



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 10:44 AM EST

PDB ID : 6EMQ  
BMRB ID : 34181  
Title : Solution structure of the LEDGF/p75 IBD - MLL1 (aa 111-160) complex  
Authors : Veverka, V.  
Deposited on : 2017-10-03

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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

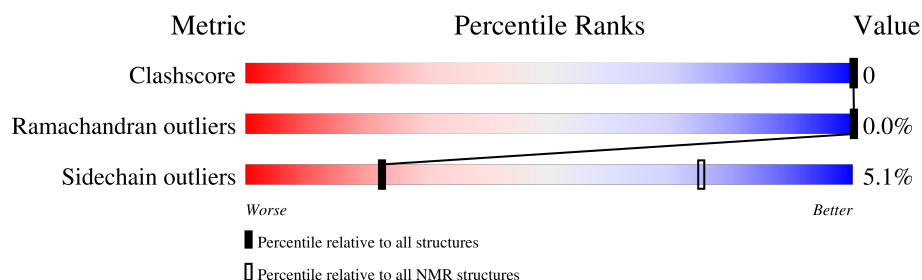
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

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	A	165	

## 2 Ensemble composition and analysis

This entry contains 40 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:348-A:426, A:497-A:500 (83)	0.31	10

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 6 clusters and 1 single-model cluster was found.

Cluster number	Models
1	3, 5, 7, 10, 11, 12, 16, 22, 23, 24, 25, 26, 28, 29, 30, 35, 38, 40
2	2, 4, 6, 9, 13, 14, 19, 27, 32, 36
3	17, 20, 34, 39
4	1, 18, 33
5	15, 31
6	8, 37
Single-model clusters	21

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2507 atoms, of which 1251 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PC4 and SFRS1-interacting protein, Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2507	771	1251	227	251	7	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	SER	-	expression tag	UNP O75475
A	340	ASN	-	expression tag	UNP O75475
A	341	ALA	-	expression tag	UNP O75475
A	342	ALA	-	expression tag	UNP O75475
A	343	SER	-	expression tag	UNP O75475
A	344	TRP	-	expression tag	UNP O75475
A	450	GLY	-	linker	UNP O75475
A	451	GLY	-	linker	UNP O75475
A	452	SER	-	linker	UNP O75475
A	453	GLY	-	linker	UNP O75475
A	454	SER	-	linker	UNP O75475
A	455	GLY	-	linker	UNP O75475
A	456	SER	-	linker	UNP O75475
A	457	GLY	-	linker	UNP O75475
A	458	SER	-	linker	UNP O75475
A	459	SER	PRO	linker	UNP Q03164

## 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: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

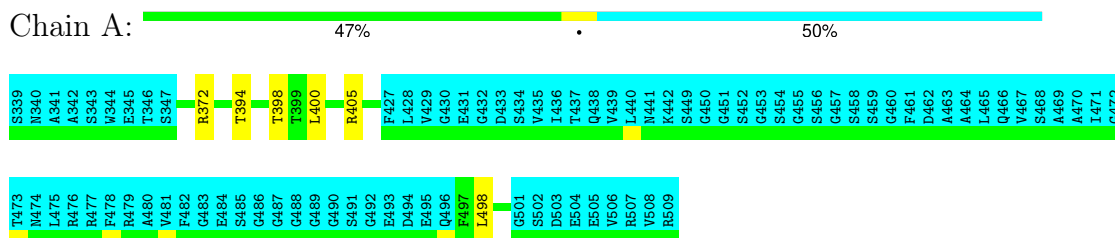


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

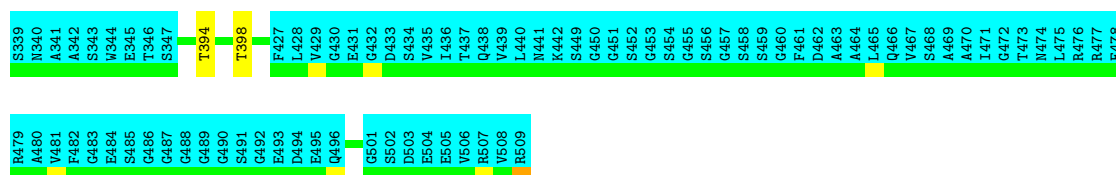
- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.2 Score per residue for model 2

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

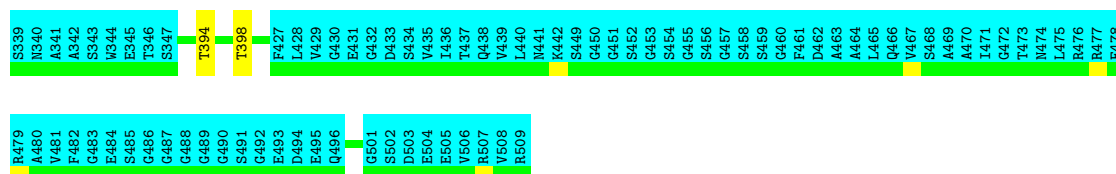




### 4.2.3 Score per residue for model 3

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

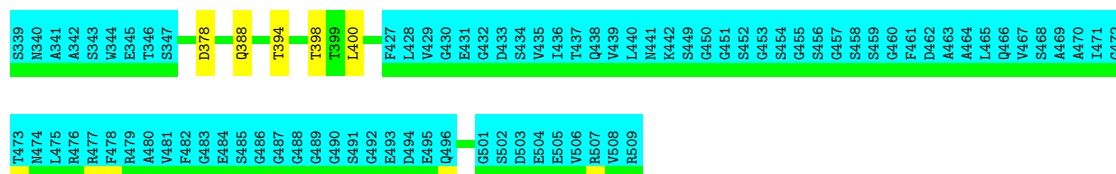
Chain A: 49% 50%



### 4.2.4 Score per residue for model 4

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

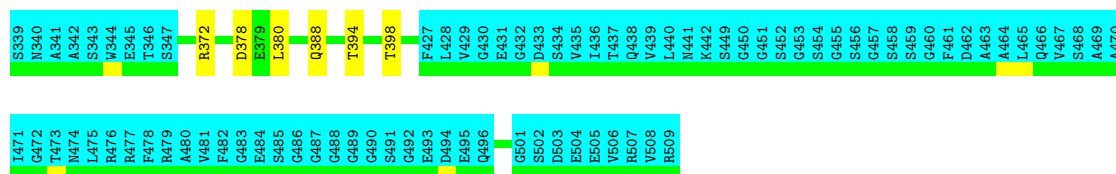
Chain A: 47% 50%



### 4.2.5 Score per residue for model 5

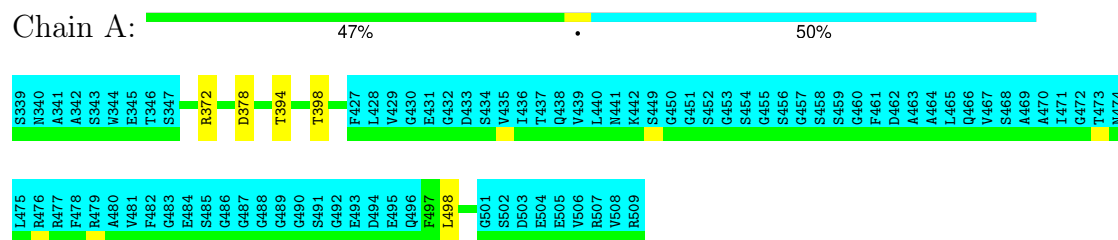
- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

