X:LEU:HB3	7	0.13
(1,419)	1:43:X:ILE:HD13	1:54:X:LEU:HB3	7	0.13
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD11	1	0.13
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD12	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD13	1	0.13
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	1	0.13
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	5	0.13
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	5	0.13
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	5	0.13
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD21	2	0.13
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD22	2	0.13
(1,272)	1:140:X:LEU:HA	1:140:X:LEU:HD23	2	0.13
(1,264)	1:111:X:ASP:HA	1:112:X:LEU:HB3	4	0.13
(1,236)	1:58:X:ILE:HD11	1:127:X:PRO:HD2	7	0.13
(1,236)	1:58:X:ILE:HD12	1:127:X:PRO:HD2	7	0.13
(1,236)	1:58:X:ILE:HD13	1:127:X:PRO:HD2	7	0.13
(1,231)	1:43:X:ILE:HG13	1:54:X:LEU:HA	1	0.13
(1,211)	1:137:X:PHE:HA	1:138:X:PRO:HD3	8	0.13
(1,209)	1:77:X:LYS:HD3	1:78:X:PRO:HD3	1	0.13
(1,206)	1:78:X:PRO:HD2	1:106:X:PHE:HE1	3	0.13
(1,205)	1:78:X:PRO:HD2	1:106:X:PHE:HD1	4	0.13
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	1	0.13
(1,153)	1:121:X:ASP:HA	1:124:X:TRP:HB3	10	0.13
(1,149)	1:133:X:THR:HG21	1:134:X:SER:HA	3	0.13
(1,149)	1:133:X:THR:HG22	1:134:X:SER:HA	3	0.13
(1,149)	1:133:X:THR:HG23	1:134:X:SER:HA	3	0.13
(1,141)	1:70:X:PRO:HD3	1:73:X:PHE:HA	7	0.13
(1,122)	1:139:X:TYR:HA	1:139:X:TYR:HD1	3	0.13
(1,63)	1:29:X:LYS:HA	1:32:X:LEU:HB3	8	0.13
(1,62)	1:29:X:LYS:HA	1:74:X:PRO:HD2	6	0.13
(1,62)	1:29:X:LYS:HA	1:74:X:PRO:HD2	10	0.13
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB2	9	0.12
(1,2351)	1:125:X:LYS:HB3	1:126:X:ASN:HB3	9	0.12
(1,2328)	1:119:X:LEU:HD11	1:122:X:GLU:HG3	10	0.12
(1,2328)	1:119:X:LEU:HD12	1:122:X:GLU:HG3	10	0.12
(1,2328)	1:119:X:LEU:HD13	1:122:X:GLU:HG3	10	0.12
(1,2328)	1:119:X:LEU:HD21	1:122:X:GLU:HG3	10	0.12
(1,2328)	1:119:X:LEU:HD22	1:122:X:GLU:HG3	10	0.12
(1,2328)	1:119:X:LEU:HD23	1:122:X:GLU:HG3	10	0.12
(1,2317)	1:117:X:GLN:HG2	1:118:X:SER:H	7	0.12
(1,2317)	1:117:X:GLN:HG3	1:118:X:SER:H	7	0.12
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG2	1	0.12
(1,2302)	1:114:X:LYS:HA	1:117:X:GLN:HG3	1	0.12
(1,2235)	1:100:X:SER:HB2	1:103:X:VAL:HG11	6	0.12
(1,2235)	1:100:X:SER:HB2	1:103:X:VAL:HG12	6	0.12
(1,2235)	1:100:X:SER:HB2	1:103:X:VAL:HG13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:100:X:SER:HB2	1:103:X:VAL:HG21	6	0.12
(1,2235)	1:100:X:SER:HB2	1:103:X:VAL:HG22	6	0.12
(1,2235)	1:100:X:SER:HB2	1:103:X:VAL:HG23	6	0.12
(1,2235)	1:100:X:SER:HB3	1:103:X:VAL:HG11	6	0.12
(1,2235)	1:100:X:SER:HB3	1:103:X:VAL:HG12	6	0.12
(1,2235)	1:100:X:SER:HB3	1:103:X:VAL:HG13	6	0.12
(1,2235)	1:100:X:SER:HB3	1:103:X:VAL:HG21	6	0.12
(1,2235)	1:100:X:SER:HB3	1:103:X:VAL:HG22	6	0.12
(1,2235)	1:100:X:SER:HB3	1:103:X:VAL:HG23	6	0.12
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	6	0.12
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	6	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG11	5	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG12	5	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG13	5	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG21	5	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG22	5	0.12
(1,2200)	1:94:X:GLN:HB2	1:96:X:VAL:HG23	5	0.12
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG11	5	0.12
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG12	5	0.12
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG13	5	0.12
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG21	5	0.12
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG22	5	0.12
(1,2200)	1:94:X:GLN:HB3	1:96:X:VAL:HG23	5	0.12
(1,2166)	1:90:X:LEU:HD11	1:122:X:GLU:HB3	1	0.12
(1,2166)	1:90:X:LEU:HD12	1:122:X:GLU:HB3	1	0.12
(1,2166)	1:90:X:LEU:HD13	1:122:X:GLU:HB3	1	0.12
(1,2166)	1:90:X:LEU:HD21	1:122:X:GLU:HB3	1	0.12
(1,2166)	1:90:X:LEU:HD22	1:122:X:GLU:HB3	1	0.12
(1,2166)	1:90:X:LEU:HD23	1:122:X:GLU:HB3	1	0.12
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB2	10	0.12
(1,2159)	1:90:X:LEU:HD11	1:100:X:SER:HB3	10	0.12
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB2	10	0.12
(1,2159)	1:90:X:LEU:HD12	1:100:X:SER:HB3	10	0.12
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB2	10	0.12
(1,2159)	1:90:X:LEU:HD13	1:100:X:SER:HB3	10	0.12
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB2	10	0.12
(1,2159)	1:90:X:LEU:HD21	1:100:X:SER:HB3	10	0.12
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB2	10	0.12
(1,2159)	1:90:X:LEU:HD22	1:100:X:SER:HB3	10	0.12
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB2	10	0.12
(1,2159)	1:90:X:LEU:HD23	1:100:X:SER:HB3	10	0.12
(1,2132)	1:87:X:ARG:HB2	1:131:X:ALA:HA	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:87:X:ARG:HB3	1:131:X:ALA:HA	5	0.12
(1,2095)	1:81:X:SER:HB2	1:98:X:VAL:H	4	0.12
(1,2095)	1:81:X:SER:HB3	1:98:X:VAL:H	4	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG11	8	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG12	8	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG13	8	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG21	8	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG22	8	0.12
(1,2092)	1:81:X:SER:HB2	1:96:X:VAL:HG23	8	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG11	8	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG12	8	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG13	8	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG21	8	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG22	8	0.12
(1,2092)	1:81:X:SER:HB3	1:96:X:VAL:HG23	8	0.12
(1,2077)	1:79:X:VAL:HG11	1:81:X:SER:H	5	0.12
(1,2077)	1:79:X:VAL:HG12	1:81:X:SER:H	5	0.12
(1,2077)	1:79:X:VAL:HG13	1:81:X:SER:H	5	0.12
(1,2077)	1:79:X:VAL:HG21	1:81:X:SER:H	5	0.12
(1,2077)	1:79:X:VAL:HG22	1:81:X:SER:H	5	0.12
(1,2077)	1:79:X:VAL:HG23	1:81:X:SER:H	5	0.12
(1,1989)	1:61:X:LEU:HD11	1:128:X:PRO:HG3	4	0.12
(1,1989)	1:61:X:LEU:HD12	1:128:X:PRO:HG3	4	0.12
(1,1989)	1:61:X:LEU:HD13	1:128:X:PRO:HG3	4	0.12
(1,1989)	1:61:X:LEU:HD21	1:128:X:PRO:HG3	4	0.12
(1,1989)	1:61:X:LEU:HD22	1:128:X:PRO:HG3	4	0.12
(1,1989)	1:61:X:LEU:HD23	1:128:X:PRO:HG3	4	0.12
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	4	0.12
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	4	0.12
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	3	0.12
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	3	0.12
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	3	0.12
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	3	0.12
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	3	0.12
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	3	0.12
(1,1906)	1:49:X:ASP:HA	1:69:X:LEU:HD11	2	0.12
(1,1906)	1:49:X:ASP:HA	1:69:X:LEU:HD12	2	0.12
(1,1906)	1:49:X:ASP:HA	1:69:X:LEU:HD13	2	0.12
(1,1906)	1:49:X:ASP:HA	1:69:X:LEU:HD21	2	0.12
(1,1906)	1:49:X:ASP:HA	1:69:X:LEU:HD22	2	0.12
(1,1906)	1:49:X:ASP:HA	1:69:X:LEU:HD23	2	0.12
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	1	0.12
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	1	0.12
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	1	0.12
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	1	0.12
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	1	0.12
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	4	0.12
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	4	0.12
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	4	0.12
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	4	0.12
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	4	0.12
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	4	0.12
(1,1850)	1:37:X:ARG:HB3	1:37:X:ARG:HD2	10	0.12
(1,1850)	1:37:X:ARG:HB3	1:37:X:ARG:HD3	10	0.12
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB2	2	0.12
(1,1814)	1:36:X:LEU:HB3	1:39:X:SER:HB3	2	0.12
(1,1784)	1:32:X:LEU:HD11	1:111:X:ASP:HA	8	0.12
(1,1784)	1:32:X:LEU:HD12	1:111:X:ASP:HA	8	0.12
(1,1784)	1:32:X:LEU:HD13	1:111:X:ASP:HA	8	0.12
(1,1784)	1:32:X:LEU:HD21	1:111:X:ASP:HA	8	0.12
(1,1784)	1:32:X:LEU:HD22	1:111:X:ASP:HA	8	0.12
(1,1784)	1:32:X:LEU:HD23	1:111:X:ASP:HA	8	0.12
(1,1654)	1:63:X:ILE:HD11	1:123:X:PHE:HE1	3	0.12
(1,1654)	1:63:X:ILE:HD12	1:123:X:PHE:HE1	3	0.12
(1,1654)	1:63:X:ILE:HD13	1:123:X:PHE:HE1	3	0.12