Chain A: 47% 50%



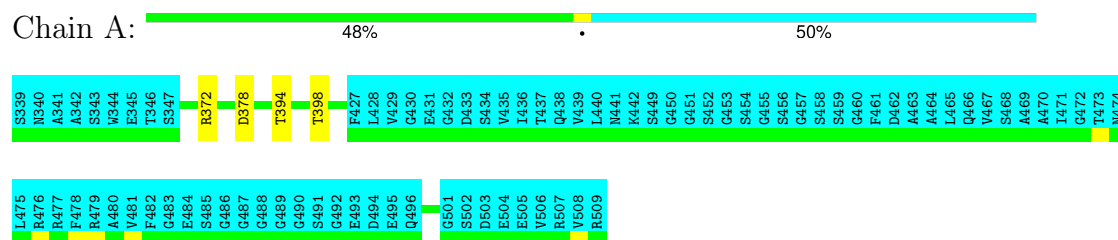
### 4.2.6 Score per residue for model 6

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



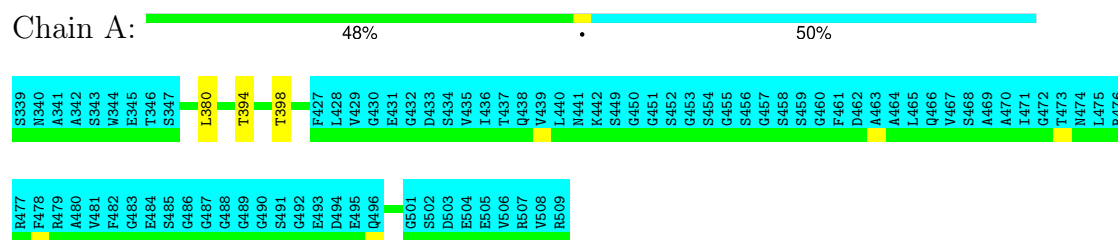
#### 4.2.7 Score per residue for model 7

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.8 Score per residue for model 8

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



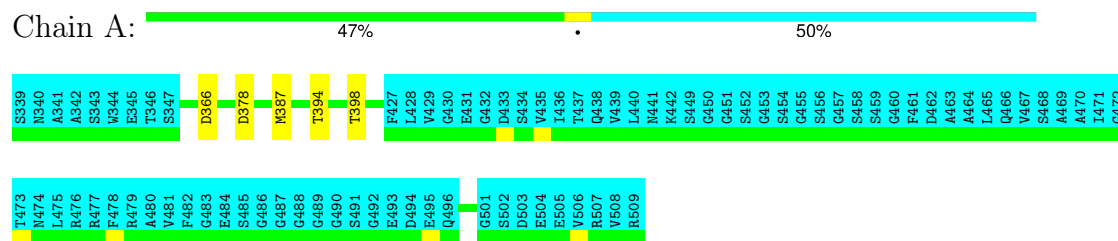
#### 4.2.9 Score per residue for model 9

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



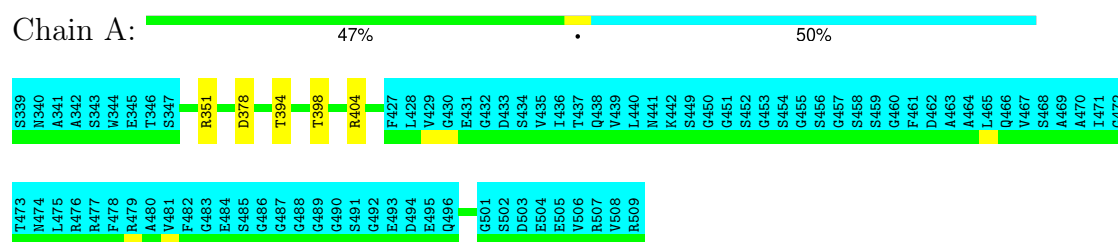
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



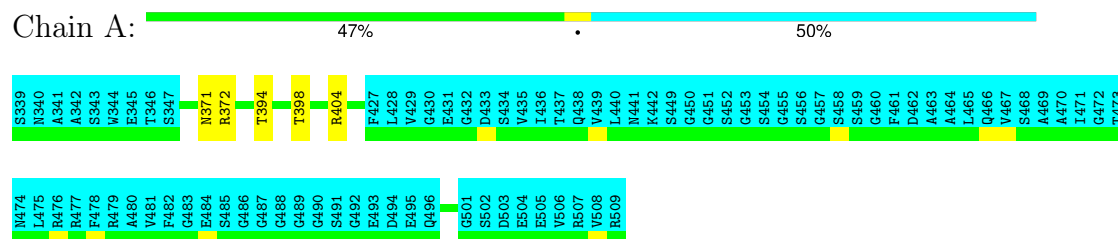
#### 4.2.11 Score per residue for model 11

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



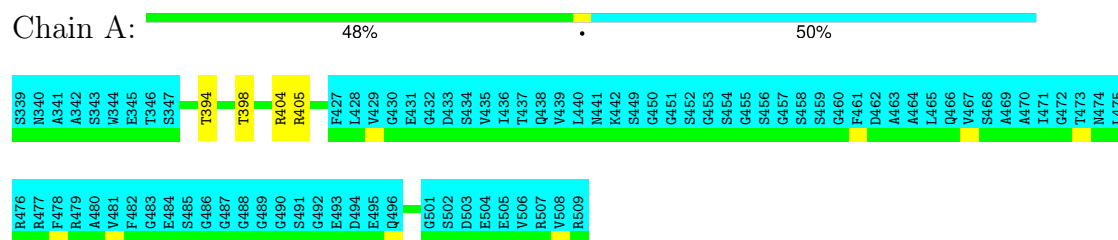
#### 4.2.12 Score per residue for model 12