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	6	0.12
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	6	0.12
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	6	0.12
(1,1640)	1:138:X:PRO:HB2	1:139:X:TYR:HD1	5	0.12
(1,1614)	1:57:X:THR:HG21	1:60:X:ASN:H	1	0.12
(1,1614)	1:57:X:THR:HG22	1:60:X:ASN:H	1	0.12
(1,1614)	1:57:X:THR:HG23	1:60:X:ASN:H	1	0.12
(1,1595)	1:43:X:ILE:HG13	1:44:X:ALA:H	6	0.12
(1,1530)	1:130:X:LEU:HD11	1:131:X:ALA:H	3	0.12
(1,1530)	1:130:X:LEU:HD12	1:131:X:ALA:H	3	0.12
(1,1530)	1:130:X:LEU:HD13	1:131:X:ALA:H	3	0.12
(1,1513)	1:73:X:PHE:HD1	1:75:X:GLN:H	9	0.12
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	2	0.12
(1,1376)	1:81:X:SER:HA	1:98:X:VAL:H	4	0.12
(1,1285)	1:48:X:LYS:HD3	1:49:X:ASP:H	5	0.12
(1,1260)	1:137:X:PHE:HA	1:139:X:TYR:H	3	0.12
(1,1212)	1:50:X:VAL:HB	1:51:X:GLU:H	2	0.12
(1,1212)	1:50:X:VAL:HB	1:51:X:GLU:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1208)	1:47:X:GLN:HG2	1:51:X:GLU:H	1	0.12
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	2	0.12
(1,1198)	1:92:X:ASP:H	1:96:X:VAL:HA	7	0.12
(1,1134)	1:50:X:VAL:H	1:52:X:TYR:HE1	3	0.12
(1,1055)	1:73:X:PHE:HD1	1:76:X:GLU:H	1	0.12
(1,1052)	1:72:X:GLN:HB3	1:76:X:GLU:H	5	0.12
(1,1050)	1:73:X:PHE:HB2	1:76:X:GLU:H	9	0.12
(1,1027)	1:96:X:VAL:H	1:97:X:TYR:H	5	0.12
(1,965)	1:91:X:MET:H	1:91:X:MET:HG3	4	0.12
(1,962)	1:91:X:MET:H	1:91:X:MET:HE1	7	0.12
(1,962)	1:91:X:MET:H	1:91:X:MET:HE2	7	0.12
(1,962)	1:91:X:MET:H	1:91:X:MET:HE3	7	0.12
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	1	0.12
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	3	0.12
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	8	0.12
(1,919)	1:52:X:TYR:HB2	1:52:X:TYR:HE1	10	0.12
(1,912)	1:50:X:VAL:HA	1:68:X:LEU:HG	9	0.12
(1,894)	1:43:X:ILE:HG13	1:52:X:TYR:HB2	2	0.12
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	1	0.12
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	10	0.12
(1,808)	1:57:X:THR:HA	1:63:X:ILE:HG13	9	0.12
(1,733)	1:82:X:VAL:HB	1:96:X:VAL:HA	3	0.12
(1,726)	1:46:X:ILE:HB	1:47:X:GLN:HB3	1	0.12
(1,721)	1:47:X:GLN:HG2	1:50:X:VAL:HB	5	0.12
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD11	1	0.12
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD12	1	0.12
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD13	1	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	6	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	6	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	6	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	7	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	7	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	7	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	10	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	10	0.12
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	10	0.12
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	3	0.12
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	9	0.12
(1,657)	1:86:X:ILE:HG13	1:91:X:MET:HB3	4	0.12
(1,653)	1:32:X:LEU:HD11	1:74:X:PRO:HB2	4	0.12
(1,653)	1:32:X:LEU:HD12	1:74:X:PRO:HB2	4	0.12
(1,653)	1:32:X:LEU:HD13	1:74:X:PRO:HB2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	7	0.12
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	7	0.12
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	7	0.12
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD11	3	0.12
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD12	3	0.12
(1,624)	1:140:X:LEU:HA	1:140:X:LEU:HD13	3	0.12
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD11	5	0.12
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD12	5	0.12
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD13	5	0.12
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD11	5	0.12
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD12	5	0.12
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD13	5	0.12
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD11	5	0.12
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD12	5	0.12
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD13	5	0.12
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD11	8	0.12
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD12	8	0.12
(1,621)	1:116:X:ILE:HG21	1:120:X:LEU:HD13	8	0.12
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD11	8	0.12
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD12	8	0.12
(1,621)	1:116:X:ILE:HG22	1:120:X:LEU:HD13	8	0.12
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD11	8	0.12
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD12	8	0.12
(1,621)	1:116:X:ILE:HG23	1:120:X:LEU:HD13	8	0.12
(1,568)	1:99:X:THR:HG21	1:100:X:SER:HA	2	0.12
(1,568)	1:99:X:THR:HG22	1:100:X:SER:HA	2	0.12
(1,568)	1:99:X:THR:HG23	1:100:X:SER:HA	2	0.12
(1,568)	1:99:X:THR:HG21	1:100:X:SER:HA	4	0.12
(1,568)	1:99:X:THR:HG22	1:100:X:SER:HA	4	0.12
(1,568)	1:99:X:THR:HG23	1:100:X:SER:HA	4	0.12
(1,512)	1:67:X:ILE:HG21	1:78:X:PRO:HD3	2	0.12
(1,512)	1:67:X:ILE:HG22	1:78:X:PRO:HD3	2	0.12
(1,512)	1:67:X:ILE:HG23	1:78:X:PRO:HD3	2	0.12
(1,501)	1:67:X:ILE:HG21	1:80:X:ILE:HA	7	0.12
(1,501)	1:67:X:ILE:HG22	1:80:X:ILE:HA	7	0.12
(1,501)	1:67:X:ILE:HG23	1:80:X:ILE:HA	7	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG21	1	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG22	1	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG23	1	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG21	1	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG22	1	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG23	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG21	1	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG22	1	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG23	1	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG21	5	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG22	5	0.12
(1,475)	1:54:X:LEU:HD21	1:116:X:ILE:HG23	5	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG21	5	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG22	5	0.12
(1,475)	1:54:X:LEU:HD22	1:116:X:ILE:HG23	5	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG21	5	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG22	5	0.12
(1,475)	1:54:X:LEU:HD23	1:116:X:ILE:HG23	5	0.12
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	2	0.12
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	2	0.12
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	2	0.12
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	10	0.12
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	10	0.12
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	10	0.12
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD11	6	0.12
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD12	6	0.12
(1,424)	1:43:X:ILE:HG21	1:43:X:ILE:HD13	6	0.12
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD11	6	0.12
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD12	6	0.12
(1,424)	1:43:X:ILE:HG22	1:43:X:ILE:HD13	6	0.12
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD11	6	0.12
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD12	6	0.12
(1,424)	1:43:X:ILE:HG23	1:43:X:ILE:HD13	6	0.12
(1,420)	1:63:X:ILE:HG12	1:65:X:ILE:HD11	10	0.12
(1,420)	1:63:X:ILE:HG12	1:65:X:ILE:HD12	10	0.12
(1,420)	1:63:X:ILE:HG12	1:65:X:ILE:HD13	10	0.12
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD11	2	0.12
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD12	2	0.12
(1,417)	1:32:X:LEU:HB2	1:33:X:ILE:HD13	2	0.12
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	4	0.12
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	4	0.12
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	4	0.12
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	4	0.12
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	4	0.12
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	4	0.12
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	4	0.12
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	4	0.12
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE1	1	0.12
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE2	1	0.12
(1,374)	1:86:X:ILE:HA	1:91:X:MET:HE3	1	0.12
(1,359)	1:63:X:ILE:HD11	1:123:X:PHE:HB2	3	0.12
(1,359)	1:63:X:ILE:HD12	1:123:X:PHE:HB2	3	0.12
(1,359)	1:63:X:ILE:HD13	1:123:X:PHE:HB2	3	0.12
(1,334)	1:93:X:LYS:HA	1:93:X:LYS:HD3	4	0.12
(1,325)	1:86:X:ILE:HA	1:128:X:PRO:HB3	3	0.12
(1,319)	1:86:X:ILE:HD11	1:130:X:LEU:HA	8	0.12
(1,319)	1:86:X:ILE:HD12	1:130:X:LEU:HA	8	0.12
(1,319)	1:86:X:ILE:HD13	1:130:X:LEU:HA	8	0.12
(1,267)	1:76:X:GLU:HA	1:76:X:GLU:HG3	3	0.12
(1,209)	1:77:X:LYS:HD3	1:78:X:PRO:HD3	9	0.12
(1,193)	1:129:X:VAL:HA	1:130:X:LEU:HB3	2	0.12
(1,150)	1:33:X:ILE:HB	1:49:X:ASP:HA	4	0.12
(1,2339)	1:122:X:GLU:HA	1:125:X:LYS:HG2	9	0.11
(1,2339)	1:122:X:GLU:HA	1:125:X:LYS:HG3	9	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	3	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	3	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	3	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	3	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	3	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	3	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	3	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	3	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	3	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	3	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	3	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	3	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	5	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	5	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	5	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	5	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	5	0.11
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	5	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	5	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	5	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	5	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	5	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	5	0.11
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	5	0.11
(1,2322)	1:119:X:LEU:HA	1:119:X:LEU:HD11	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2322)	1:119:X:LEU:HA	1:119:X:LEU:HD12	3	0.11
(1,2322)	1:119:X:LEU:HA	1:119:X:LEU:HD13	3	0.11
(1,2322)	1:119:X:LEU:HA	1:119:X:LEU:HD21	3	0.11
(1,2322)	1:119:X:LEU:HA	1:119:X:LEU:HD22	3	0.11
(1,2322)	1:119:X:LEU:HA	1:119:X:LEU:HD23	3	0.11
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB2	4	0.11
(1,2277)	1:107:X:THR:H	1:110:X:SER:HB3	4	0.11
(1,2260)	1:102:X:LEU:HD11	1:122:X:GLU:HG2	3	0.11
(1,2260)	1:102:X:LEU:HD12	1:122:X:GLU:HG2	3	0.11
(1,2260)	1:102:X:LEU:HD13	1:122:X:GLU:HG2	3	0.11
(1,2260)	1:102:X:LEU:HD21	1:122:X:GLU:HG2	3	0.11
(1,2260)	1:102:X:LEU:HD22	1:122:X:GLU:HG2	3	0.11
(1,2260)	1:102:X:LEU:HD23	1:122:X:GLU:HG2	3	0.11
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD11	10	0.11
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD12	10	0.11
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD13	10	0.11
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD21	10	0.11
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD22	10	0.11
(1,2257)	1:102:X:LEU:HD11	1:119:X:LEU:HD23	10	0.11
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD11	10	0.11
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD12	10	0.11
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD13	10	0.11
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD21	10	0.11
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD22	10	0.11
(1,2257)	1:102:X:LEU:HD12	1:119:X:LEU:HD23	10	0.11
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD11	10	0.11
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD12	10	0.11
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD13	10	0.11
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD21	10	0.11
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD22	10	0.11
(1,2257)	1:102:X:LEU:HD13	1:119:X:LEU:HD23	10	0.11
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD11	10	0.11
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD12	10	0.11
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD13	10	0.11
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD21	10	0.11
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD22	10	0.11
(1,2257)	1:102:X:LEU:HD21	1:119:X:LEU:HD23	10	0.11
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD11	10	0.11
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD12	10	0.11
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD13	10	0.11
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD21	10	0.11
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2257)	1:102:X:LEU:HD22	1:119:X:LEU:HD23	10	0.11
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD11	10	0.11
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD12	10	0.11
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD13	10	0.11
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD21	10	0.11
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD22	10	0.11
(1,2257)	1:102:X:LEU:HD23	1:119:X:LEU:HD23	10	0.11
(1,2204)	1:94:X:GLN:HG2	1:97:X:TYR:HA	1	0.11
(1,2204)	1:94:X:GLN:HG3	1:97:X:TYR:HA	1	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG11	6	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG12	6	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG13	6	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG21	6	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG22	6	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG23	6	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG11	6	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG12	6	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG13	6	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG21	6	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG22	6	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG23	6	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG11	8	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG12	8	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG13	8	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG21	8	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG22	8	0.11
(1,2203)	1:94:X:GLN:HG2	1:96:X:VAL:HG23	8	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG11	8	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG12	8	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG13	8	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG21	8	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG22	8	0.11
(1,2203)	1:94:X:GLN:HG3	1:96:X:VAL:HG23	8	0.11
(1,2186)	1:92:X:ASP:HB2	1:99:X:THR:HB	7	0.11
(1,2186)	1:92:X:ASP:HB3	1:99:X:THR:HB	7	0.11
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD11	7	0.11
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD12	7	0.11
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD13	7	0.11
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD21	7	0.11
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD22	7	0.11
(1,2172)	1:91:X:MET:H	1:119:X:LEU:HD23	7	0.11
(1,2151)	1:90:X:LEU:HB3	1:100:X:SER:HB2	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2151)	1:90:X:LEU:HB3	1:100:X:SER:HB3	10	0.11
(1,2144)	1:89:X:HIS:HE1	1:90:X:LEU:HD11	7	0.11
(1,2144)	1:89:X:HIS:HE1	1:90:X:LEU:HD12	7	0.11
(1,2144)	1:89:X:HIS:HE1	1:90:X:LEU:HD13	7	0.11
(1,2144)	1:89:X:HIS:HE1	1:90:X:LEU:HD21	7	0.11
(1,2144)	1:89:X:HIS:HE1	1:90:X:LEU:HD22	7	0.11
(1,2144)	1:89:X:HIS:HE1	1:90:X:LEU:HD23	7	0.11
(1,2137)	1:87:X:ARG:HD2	1:131:X:ALA:HA	9	0.11
(1,2137)	1:87:X:ARG:HD3	1:131:X:ALA:HA	9	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	2	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	2	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	2	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	2	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	2	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	2	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG11	3	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG12	3	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG13	3	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG21	3	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG22	3	0.11
(1,2117)	1:85:X:PRO:HD2	1:96:X:VAL:HG23	3	0.11
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	3	0.11