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.13 Score per residue for model 13

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A

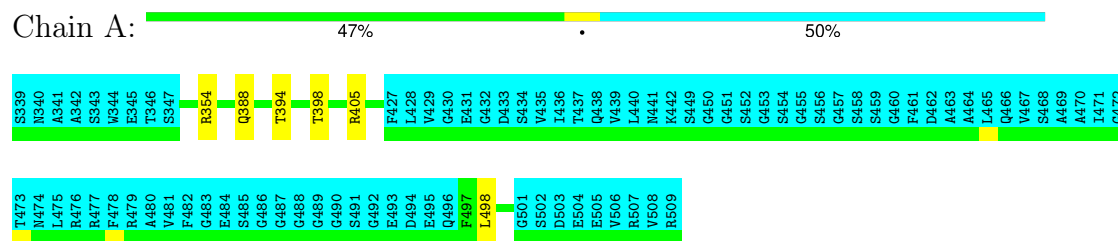






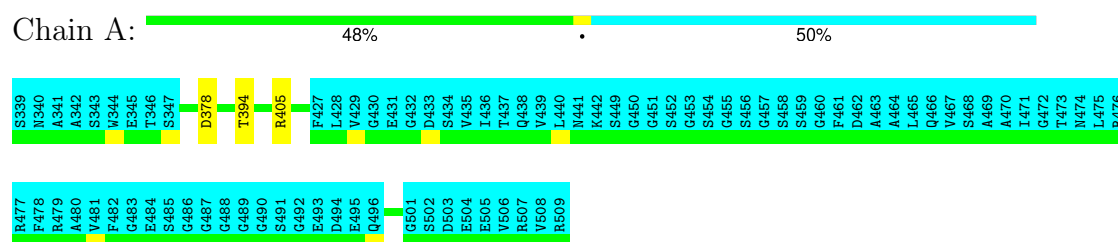
### 4.2.18 Score per residue for model 18

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



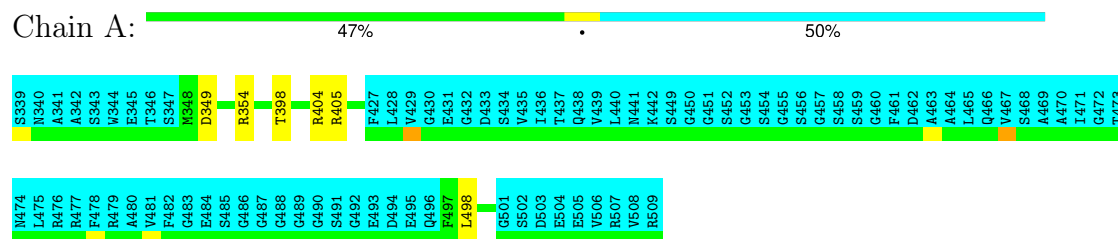
### 4.2.19 Score per residue for model 19

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



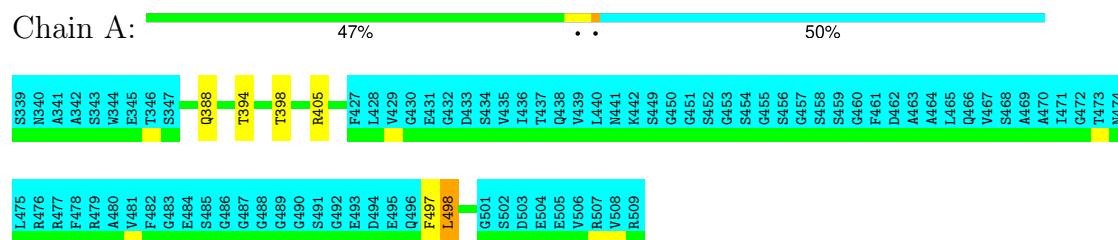
### 4.2.20 Score per residue for model 20

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



### 4.2.21 Score per residue for model 21

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



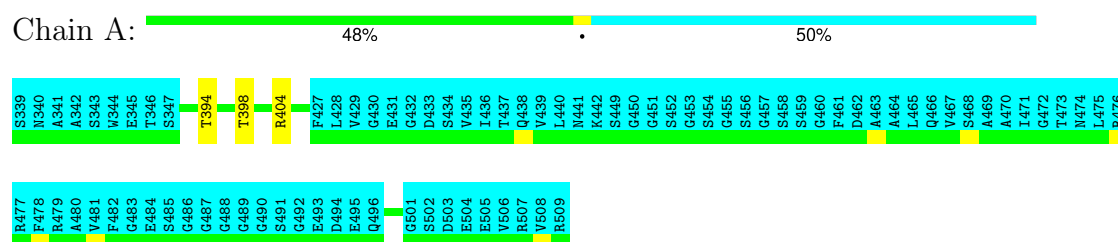
### 4.2.22 Score per residue for model 22

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



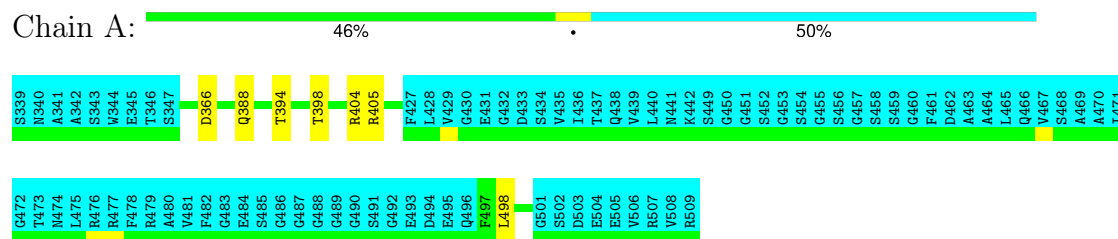
### 4.2.23 Score per residue for model 23

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



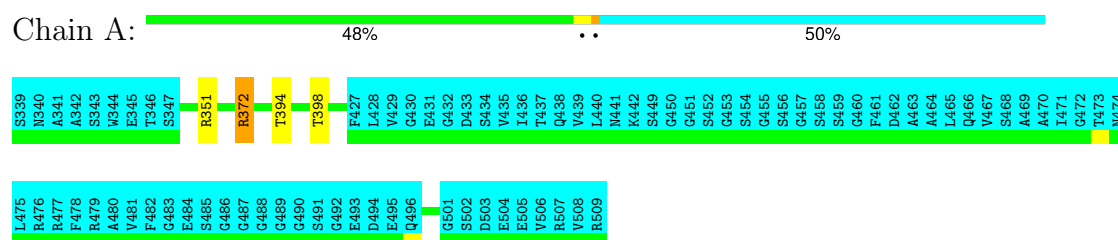
### 4.2.24 Score per residue for model 24