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	3	0.11
(1,2113)	1:84:X:PRO:HB2	1:85:X:PRO:HD3	5	0.11
(1,2113)	1:84:X:PRO:HB3	1:85:X:PRO:HD3	5	0.11
(1,2105)	1:82:X:VAL:HG11	1:86:X:ILE:HA	7	0.11
(1,2105)	1:82:X:VAL:HG12	1:86:X:ILE:HA	7	0.11
(1,2105)	1:82:X:VAL:HG13	1:86:X:ILE:HA	7	0.11
(1,2105)	1:82:X:VAL:HG21	1:86:X:ILE:HA	7	0.11
(1,2105)	1:82:X:VAL:HG22	1:86:X:ILE:HA	7	0.11
(1,2105)	1:82:X:VAL:HG23	1:86:X:ILE:HA	7	0.11
(1,2103)	1:82:X:VAL:HG11	1:85:X:PRO:HA	2	0.11
(1,2103)	1:82:X:VAL:HG12	1:85:X:PRO:HA	2	0.11
(1,2103)	1:82:X:VAL:HG13	1:85:X:PRO:HA	2	0.11
(1,2103)	1:82:X:VAL:HG21	1:85:X:PRO:HA	2	0.11
(1,2103)	1:82:X:VAL:HG22	1:85:X:PRO:HA	2	0.11
(1,2103)	1:82:X:VAL:HG23	1:85:X:PRO:HA	2	0.11
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG11	10	0.11
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG12	10	0.11
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG13	10	0.11
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG21	10	0.11
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG22	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2082)	1:80:X:ILE:HB	1:103:X:VAL:HG23	10	0.11
(1,2032)	1:69:X:LEU:HA	1:69:X:LEU:HD11	10	0.11
(1,2032)	1:69:X:LEU:HA	1:69:X:LEU:HD12	10	0.11
(1,2032)	1:69:X:LEU:HA	1:69:X:LEU:HD13	10	0.11
(1,2032)	1:69:X:LEU:HA	1:69:X:LEU:HD21	10	0.11
(1,2032)	1:69:X:LEU:HA	1:69:X:LEU:HD22	10	0.11
(1,2032)	1:69:X:LEU:HA	1:69:X:LEU:HD23	10	0.11
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	5	0.11
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	5	0.11
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	6	0.11
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	6	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD11	1	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD12	1	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD13	1	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD21	1	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD22	1	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD23	1	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD11	3	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD12	3	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD13	3	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD21	3	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD22	3	0.11
(1,1994)	1:63:X:ILE:HG12	1:120:X:LEU:HD23	3	0.11
(1,1989)	1:61:X:LEU:HD11	1:128:X:PRO:HG3	5	0.11
(1,1989)	1:61:X:LEU:HD12	1:128:X:PRO:HG3	5	0.11
(1,1989)	1:61:X:LEU:HD13	1:128:X:PRO:HG3	5	0.11
(1,1989)	1:61:X:LEU:HD21	1:128:X:PRO:HG3	5	0.11
(1,1989)	1:61:X:LEU:HD22	1:128:X:PRO:HG3	5	0.11
(1,1989)	1:61:X:LEU:HD23	1:128:X:PRO:HG3	5	0.11
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	7	0.11
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	7	0.11
(1,1976)	1:59:X:ASN:HB2	1:127:X:PRO:HD2	8	0.11
(1,1976)	1:59:X:ASN:HB3	1:127:X:PRO:HD2	8	0.11
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	4	0.11
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	4	0.11
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	4	0.11
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	4	0.11
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	4	0.11
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	4	0.11
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	7	0.11
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	7	0.11
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	7	0.11
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	7	0.11
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	7	0.11
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD11	7	0.11
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD12	7	0.11
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD13	7	0.11
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD21	7	0.11
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD22	7	0.11
(1,1949)	1:56:X:PHE:HD2	1:120:X:LEU:HD23	7	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	5	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	5	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	5	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	5	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	5	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	5	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD11	9	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD12	9	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD13	9	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD21	9	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD22	9	0.11
(1,1943)	1:56:X:PHE:HB3	1:120:X:LEU:HD23	9	0.11
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG2	1	0.11
(1,1931)	1:53:X:ARG:HD2	1:55:X:PRO:HG3	1	0.11
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG2	1	0.11
(1,1931)	1:53:X:ARG:HD3	1:55:X:PRO:HG3	1	0.11
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB2	10	0.11
(1,1925)	1:53:X:ARG:HA	1:64:X:ASN:HB3	10	0.11
(1,1882)	1:45:X:GLU:HG2	1:48:X:LYS:HD2	4	0.11
(1,1882)	1:45:X:GLU:HG3	1:48:X:LYS:HD2	4	0.11
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD11	6	0.11
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD12	6	0.11
(1,1870)	1:42:X:SER:HB2	1:54:X:LEU:HD13	6	0.11
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD11	6	0.11
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD12	6	0.11
(1,1870)	1:42:X:SER:HB3	1:54:X:LEU:HD13	6	0.11
(1,1866)	1:39:X:SER:HB2	1:113:X:GLY:HA2	10	0.11
(1,1866)	1:39:X:SER:HB3	1:113:X:GLY:HA2	10	0.11
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD2	7	0.11
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD3	7	0.11
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD2	7	0.11
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD3	7	0.11
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD3	7	0.11
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	4	0.11
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	4	0.11
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	4	0.11
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	4	0.11
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	4	0.11
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	4	0.11
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	6	0.11
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	6	0.11
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	6	0.11
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	6	0.11
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	6	0.11
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	6	0.11
(1,1784)	1:32:X:LEU:HD11	1:111:X:ASP:HA	1	0.11
(1,1784)	1:32:X:LEU:HD12	1:111:X:ASP:HA	1	0.11
(1,1784)	1:32:X:LEU:HD13	1:111:X:ASP:HA	1	0.11
(1,1784)	1:32:X:LEU:HD21	1:111:X:ASP:HA	1	0.11
(1,1784)	1:32:X:LEU:HD22	1:111:X:ASP:HA	1	0.11
(1,1784)	1:32:X:LEU:HD23	1:111:X:ASP:HA	1	0.11
(1,1784)	1:32:X:LEU:HD11	1:111:X:ASP:HA	4	0.11
(1,1784)	1:32:X:LEU:HD12	1:111:X:ASP:HA	4	0.11
(1,1784)	1:32:X:LEU:HD13	1:111:X:ASP:HA	4	0.11
(1,1784)	1:32:X:LEU:HD21	1:111:X:ASP:HA	4	0.11
(1,1784)	1:32:X:LEU:HD22	1:111:X:ASP:HA	4	0.11
(1,1784)	1:32:X:LEU:HD23	1:111:X:ASP:HA	4	0.11
(1,1760)	1:30:X:GLN:HG2	1:33:X:ILE:HD11	8	0.11
(1,1760)	1:30:X:GLN:HG2	1:33:X:ILE:HD12	8	0.11
(1,1760)	1:30:X:GLN:HG2	1:33:X:ILE:HD13	8	0.11
(1,1760)	1:30:X:GLN:HG3	1:33:X:ILE:HD11	8	0.11
(1,1760)	1:30:X:GLN:HG3	1:33:X:ILE:HD12	8	0.11
(1,1760)	1:30:X:GLN:HG3	1:33:X:ILE:HD13	8	0.11
(1,1753)	1:29:X:LYS:HE2	1:69:X:LEU:HB2	7	0.11
(1,1753)	1:29:X:LYS:HE3	1:69:X:LEU:HB2	7	0.11
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG2	9	0.11
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG3	9	0.11
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG2	9	0.11
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG3	9	0.11
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG2	10	0.11
(1,1746)	1:29:X:LYS:HE2	1:30:X:GLN:HG3	10	0.11
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG2	10	0.11
(1,1746)	1:29:X:LYS:HE3	1:30:X:GLN:HG3	10	0.11
(1,1743)	1:29:X:LYS:HG2	1:49:X:ASP:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1743)	1:29:X:LYS:HG2	1:49:X:ASP:HB3	7	0.11
(1,1743)	1:29:X:LYS:HG3	1:49:X:ASP:HB2	7	0.11
(1,1743)	1:29:X:LYS:HG3	1:49:X:ASP:HB3	7	0.11
(1,1742)	1:29:X:LYS:HG2	1:33:X:ILE:HD11	7	0.11
(1,1742)	1:29:X:LYS:HG2	1:33:X:ILE:HD12	7	0.11
(1,1742)	1:29:X:LYS:HG2	1:33:X:ILE:HD13	7	0.11
(1,1742)	1:29:X:LYS:HG3	1:33:X:ILE:HD11	7	0.11
(1,1742)	1:29:X:LYS:HG3	1:33:X:ILE:HD12	7	0.11
(1,1742)	1:29:X:LYS:HG3	1:33:X:ILE:HD13	7	0.11
(1,1699)	1:24:X:SER:HA	1:27:X:GLN:HG2	10	0.11
(1,1699)	1:24:X:SER:HA	1:27:X:GLN:HG3	10	0.11
(1,1679)	1:138:X:PRO:HB3	1:139:X:TYR:HE1	9	0.11
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	7	0.11
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	7	0.11
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	7	0.11
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD11	8	0.11
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD12	8	0.11
(1,1648)	1:56:X:PHE:HD2	1:65:X:ILE:HD13	8	0.11
(1,1642)	1:73:X:PHE:HD1	1:74:X:PRO:HA	8	0.11
(1,1640)	1:138:X:PRO:HB2	1:139:X:TYR:HD1	1	0.11
(1,1614)	1:57:X:THR:HG21	1:60:X:ASN:H	2	0.11
(1,1614)	1:57:X:THR:HG22	1:60:X:ASN:H	2	0.11
(1,1614)	1:57:X:THR:HG23	1:60:X:ASN:H	2	0.11
(1,1595)	1:43:X:ILE:HG13	1:44:X:ALA:H	5	0.11
(1,1578)	1:68:X:LEU:H	1:78:X:PRO:HB3	3	0.11
(1,1578)	1:68:X:LEU:H	1:78:X:PRO:HB3	4	0.11
(1,1578)	1:68:X:LEU:H	1:78:X:PRO:HB3	5	0.11
(1,1573)	1:43:X:ILE:HG13	1:54:X:LEU:H	4	0.11
(1,1573)	1:43:X:ILE:HG13	1:54:X:LEU:H	5	0.11
(1,1573)	1:43:X:ILE:HG13	1:54:X:LEU:H	7	0.11
(1,1564)	1:65:X:ILE:HG12	1:66:X:ASN:H	2	0.11
(1,1489)	1:88:X:HIS:H	1:91:X:MET:HB2	1	0.11
(1,1441)	1:90:X:LEU:H	1:91:X:MET:HB3	6	0.11
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD11	7	0.11
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD12	7	0.11
(1,1431)	1:83:X:TYR:H	1:86:X:ILE:HD13	7	0.11
(1,1421)	1:91:X:MET:HE1	1:98:X:VAL:H	3	0.11
(1,1421)	1:91:X:MET:HE2	1:98:X:VAL:H	3	0.11
(1,1421)	1:91:X:MET:HE3	1:98:X:VAL:H	3	0.11
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	1	0.11
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	7	0.11
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1394)	1:25:X:LEU:H	1:25:X:LEU:HB3	9	0.11
(1,1320)	1:115:X:ILE:H	1:115:X:ILE:HG12	6	0.11
(1,1229)	1:76:X:GLU:HG3	1:77:X:LYS:H	10	0.11
(1,1212)	1:50:X:VAL:HB	1:51:X:GLU:H	7	0.11
(1,1208)	1:47:X:GLN:HG2	1:51:X:GLU:H	9	0.11
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD11	5	0.11
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD12	5	0.11
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD13	5	0.11
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD11	6	0.11
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD12	6	0.11
(1,1206)	1:64:X:ASN:H	1:65:X:ILE:HD13	6	0.11
(1,1100)	1:120:X:LEU:H	1:120:X:LEU:HG	3	0.11
(1,1100)	1:120:X:LEU:H	1:120:X:LEU:HG	10	0.11
(1,1050)	1:73:X:PHE:HB2	1:76:X:GLU:H	5	0.11
(1,1050)	1:73:X:PHE:HB2	1:76:X:GLU:H	10	0.11
(1,1027)	1:96:X:VAL:H	1:97:X:TYR:H	4	0.11
(1,966)	1:91:X:MET:H	1:91:X:MET:HG2	9	0.11
(1,956)	1:72:X:GLN:H	1:72:X:GLN:HB3	6	0.11
(1,888)	1:121:X:ASP:HB2	1:122:X:GLU:HG3	5	0.11
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	2	0.11
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	3	0.11
(1,788)	1:37:X:ARG:HA	1:43:X:ILE:HG12	5	0.11
(1,770)	1:50:X:VAL:HA	1:69:X:LEU:HB2	9	0.11
(1,723)	1:46:X:ILE:HB	1:47:X:GLN:HG2	6	0.11
(1,706)	1:63:X:ILE:HB	1:82:X:VAL:HB	9	0.11
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD11	10	0.11
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD12	10	0.11
(1,702)	1:63:X:ILE:HB	1:86:X:ILE:HD13	10	0.11
(1,699)	1:52:X:TYR:HB2	1:67:X:ILE:HB	1	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	3	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	3	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	3	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	9	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	9	0.11
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	9	0.11
(1,679)	1:43:X:ILE:HG12	1:54:X:LEU:HB2	1	0.11
(1,675)	1:77:X:LYS:HG2	1:106:X:PHE:HD1	1	0.11
(1,675)	1:77:X:LYS:HG2	1:106:X:PHE:HD1	9	0.11
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	5	0.11
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	6	0.11
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	7	0.11
(1,653)	1:32:X:LEU:HD11	1:74:X:PRO:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:32:X:LEU:HD12	1:74:X:PRO:HB2	7	0.11
(1,653)	1:32:X:LEU:HD13	1:74:X:PRO:HB2	7	0.11
(1,651)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	2	0.11
(1,651)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	2	0.11
(1,651)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	2	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	1	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	1	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	1	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	3	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	3	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	3	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	4	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	4	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	4	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	5	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	5	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	5	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	6	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	6	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	6	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	8	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	8	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	8	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	9	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	9	0.11
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	9	0.11
(1,625)	1:40:X:HIS:HB3	1:54:X:LEU:HD11	2	0.11
(1,625)	1:40:X:HIS:HB3	1:54:X:LEU:HD12	2	0.11
(1,625)	1:40:X:HIS:HB3	1:54:X:LEU:HD13	2	0.11
(1,574)	1:23:X:THR:HG21	1:26:X:GLN:HB3	2	0.11
(1,574)	1:23:X:THR:HG22	1:26:X:GLN:HB3	2	0.11
(1,574)	1:23:X:THR:HG23	1:26:X:GLN:HB3	2	0.11
(1,514)	1:63:X:ILE:HG21	1:84:X:PRO:HD3	7	0.11
(1,514)	1:63:X:ILE:HG22	1:84:X:PRO:HD3	7	0.11
(1,514)	1:63:X:ILE:HG23	1:84:X:PRO:HD3	7	0.11
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG21	2	0.11
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG22	2	0.11
(1,469)	1:113:X:GLY:HA3	1:116:X:ILE:HG23	2	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE1	4	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE2	4	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE3	4	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE1	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE2	4	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE3	4	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE1	4	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE2	4	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE3	4	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE1	8	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE2	8	0.11
(1,450)	1:86:X:ILE:HD11	1:91:X:MET:HE3	8	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE1	8	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE2	8	0.11
(1,450)	1:86:X:ILE:HD12	1:91:X:MET:HE3	8	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE1	8	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE2	8	0.11
(1,450)	1:86:X:ILE:HD13	1:91:X:MET:HE3	8	0.11
(1,441)	1:58:X:ILE:HD11	1:126:X:ASN:HA	2	0.11
(1,441)	1:58:X:ILE:HD12	1:126:X:ASN:HA	2	0.11
(1,441)	1:58:X:ILE:HD13	1:126:X:ASN:HA	2	0.11
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	1	0.11
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	1	0.11
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	1	0.11
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	3	0.11
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	3	0.11
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	3	0.11
(1,439)	1:58:X:ILE:HD11	1:124:X:TRP:HA	4	0.11
(1,439)	1:58:X:ILE:HD12	1:124:X:TRP:HA	4	0.11
(1,439)	1:58:X:ILE:HD13	1:124:X:TRP:HA	4	0.11
(1,431)	1:86:X:ILE:HD11	1:91:X:MET:HA	2	0.11
(1,431)	1:86:X:ILE:HD12	1:91:X:MET:HA	2	0.11
(1,431)	1:86:X:ILE:HD13	1:91:X:MET:HA	2	0.11
(1,431)	1:86:X:ILE:HD11	1:91:X:MET:HA	6	0.11
(1,431)	1:86:X:ILE:HD12	1:91:X:MET:HA	6	0.11