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



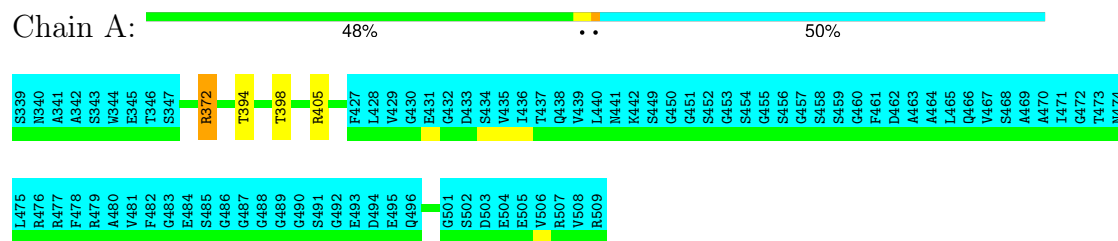
### 4.2.25 Score per residue for model 25

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



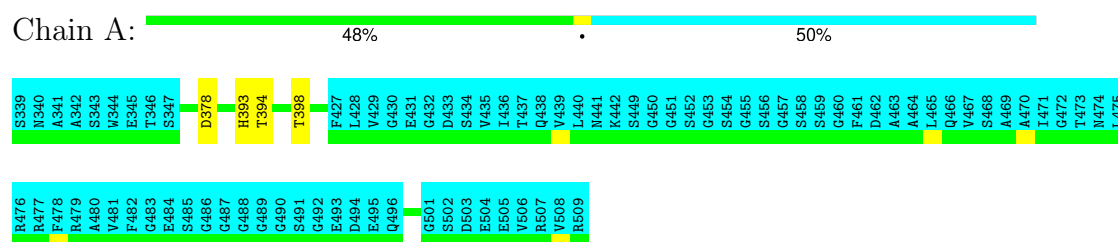
#### 4.2.26 Score per residue for model 26

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.27 Score per residue for model 27

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



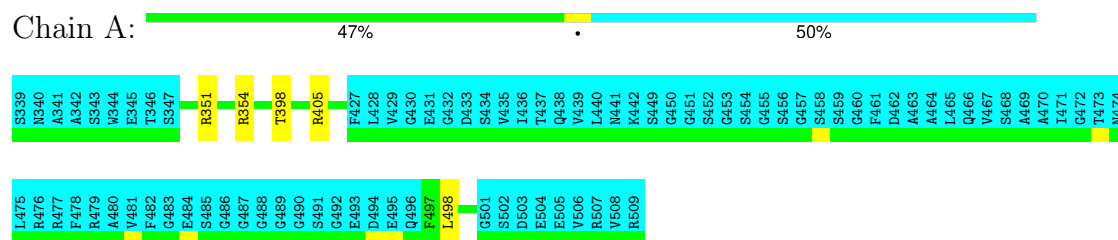
#### 4.2.28 Score per residue for model 28

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



#### 4.2.29 Score per residue for model 29

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



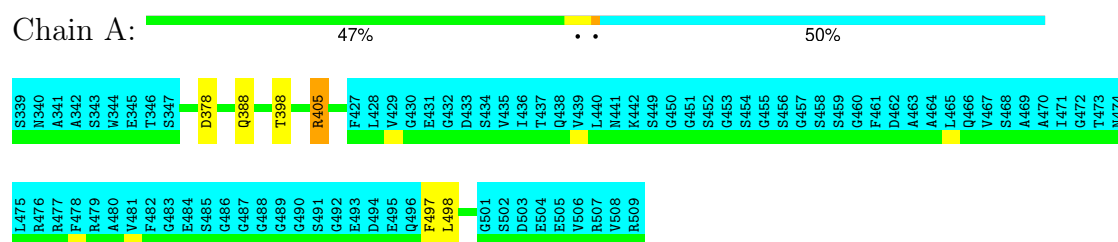
### 4.2.30 Score per residue for model 30

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



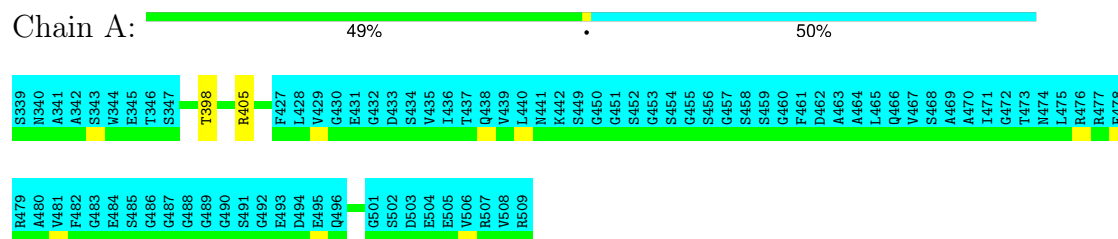
### 4.2.31 Score per residue for model 31

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



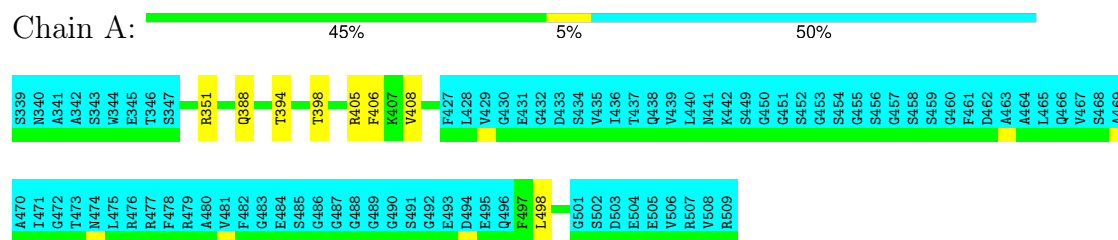
### 4.2.32 Score per residue for model 32