(1,431)	1:86:X:ILE:HD13	1:91:X:MET:HA	6	0.11
(1,425)	1:33:X:ILE:HD11	1:69:X:LEU:HG	7	0.11
(1,425)	1:33:X:ILE:HD12	1:69:X:LEU:HG	7	0.11
(1,425)	1:33:X:ILE:HD13	1:69:X:LEU:HG	7	0.11
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	2	0.11
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	2	0.11
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	2	0.11
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	2	0.11
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	2	0.11
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	2	0.11
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	2	0.11
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	2	0.11
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	9	0.11
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	9	0.11
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	9	0.11
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	9	0.11
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	9	0.11
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	9	0.11
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	9	0.11
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	9	0.11
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	9	0.11
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	1	0.11
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	1	0.11
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	1	0.11
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD11	8	0.11
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD12	8	0.11
(1,389)	1:64:X:ASN:HA	1:65:X:ILE:HD13	8	0.11
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD11	3	0.11
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD12	3	0.11
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD13	3	0.11
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD11	8	0.11
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD12	8	0.11
(1,385)	1:63:X:ILE:H	1:65:X:ILE:HD13	8	0.11
(1,380)	1:43:X:ILE:HD11	1:52:X:TYR:HE1	1	0.11
(1,380)	1:43:X:ILE:HD12	1:52:X:TYR:HE1	1	0.11
(1,380)	1:43:X:ILE:HD13	1:52:X:TYR:HE1	1	0.11
(1,352)	1:63:X:ILE:HD11	1:123:X:PHE:HD1	9	0.11
(1,352)	1:63:X:ILE:HD12	1:123:X:PHE:HD1	9	0.11
(1,352)	1:63:X:ILE:HD13	1:123:X:PHE:HD1	9	0.11
(1,313)	1:45:X:GLU:HA	1:48:X:LYS:HA	1	0.11
(1,276)	1:77:X:LYS:HA	1:77:X:LYS:HG2	2	0.11
(1,264)	1:111:X:ASP:HA	1:112:X:LEU:HB3	2	0.11
(1,236)	1:58:X:ILE:HD11	1:127:X:PRO:HD2	2	0.11
(1,236)	1:58:X:ILE:HD12	1:127:X:PRO:HD2	2	0.11
(1,236)	1:58:X:ILE:HD13	1:127:X:PRO:HD2	2	0.11
(1,231)	1:43:X:ILE:HG13	1:54:X:LEU:HA	9	0.11
(1,153)	1:121:X:ASP:HA	1:124:X:TRP:HB3	3	0.11
(1,136)	1:46:X:ILE:HG13	1:52:X:TYR:HA	9	0.11
(1,96)	1:29:X:LYS:HA	1:73:X:PHE:HD1	3	0.11
(1,47)	1:70:X:PRO:HA	1:73:X:PHE:HB2	4	0.11
(1,25)	1:50:X:VAL:HA	1:69:X:LEU:HB3	2	0.11
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD2	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2384)	1:143:X:ASN:HB2	1:144:X:PRO:HD3	4	0.1
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD2	4	0.1
(1,2384)	1:143:X:ASN:HB3	1:144:X:PRO:HD3	4	0.1
(1,2350)	1:125:X:LYS:HB3	1:125:X:LYS:HE2	9	0.1
(1,2350)	1:125:X:LYS:HB3	1:125:X:LYS:HE3	9	0.1
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD11	7	0.1
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD12	7	0.1
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD13	7	0.1
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD21	7	0.1
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD22	7	0.1
(1,2323)	1:119:X:LEU:HB2	1:119:X:LEU:HD23	7	0.1
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD11	7	0.1
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD12	7	0.1
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD13	7	0.1
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD21	7	0.1
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD22	7	0.1
(1,2323)	1:119:X:LEU:HB3	1:119:X:LEU:HD23	7	0.1
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD11	1	0.1
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD12	1	0.1
(1,2297)	1:112:X:LEU:HD11	1:116:X:ILE:HD13	1	0.1
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD11	1	0.1
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD12	1	0.1
(1,2297)	1:112:X:LEU:HD12	1:116:X:ILE:HD13	1	0.1
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD11	1	0.1
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD12	1	0.1
(1,2297)	1:112:X:LEU:HD13	1:116:X:ILE:HD13	1	0.1
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD11	1	0.1
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD12	1	0.1
(1,2297)	1:112:X:LEU:HD21	1:116:X:ILE:HD13	1	0.1
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD11	1	0.1
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD12	1	0.1
(1,2297)	1:112:X:LEU:HD22	1:116:X:ILE:HD13	1	0.1
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD11	1	0.1
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD12	1	0.1
(1,2297)	1:112:X:LEU:HD23	1:116:X:ILE:HD13	1	0.1
(1,2240)	1:101:X:PRO:HD2	1:119:X:LEU:HD11	9	0.1
(1,2240)	1:101:X:PRO:HD2	1:119:X:LEU:HD12	9	0.1
(1,2240)	1:101:X:PRO:HD2	1:119:X:LEU:HD13	9	0.1
(1,2240)	1:101:X:PRO:HD2	1:119:X:LEU:HD21	9	0.1
(1,2240)	1:101:X:PRO:HD2	1:119:X:LEU:HD22	9	0.1
(1,2240)	1:101:X:PRO:HD2	1:119:X:LEU:HD23	9	0.1
(1,2240)	1:101:X:PRO:HD3	1:119:X:LEU:HD11	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2240)	1:101:X:PRO:HD3	1:119:X:LEU:HD12	9	0.1
(1,2240)	1:101:X:PRO:HD3	1:119:X:LEU:HD13	9	0.1
(1,2240)	1:101:X:PRO:HD3	1:119:X:LEU:HD21	9	0.1
(1,2240)	1:101:X:PRO:HD3	1:119:X:LEU:HD22	9	0.1
(1,2240)	1:101:X:PRO:HD3	1:119:X:LEU:HD23	9	0.1
(1,2151)	1:90:X:LEU:HB3	1:100:X:SER:HB2	1	0.1
(1,2151)	1:90:X:LEU:HB3	1:100:X:SER:HB3	1	0.1
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB2	6	0.1
(1,2112)	1:83:X:TYR:HE1	1:84:X:PRO:HB3	6	0.1
(1,2105)	1:82:X:VAL:HG11	1:86:X:ILE:HA	10	0.1
(1,2105)	1:82:X:VAL:HG12	1:86:X:ILE:HA	10	0.1
(1,2105)	1:82:X:VAL:HG13	1:86:X:ILE:HA	10	0.1
(1,2105)	1:82:X:VAL:HG21	1:86:X:ILE:HA	10	0.1
(1,2105)	1:82:X:VAL:HG22	1:86:X:ILE:HA	10	0.1
(1,2105)	1:82:X:VAL:HG23	1:86:X:ILE:HA	10	0.1
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD11	4	0.1
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD12	4	0.1
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD13	4	0.1
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD21	4	0.1
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD22	4	0.1
(1,2044)	1:69:X:LEU:HD11	1:112:X:LEU:HD23	4	0.1
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD11	4	0.1
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD12	4	0.1
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD13	4	0.1
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD21	4	0.1
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD22	4	0.1
(1,2044)	1:69:X:LEU:HD12	1:112:X:LEU:HD23	4	0.1
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD11	4	0.1
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD12	4	0.1
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD13	4	0.1
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD21	4	0.1
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD22	4	0.1
(1,2044)	1:69:X:LEU:HD13	1:112:X:LEU:HD23	4	0.1
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD11	4	0.1
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD12	4	0.1
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD13	4	0.1
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD21	4	0.1
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD22	4	0.1
(1,2044)	1:69:X:LEU:HD21	1:112:X:LEU:HD23	4	0.1
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD11	4	0.1
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD12	4	0.1
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD13	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD21	4	0.1
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD22	4	0.1
(1,2044)	1:69:X:LEU:HD22	1:112:X:LEU:HD23	4	0.1
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD11	4	0.1
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD12	4	0.1
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD13	4	0.1
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD21	4	0.1
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD22	4	0.1