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



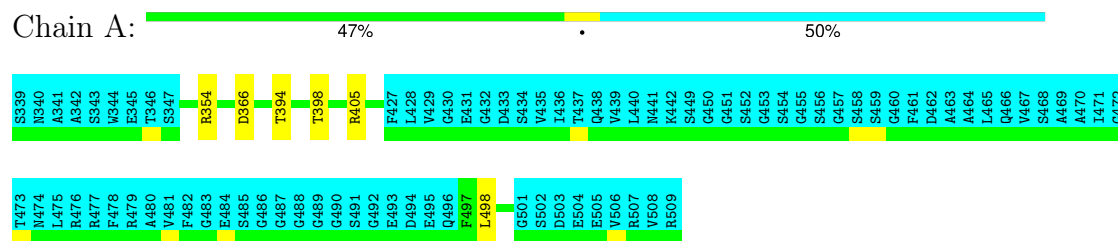
### 4.2.33 Score per residue for model 33

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



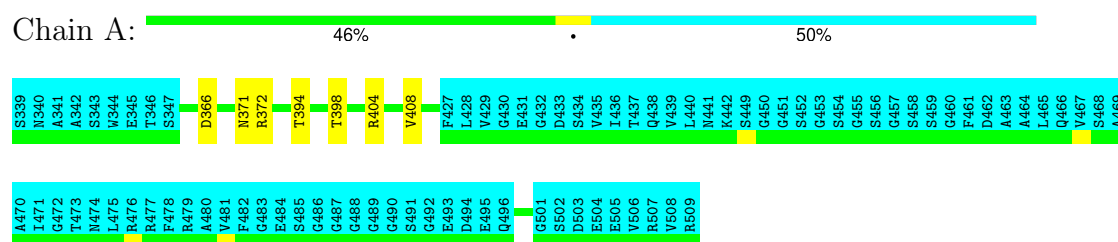
#### 4.2.34 Score per residue for model 34

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



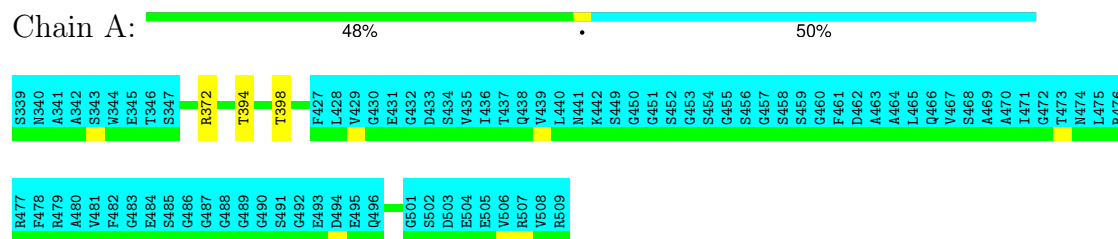
#### 4.2.35 Score per residue for model 35

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



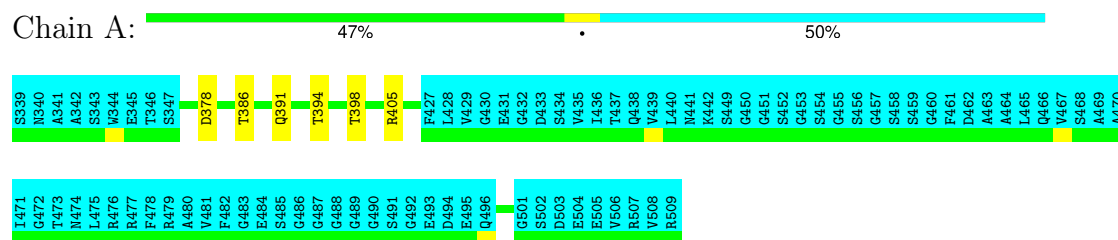
#### 4.2.36 Score per residue for model 36

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



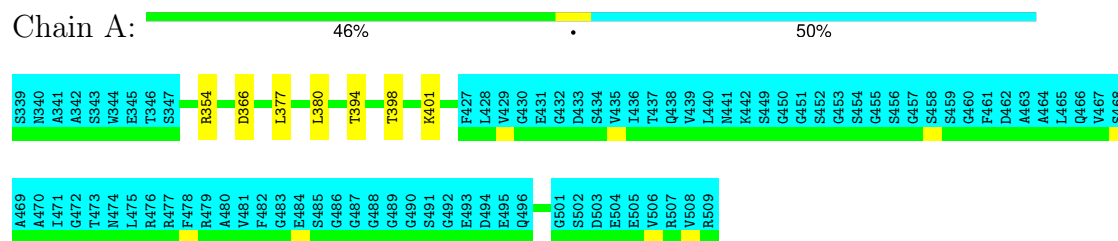
#### 4.2.37 Score per residue for model 37

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



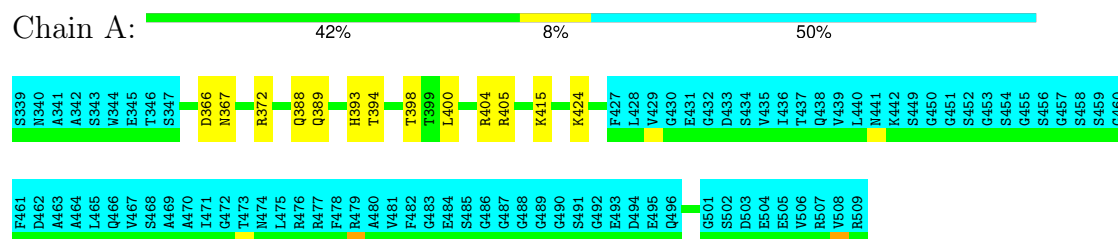
#### 4.2.38 Score per residue for model 38

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



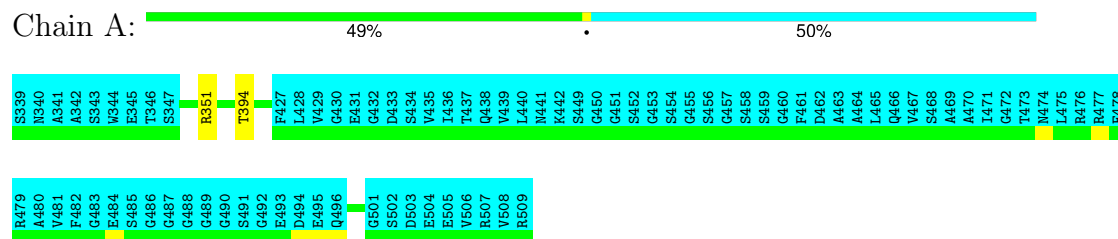
#### 4.2.39 Score per residue for model 39

- Molecule 1: PC4 and SFRS1-interacting protein, Histone-lysine N-methyltransferase 2A



#### 4.2.40 Score per residue for model 40

- Molecule 1: PC4 and SFRS1-interacting protein,Histone-lysine N-methyltransferase 2A