(1,2044)	1:69:X:LEU:HD23	1:112:X:LEU:HD23	4	0.1
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	1	0.1
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	1	0.1
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	7	0.1
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	7	0.1
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	8	0.1
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	8	0.1
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	9	0.1
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	9	0.1
(1,2025)	1:68:X:LEU:HB2	1:79:X:VAL:HB	10	0.1
(1,2025)	1:68:X:LEU:HB3	1:79:X:VAL:HB	10	0.1
(1,1990)	1:61:X:LEU:HD11	1:128:X:PRO:HG2	9	0.1
(1,1990)	1:61:X:LEU:HD12	1:128:X:PRO:HG2	9	0.1
(1,1990)	1:61:X:LEU:HD13	1:128:X:PRO:HG2	9	0.1
(1,1990)	1:61:X:LEU:HD21	1:128:X:PRO:HG2	9	0.1
(1,1990)	1:61:X:LEU:HD22	1:128:X:PRO:HG2	9	0.1
(1,1990)	1:61:X:LEU:HD23	1:128:X:PRO:HG2	9	0.1
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD2	1	0.1
(1,1954)	1:58:X:ILE:HG21	1:128:X:PRO:HD3	1	0.1
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD2	1	0.1
(1,1954)	1:58:X:ILE:HG22	1:128:X:PRO:HD3	1	0.1
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD2	1	0.1
(1,1954)	1:58:X:ILE:HG23	1:128:X:PRO:HD3	1	0.1
(1,1851)	1:37:X:ARG:HG2	1:37:X:ARG:HD2	6	0.1
(1,1851)	1:37:X:ARG:HG2	1:37:X:ARG:HD3	6	0.1
(1,1851)	1:37:X:ARG:HG3	1:37:X:ARG:HD2	6	0.1
(1,1851)	1:37:X:ARG:HG3	1:37:X:ARG:HD3	6	0.1
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD2	2	0.1
(1,1797)	1:33:X:ILE:HG21	1:37:X:ARG:HD3	2	0.1
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD2	2	0.1
(1,1797)	1:33:X:ILE:HG22	1:37:X:ARG:HD3	2	0.1
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD2	2	0.1
(1,1797)	1:33:X:ILE:HG23	1:37:X:ARG:HD3	2	0.1
(1,1785)	1:32:X:LEU:HD11	1:111:X:ASP:HB2	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1785)	1:32:X:LEU:HD12	1:111:X:ASP:HB2	8	0.1
(1,1785)	1:32:X:LEU:HD13	1:111:X:ASP:HB2	8	0.1
(1,1785)	1:32:X:LEU:HD21	1:111:X:ASP:HB2	8	0.1
(1,1785)	1:32:X:LEU:HD22	1:111:X:ASP:HB2	8	0.1
(1,1785)	1:32:X:LEU:HD23	1:111:X:ASP:HB2	8	0.1
(1,1781)	1:32:X:LEU:HD11	1:74:X:PRO:HD2	9	0.1
(1,1781)	1:32:X:LEU:HD12	1:74:X:PRO:HD2	9	0.1
(1,1781)	1:32:X:LEU:HD13	1:74:X:PRO:HD2	9	0.1
(1,1781)	1:32:X:LEU:HD21	1:74:X:PRO:HD2	9	0.1
(1,1781)	1:32:X:LEU:HD22	1:74:X:PRO:HD2	9	0.1
(1,1781)	1:32:X:LEU:HD23	1:74:X:PRO:HD2	9	0.1
(1,1728)	1:28:X:GLN:HG2	1:74:X:PRO:HD3	7	0.1
(1,1728)	1:28:X:GLN:HG3	1:74:X:PRO:HD3	7	0.1
(1,1600)	1:46:X:ILE:H	1:47:X:GLN:HB3	3	0.1
(1,1513)	1:73:X:PHE:HD1	1:75:X:GLN:H	1	0.1
(1,1486)	1:73:X:PHE:H	1:76:X:GLU:HG2	10	0.1
(1,1421)	1:91:X:MET:HE1	1:98:X:VAL:H	6	0.1
(1,1421)	1:91:X:MET:HE2	1:98:X:VAL:H	6	0.1
(1,1421)	1:91:X:MET:HE3	1:98:X:VAL:H	6	0.1
(1,1421)	1:91:X:MET:HE1	1:98:X:VAL:H	9	0.1
(1,1421)	1:91:X:MET:HE2	1:98:X:VAL:H	9	0.1
(1,1421)	1:91:X:MET:HE3	1:98:X:VAL:H	9	0.1
(1,1055)	1:73:X:PHE:HD1	1:76:X:GLU:H	6	0.1
(1,1055)	1:73:X:PHE:HD1	1:76:X:GLU:H	10	0.1
(1,1027)	1:96:X:VAL:H	1:97:X:TYR:H	1	0.1
(1,912)	1:50:X:VAL:HA	1:68:X:LEU:HG	7	0.1
(1,894)	1:43:X:ILE:HG13	1:52:X:TYR:HB2	10	0.1
(1,886)	1:77:X:LYS:HD3	1:106:X:PHE:HB2	3	0.1
(1,885)	1:69:X:LEU:HB2	1:73:X:PHE:HB2	5	0.1
(1,866)	1:72:X:GLN:HB3	1:73:X:PHE:HB2	9	0.1
(1,835)	1:119:X:LEU:HA	1:122:X:GLU:HG2	6	0.1
(1,826)	1:137:X:PHE:HB2	1:138:X:PRO:HD3	10	0.1
(1,810)	1:53:X:ARG:HA	1:53:X:ARG:HD2	10	0.1
(1,783)	1:74:X:PRO:HB2	1:106:X:PHE:HE1	7	0.1
(1,764)	1:32:X:LEU:HG	1:74:X:PRO:HB2	1	0.1
(1,764)	1:32:X:LEU:HG	1:74:X:PRO:HB2	10	0.1
(1,699)	1:52:X:TYR:HB2	1:67:X:ILE:HB	7	0.1
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD21	4	0.1
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD22	4	0.1
(1,692)	1:130:X:LEU:HB3	1:130:X:LEU:HD23	4	0.1
(1,671)	1:124:X:TRP:HB3	1:125:X:LYS:HB3	1	0.1
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:56:X:PHE:HB2	1:63:X:ILE:HG12	8	0.1
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD11	10	0.1
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD12	10	0.1
(1,631)	1:54:X:LEU:HB3	1:54:X:LEU:HD13	10	0.1
(1,574)	1:23:X:THR:HG21	1:26:X:GLN:HB3	6	0.1
(1,574)	1:23:X:THR:HG22	1:26:X:GLN:HB3	6	0.1
(1,574)	1:23:X:THR:HG23	1:26:X:GLN:HB3	6	0.1
(1,550)	1:91:X:MET:HA	1:99:X:THR:HG21	4	0.1
(1,550)	1:91:X:MET:HA	1:99:X:THR:HG22	4	0.1
(1,550)	1:91:X:MET:HA	1:99:X:THR:HG23	4	0.1
(1,512)	1:67:X:ILE:HG21	1:78:X:PRO:HD3	5	0.1
(1,512)	1:67:X:ILE:HG22	1:78:X:PRO:HD3	5	0.1
(1,512)	1:67:X:ILE:HG23	1:78:X:PRO:HD3	5	0.1
(1,482)	1:108:X:MET:HE1	1:109:X:HIS:HD2	2	0.1
(1,482)	1:108:X:MET:HE2	1:109:X:HIS:HD2	2	0.1
(1,482)	1:108:X:MET:HE3	1:109:X:HIS:HD2	2	0.1
(1,441)	1:58:X:ILE:HD11	1:126:X:ASN:HA	3	0.1
(1,441)	1:58:X:ILE:HD12	1:126:X:ASN:HA	3	0.1
(1,441)	1:58:X:ILE:HD13	1:126:X:ASN:HA	3	0.1
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD11	4	0.1
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD12	4	0.1
(1,421)	1:54:X:LEU:HB2	1:65:X:ILE:HD13	4	0.1
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	3	0.1
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	3	0.1
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	3	0.1
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	3	0.1
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	3	0.1
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	3	0.1
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	3	0.1
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	3	0.1
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	3	0.1
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD11	8	0.1
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD12	8	0.1
(1,408)	1:115:X:ILE:HG21	1:115:X:ILE:HD13	8	0.1
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD11	8	0.1
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD12	8	0.1
(1,408)	1:115:X:ILE:HG22	1:115:X:ILE:HD13	8	0.1
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD11	8	0.1
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD12	8	0.1
(1,408)	1:115:X:ILE:HG23	1:115:X:ILE:HD13	8	0.1
(1,406)	1:105:X:ASN:HB3	1:115:X:ILE:HD11	1	0.1
(1,406)	1:105:X:ASN:HB3	1:115:X:ILE:HD12	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,406)	1:105:X:ASN:HB3	1:115:X:ILE:HD13	1	0.1
(1,378)	1:33:X:ILE:HD11	1:52:X:TYR:HE1	7	0.1
(1,378)	1:33:X:ILE:HD12	1:52:X:TYR:HE1	7	0.1
(1,378)	1:33:X:ILE:HD13	1:52:X:TYR:HE1	7	0.1
(1,359)	1:63:X:ILE:HD11	1:123:X:PHE:HB2	4	0.1
(1,359)	1:63:X:ILE:HD12	1:123:X:PHE:HB2	4	0.1
(1,359)	1:63:X:ILE:HD13	1:123:X:PHE:HB2	4	0.1
(1,214)	1:70:X:PRO:HB2	1:71:X:PRO:HD3	10	0.1
(1,164)	1:86:X:ILE:HG21	1:129:X:VAL:HA	4	0.1
(1,164)	1:86:X:ILE:HG22	1:129:X:VAL:HA	4	0.1
(1,164)	1:86:X:ILE:HG23	1:129:X:VAL:HA	4	0.1
(1,56)	1:116:X:ILE:HA	1:116:X:ILE:HD11	10	0.1
(1,56)	1:116:X:ILE:HA	1:116:X:ILE:HD12	10	0.1
(1,56)	1:116:X:ILE:HA	1:116:X:ILE:HD13	10	0.1
(1,42)	1:91:X:MET:HG3	1:98:X:VAL:HA	1	0.1

## 10 Dihedral-angle violation analysis [i](#)

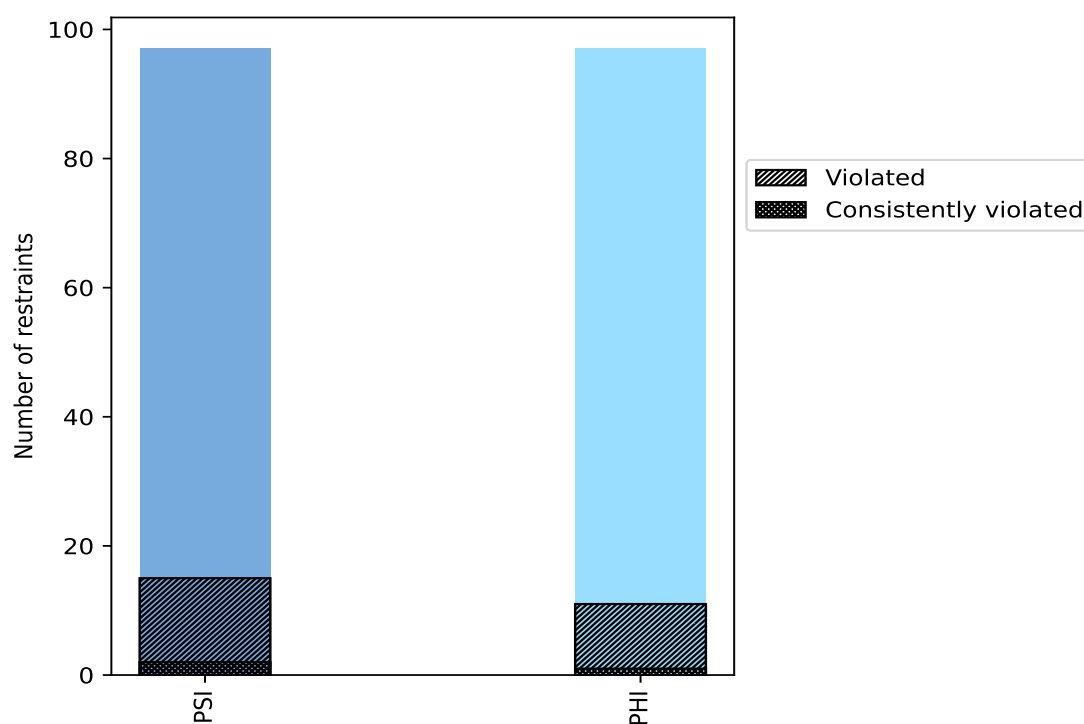
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle 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>
PSI	97	50.0	15	15.5	7.7	2	2.1	1.0
PHI	97	50.0	11	11.3	5.7	1	1.0	0.5
Total	194	100.0	26	13.4	13.4	3	1.5	1.5

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



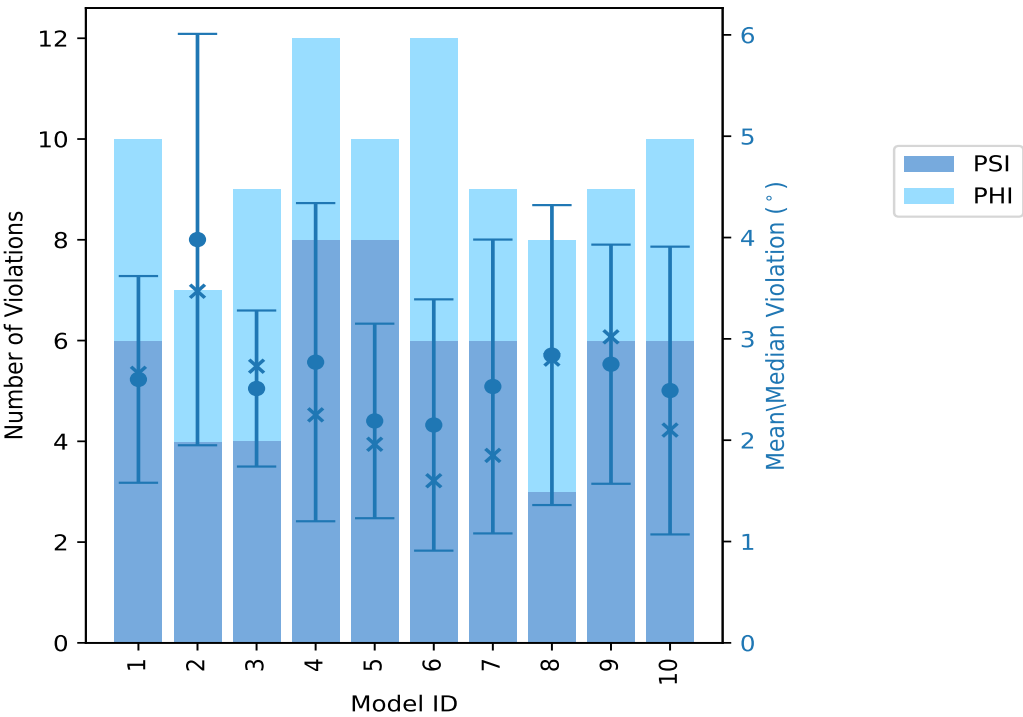
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	6	4	10	2.6	4.49	1.02	2.66
2	4	3	7	3.98	7.69	2.03	3.47
3	4	5	9	2.51	3.39	0.77	2.73
4	8	4	12	2.77	6.44	1.57	2.25
5	8	2	10	2.19	4.32	0.96	1.96
6	6	6	12	2.15	5.52	1.24	1.6
7	6	3	9	2.53	5.8	1.45	1.85
8	3	5	8	2.84	5.31	1.48	2.8
9	6	3	9	2.75	4.67	1.18	3.02
10	6	4	10	2.49	5.1	1.42	2.1

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

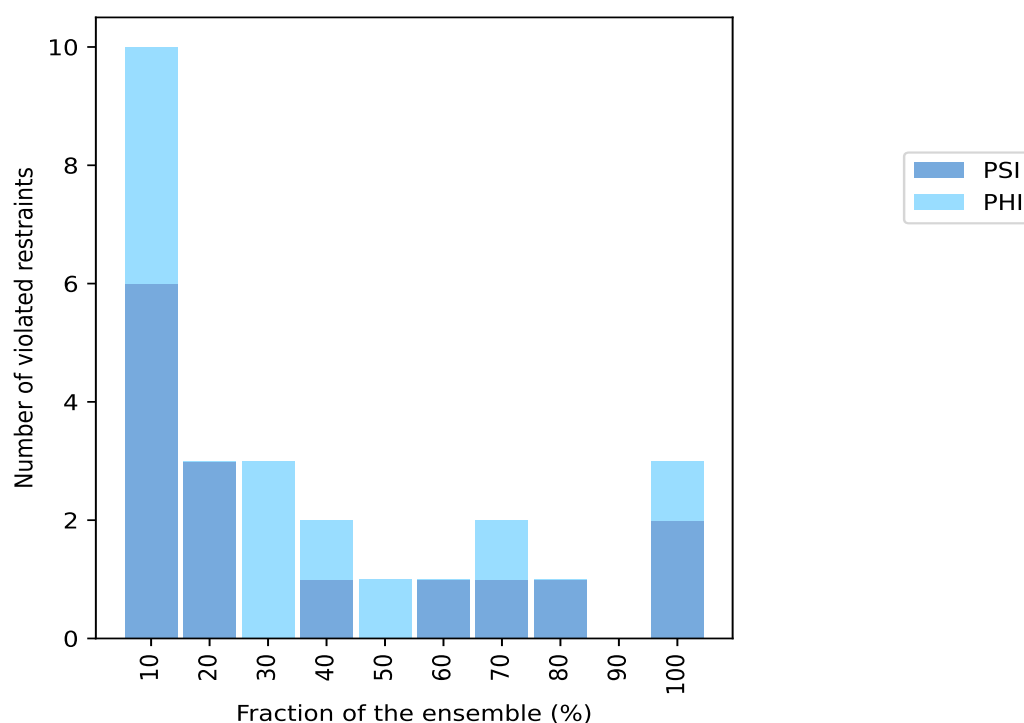
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
6	4	10	1	10.0
3	0	3	2	20.0
0	3	3	3	30.0
1	1	2	4	40.0
0	1	1	5	50.0
1	0	1	6	60.0
1	1	2	7	70.0
1	0	1	8	80.0
0	0	0	9	90.0
2	1	3	10	100.0

<sup>1</sup> Number of models with violations

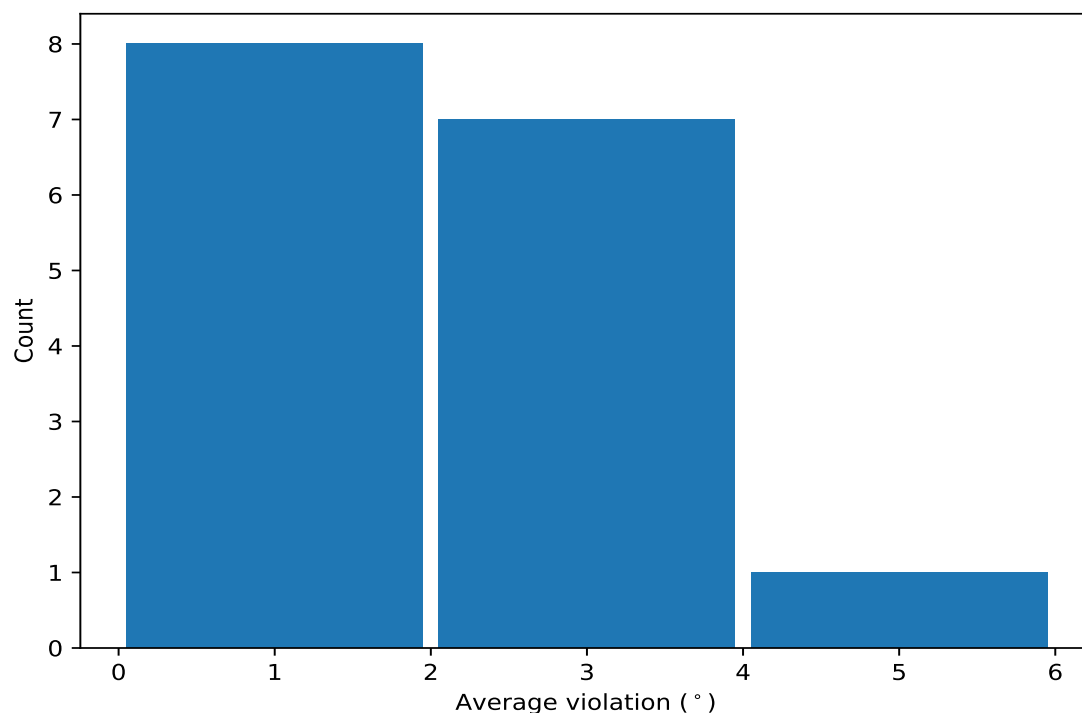
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle 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



### 10.4.2 Table: Most violated dihedral-angle 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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	10	4.53	1.26	4.64
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	10	2.78	0.69	2.84