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
YASARA	refinement	
TopSpin	structure solution	
Sparky	structure solution	
CYANA	structure solution	

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	1837
Number of shifts mapped to atoms	1837
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%



## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.60±0.03	0±0/689 ( 0.0± 0.0%)	0.69±0.03	1±1/919 ( 0.1± 0.1%)
All	All	0.60	0/27560 ( 0.0%)	0.69	43/36760 ( 0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	405	ARG	NE-CZ-NH1	6.58	123.59	120.30	39	12
1	A	351	ARG	NE-CZ-NH1	6.50	123.55	120.30	33	5
1	A	354	ARG	NE-CZ-NH1	6.49	123.54	120.30	38	5
1	A	372	ARG	NE-CZ-NH1	5.71	123.16	120.30	5	12
1	A	404	ARG	NE-CZ-NH1	5.63	123.12	120.30	39	9

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	682	719	719	0±0
All	All	27280	28760	28760	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:406:PHE:CE1	1:A:408:VAL:HG22	0.41	2.50	33	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	83/165 (50%)	82±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
All	All	3320/6600 (50%)	3269 (98%)	50 (2%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	498	LEU	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	78/136 (57%)	74±2 (95±2%)	4±2 (5±2%)	22	75
All	All	3120/5440 (57%)	2962 (95%)	158 (5%)	22	75

All 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	398	THR	38
1	A	394	THR	33
1	A	378	ASP	14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	498	LEU	13
1	A	405	ARG	10
1	A	388	GLN	8
1	A	372	ARG	7
1	A	366	ASP	6
1	A	400	LEU	4
1	A	380	LEU	4
1	A	387	MET	2
1	A	371	ASN	2
1	A	497	PHE	2
1	A	377	LEU	2
1	A	393	HIS	2
1	A	354	ARG	1
1	A	349	ASP	1
1	A	404	ARG	1
1	A	408	VAL	1
1	A	386	THR	1
1	A	391	GLN	1
1	A	401	LYS	1
1	A	367	ASN	1
1	A	389	GLN	1
1	A	415	LYS	1
1	A	424	LYS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *str*

#### 7.1.1 Bookkeeping [i](#)

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

Total number of shifts	1837
Number of shifts mapped to atoms	1837
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	$-0.62 \pm 0.16$	Should be checked
$^{13}\text{C}_\beta$	138	$0.22 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	142	$-0.39 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	144	$-0.28 \pm 0.10$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1111 atoms were assigned a chemical shift out of a possible 1225. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	403/416 (97%)	164/167 (98%)	159/166 (96%)	80/83 (96%)
Sidechain	664/746 (89%)	455/483 (94%)	198/228 (87%)	11/35 (31%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	44/63 (70%)	27/32 (84%)	17/29 (59%)	0/2 (0%)
Overall	1111/1225 (91%)	646/682 (95%)	374/423 (88%)	91/120 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1833 atoms were assigned a chemical shift out of a possible 2174. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	730/843 (87%)	295/348 (85%)	291/330 (88%)	144/165 (87%)
Sidechain	1019/1216 (84%)	701/786 (89%)	304/373 (82%)	14/57 (25%)
Aromatic	84/115 (73%)	51/58 (88%)	32/54 (59%)	1/3 (33%)
Overall	1833/2174 (84%)	1047/1192 (88%)	627/757 (83%)	159/225 (71%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

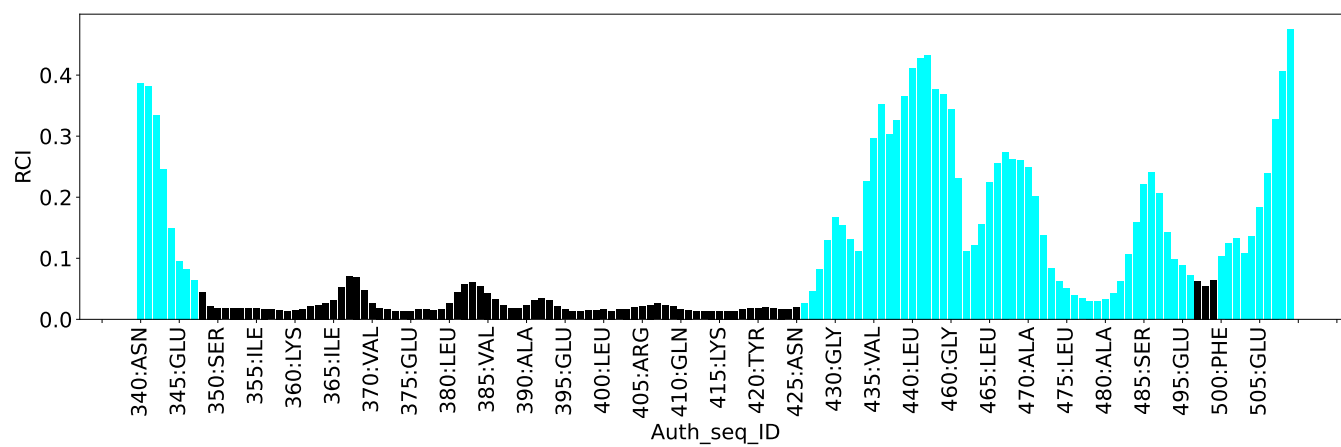
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	417	THR	HG1	5.69	0.08 – 2.19	21.6
1	A	386	THR	HG1	5.58	0.08 – 2.19	21.0

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2190
Intra-residue ( $ i-j =0$ )	688
Sequential ( $ i-j =1$ )	511
Medium range ( $ i-j >1$ and $ i-j <5$ )	445
Long range ( $ i-j \geq 5$ )	546
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	180
Number of unmapped restraints	0
Number of restraints per residue	14.4
Number of long range restraints per residue <sup>1</sup>	3.3

<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)	7.5	0.2
0.2-0.5 (Medium)	2.2	0.5
>0.5 (Large)	None	None



### 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)	2.2	5.02
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis

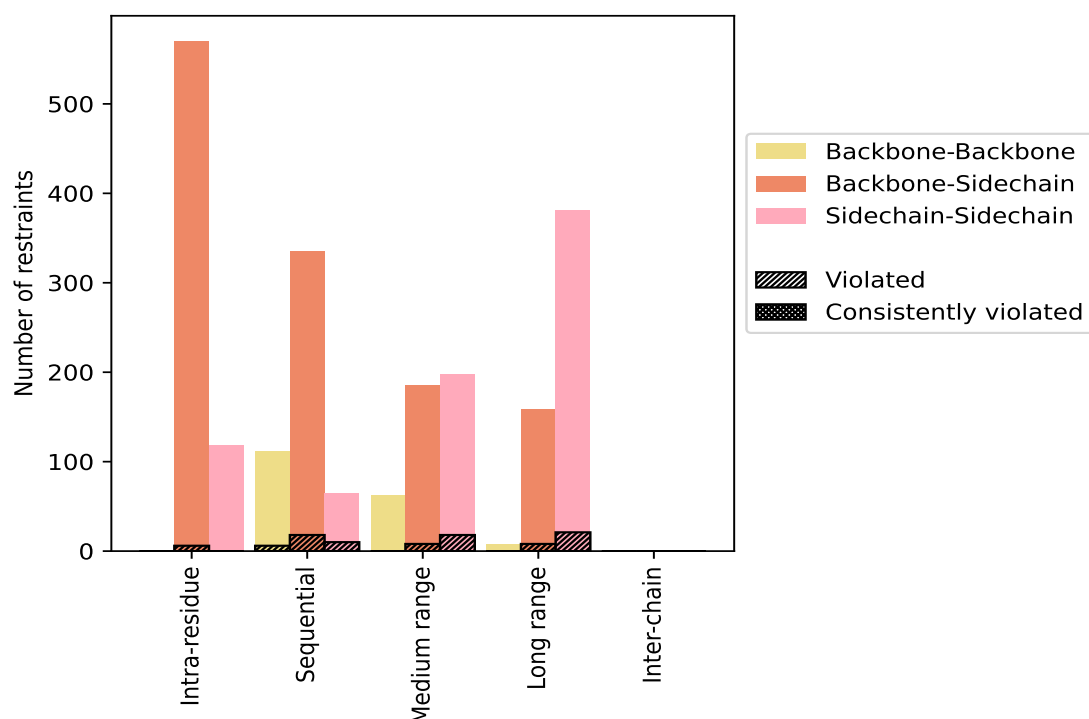
### 9.1 Summary of distance violations

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>688</b>	<b>31.4</b>	<b>6</b>	<b>0.9</b>	<b>0.3</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	570	26.0	6	1.1	0.3	0	0.0	0.0
Sidechain-Sidechain	118	5.4	0	0.0	0.0	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>511</b>	<b>23.3</b>	<b>34</b>	<b>6.7</b>	<b>1.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	112	5.1	6	5.4	0.3	0	0.0	0.0
Backbone-Sidechain	335	15.3	18	5.4	0.8	0	0.0	0.0
Sidechain-Sidechain	64	2.9	10	15.6	0.5	0	0.0	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>445</b>	<b>20.3</b>	<b>26</b>	<b>5.8</b>	<b>1.2</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	62	2.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	185	8.4	8	4.3	0.4	0	0.0	0.0
Sidechain-Sidechain	198	9.0	18	9.1	0.8	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>546</b>	<b>24.9</b>	<b>29</b>	<b>5.3</b>	<b>1.3</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	7	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	158	7.2	8	5.1	0.4	0	0.0	0.0
Sidechain-Sidechain	381	17.4	21	5.5	1.0	0	0.0	0.0
<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>2190</b>	<b>100.0</b>	<b>95</b>	<b>4.3</b>	<b>4.3</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	181	8.3	6	3.3	0.3	0	0.0	0.0
Backbone-Sidechain	1248	57.0	40	3.2	1.8	0	0.0	0.0
Sidechain-Sidechain	761	34.7	49	6.4	2.2	0	0.0	0.0

<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	0	2	1	2	0	5	0.19	0.31	0.1	0.11
2	1	8	4	5	0	18	0.19	0.35	0.08	0.16
3	0	7	6	10	0	23	0.16	0.3	0.06	0.15
4	0	4	5	6	0	15	0.16	0.24	0.04	0.14
5	0	7	2	7	0	16	0.15	0.31	0.05	0.13
6	0	2	2	2	0	6	0.12	0.13	0.01	0.11
7	0	5	3	3	0	11	0.17	0.49	0.1	0.13
8	0	4	1	2	0	7	0.17	0.29	0.05	0.15
9	0	3	5	5	0	13	0.2	0.39	0.08	0.19
10	0	2	1	4	0	7	0.19	0.3	0.07	0.16