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	10	1.87	0.71	1.64
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	8	2.79	0.6	3.02
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	7	3.28	1.82	3.11
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	7	2.87	1.1	2.91
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	6	3.71	1.15	3.98
(1,190)	1:142:X:SER:C	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	5	1.59	0.34	1.63
(1,132)	1:105:X:ASN:N	1:105:X:ASN:CA	1:105:X:ASN:C	1:106:X:PHE:N	4	1.39	0.14	1.35
(1,61)	1:57:X:THR:C	1:58:X:ILE:N	1:58:X:ILE:CA	1:58:X:ILE:C	4	1.19	0.09	1.16
(1,182)	1:138:X:PRO:C	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	3	2.51	0.74	2.81
(1,115)	1:93:X:LYS:C	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	3	1.77	0.68	1.36
(1,49)	1:50:X:VAL:C	1:51:X:GLU:N	1:51:X:GLU:CA	1:51:X:GLU:C	3	1.74	0.1	1.77

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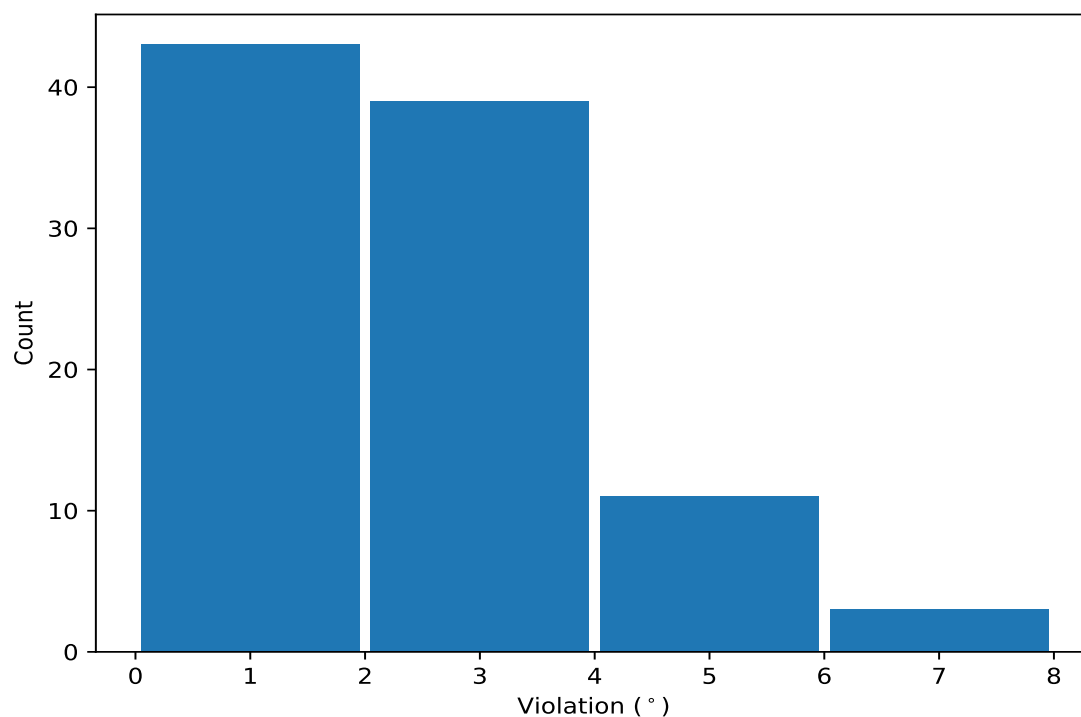
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,183)	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	1:140:X:LEU:N	2	2.23	0.56	2.23
(1,185)	1:140:X:LEU:N	1:140:X:LEU:CA	1:140:X:LEU:C	1:141:X:TYR:N	2	1.81	0.36	1.81
(1,116)	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	1:95:X:GLY:N	2	1.42	0.17	1.42

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

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



### 10.5.2 Table: All violated dihedral-angle restraints [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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:140:X:LEU:C	1:141:X:TYR:N	1:141:X:TYR:CA	1:141:X:TYR:C	2	7.69
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	4	6.44
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	2	6.25
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	7	5.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	4	5.7
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	6	5.52
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	8	5.31
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	10	5.1
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	10	4.96
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	8	4.68
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	9	4.67
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	1	4.49
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	5	4.32
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	9	4.09
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	7	3.75
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1	3.74
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	7	3.6
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	2	3.58
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	9	3.58
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	2	3.47
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	6	3.43
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	8	3.41
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	3	3.39
(1,110)	1:90:X:LEU:N	1:90:X:LEU:CA	1:90:X:LEU:C	1:91:X:MET:N	3	3.39
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	6	3.32
(1,3)	1:23:X:THR:C	1:24:X:SER:N	1:24:X:SER:CA	1:24:X:SER:C	9	3.28
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	10	3.26
(1,182)	1:138:X:PRO:C	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	3	3.23
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	1	3.13
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	1	3.11
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	2	3.02
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	9	3.02
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	5	2.91
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	5	2.89
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	4	2.87
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	4	2.85
(1,182)	1:138:X:PRO:C	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	8	2.81
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	8	2.8
(1,183)	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	1:140:X:LEU:N	1	2.79
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	4	2.75
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	3	2.75
(1,115)	1:93:X:LYS:C	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	3	2.73
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	5	2.66
(1,122)	1:99:X:THR:N	1:99:X:THR:CA	1:99:X:THR:C	1:100:X:SER:N	1	2.53
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	3	2.46
(1,106)	1:87:X:ARG:N	1:87:X:ARG:CA	1:87:X:ARG:C	1:88:X:HIS:N	10	2.45
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	4	2.34
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	5	2.32
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	10	2.28
(1,190)	1:142:X:SER:C	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	1	2.18
(1,185)	1:140:X:LEU:N	1:140:X:LEU:CA	1:140:X:LEU:C	1:141:X:TYR:N	4	2.16
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	2	2.07
(1,134)	1:106:X:PHE:N	1:106:X:PHE:CA	1:106:X:PHE:C	1:107:X:THR:N	4	2.06
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	7	1.98
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	10	1.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:72:X:GLN:N	1:72:X:GLN:CA	1:72:X:GLN:C	1:73:X:PHE:N	6	1.88
(1,49)	1:50:X:VAL:C	1:51:X:GLU:N	1:51:X:GLU:CA	1:51:X:GLU:C	7	1.85
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	3	1.82
(1,49)	1:50:X:VAL:C	1:51:X:GLU:N	1:51:X:GLU:CA	1:51:X:GLU:C	2	1.77
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	7	1.68
(1,183)	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	1:140:X:LEU:N	3	1.67
(1,176)	1:134:X:SER:C	1:135:X:THR:N	1:135:X:THR:CA	1:135:X:THR:C	4	1.66
(1,190)	1:142:X:SER:C	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	4	1.63
(1,190)	1:142:X:SER:C	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	6	1.63
(1,132)	1:105:X:ASN:N	1:105:X:ASN:CA	1:105:X:ASN:C	1:106:X:PHE:N	7	1.61
(1,49)	1:50:X:VAL:C	1:51:X:GLU:N	1:51:X:GLU:CA	1:51:X:GLU:C	6	1.6
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	5	1.59
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	9	1.59
(1,116)	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	1:95:X:GLY:N	6	1.59
(1,159)	1:119:X:LEU:C	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	9	1.54
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	1	1.53
(1,191)	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	1:144:X:PRO:N	4	1.5
(1,182)	1:138:X:PRO:C	1:139:X:TYR:N	1:139:X:TYR:CA	1:139:X:TYR:C	6	1.5
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	9	1.5
(1,66)	1:60:X:ASN:N	1:60:X:ASN:CA	1:60:X:ASN:C	1:61:X:LEU:N	9	1.5
(1,185)	1:140:X:LEU:N	1:140:X:LEU:CA	1:140:X:LEU:C	1:141:X:TYR:N	5	1.45
(1,40)	1:42:X:SER:N	1:42:X:SER:CA	1:42:X:SER:C	1:43:X:ILE:N	10	1.42
(1,174)	1:129:X:VAL:N	1:129:X:VAL:CA	1:129:X:VAL:C	1:130:X:LEU:N	7	1.39
(1,132)	1:105:X:ASN:N	1:105:X:ASN:CA	1:105:X:ASN:C	1:106:X:PHE:N	6	1.39
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	6	1.37
(1,115)	1:93:X:LYS:C	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	1	1.36
(1,61)	1:57:X:THR:C	1:58:X:ILE:N	1:58:X:ILE:CA	1:58:X:ILE:C	6	1.34
(1,132)	1:105:X:ASN:N	1:105:X:ASN:CA	1:105:X:ASN:C	1:106:X:PHE:N	5	1.31
(1,190)	1:142:X:SER:C	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	8	1.29
(1,116)	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	1:95:X:GLY:N	5	1.26
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	8	1.25
(1,132)	1:105:X:ASN:N	1:105:X:ASN:CA	1:105:X:ASN:C	1:106:X:PHE:N	4	1.24
(1,190)	1:142:X:SER:C	1:143:X:ASN:N	1:143:X:ASN:CA	1:143:X:ASN:C	10	1.22
(1,115)	1:93:X:LYS:C	1:94:X:GLN:N	1:94:X:GLN:CA	1:94:X:GLN:C	6	1.22
(1,117)	1:95:X:GLY:C	1:96:X:VAL:N	1:96:X:VAL:CA	1:96:X:VAL:C	5	1.21
(1,61)	1:57:X:THR:C	1:58:X:ILE:N	1:58:X:ILE:CA	1:58:X:ILE:C	8	1.19
(1,160)	1:120:X:LEU:N	1:120:X:LEU:CA	1:120:X:LEU:C	1:121:X:ASP:N	1	1.16
(1,192)	1:144:X:PRO:C	1:145:X:SER:N	1:145:X:SER:CA	1:145:X:SER:C	10	1.14
(1,61)	1:57:X:THR:C	1:58:X:ILE:N	1:58:X:ILE:CA	1:58:X:ILE:C	10	1.13
(1,61)	1:57:X:THR:C	1:58:X:ILE:N	1:58:X:ILE:CA	1:58:X:ILE:C	3	1.12
(1,28)	1:36:X:LEU:N	1:36:X:LEU:CA	1:36:X:LEU:C	1:37:X:ARG:N	7	1.11