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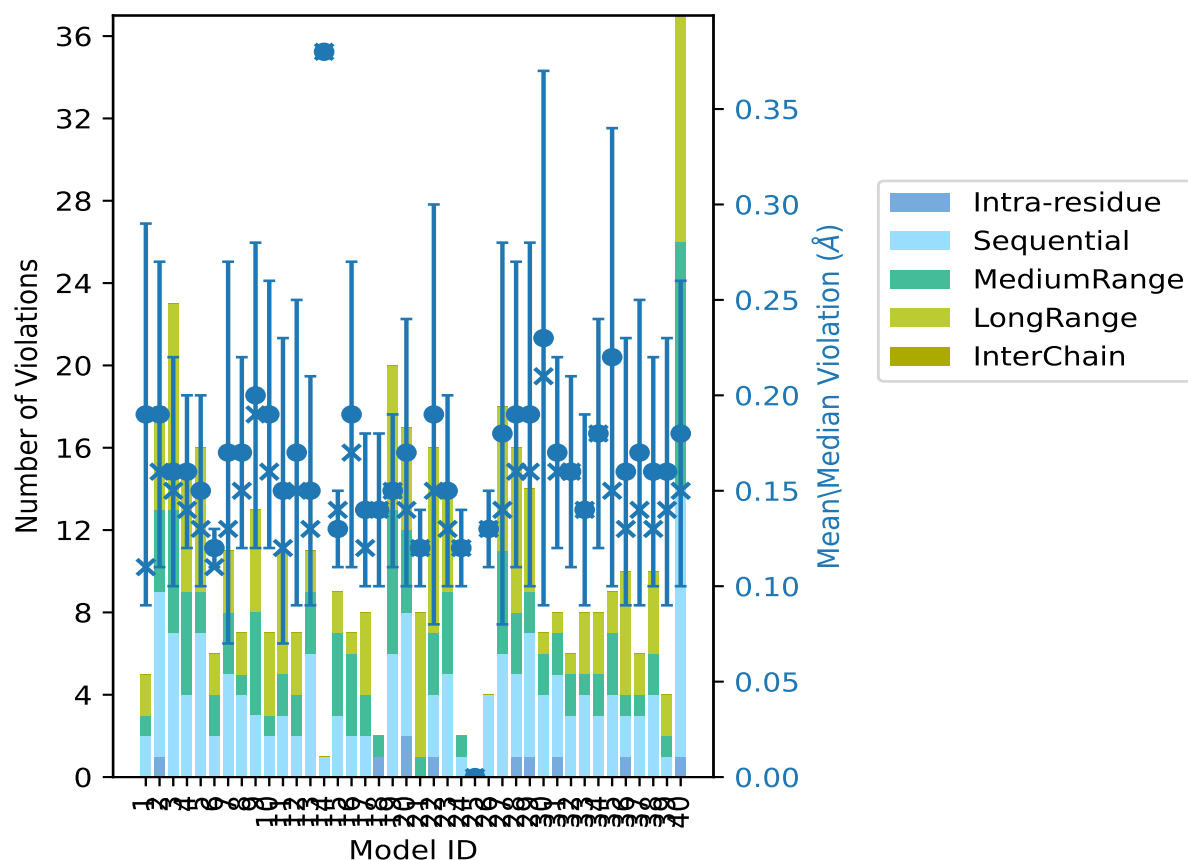
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	0	3	2	6	0	11	0.15	0.37	0.08	0.12
12	0	2	2	3	0	7	0.17	0.35	0.08	0.15
13	0	6	3	2	0	11	0.15	0.32	0.06	0.13
14	0	1	0	0	0	1	0.38	0.38	0.0	0.38
15	0	3	4	2	0	9	0.13	0.17	0.02	0.14
16	0	2	4	1	0	7	0.19	0.35	0.08	0.17
17	0	2	2	4	0	8	0.14	0.22	0.04	0.12
18	1	0	1	0	0	2	0.14	0.17	0.04	0.14
19	0	6	7	7	0	20	0.15	0.23	0.04	0.15
20	2	6	4	5	0	17	0.17	0.39	0.07	0.14
21	0	0	1	7	0	8	0.12	0.16	0.02	0.12
22	1	3	3	9	0	16	0.19	0.45	0.11	0.15
23	0	5	4	5	0	14	0.15	0.25	0.05	0.13
24	0	1	1	0	0	2	0.12	0.14	0.02	0.12
25	0	0	0	0	0	0	0.0	0.0	0.0	0.0
26	0	4	0	0	0	4	0.13	0.16	0.02	0.13
27	0	6	5	7	0	18	0.18	0.46	0.1	0.14
28	1	4	3	8	0	16	0.19	0.39	0.08	0.16
29	1	6	2	5	0	14	0.19	0.4	0.09	0.16
30	0	4	2	1	0	7	0.23	0.5	0.14	0.21
31	1	4	2	1	0	8	0.17	0.29	0.05	0.16
32	0	3	2	1	0	6	0.16	0.25	0.05	0.16
33	0	4	1	3	0	8	0.14	0.26	0.05	0.14
34	0	3	2	3	0	8	0.18	0.29	0.06	0.18
35	0	4	3	2	0	9	0.22	0.5	0.12	0.15
36	1	2	1	6	0	10	0.16	0.35	0.07	0.13
37	0	3	1	2	0	6	0.17	0.34	0.08	0.14
38	0	4	2	4	0	10	0.16	0.29	0.06	0.13
39	0	1	1	2	0	4	0.16	0.27	0.07	0.14
40	1	13	12	11	0	37	0.18	0.48	0.08	0.15

<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, 2095(IR:682, SQ:477, MR:419, LR:517, 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>	%
3	15	11	5	0	34	1	2.5
2	3	3	5	0	13	2	5.0
1	5	3	4	0	13	3	7.5
0	2	2	4	0	8	4	10.0
0	1	1	0	0	2	5	12.5
0	0	1	1	0	2	6	15.0

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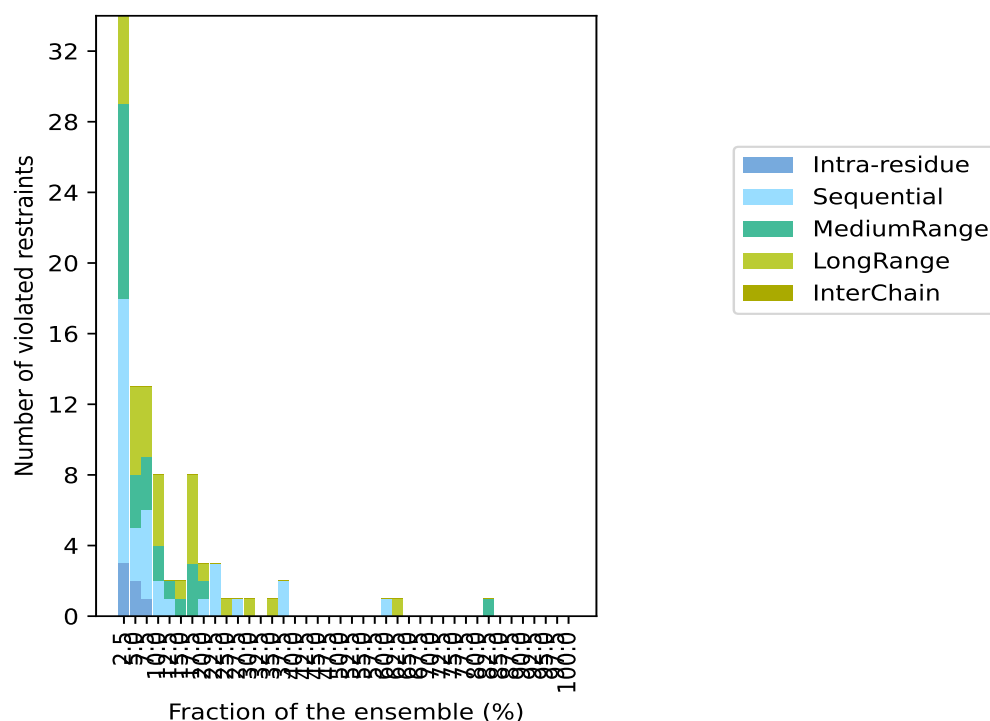
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	3	5	0	8	7	17.5
0	1	1	1	0	3	8	20.0
0	3	0	0	0	3	9	22.5
0	0	0	1	0	1	10	25.0
0	1	0	0	0	1	11	27.5
0	0	0	1	0	1	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	1	0	1	14	35.0
0	2	0	0	0	2	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	0	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	0	0	0	0	0	20	50.0
0	0	0	0	0	0	21	52.5
0	0	0	0	0	0	22	55.0
0	0	0	0	0	0	23	57.5
0	1	0	0	0	1	24	60.0
0	0	0	1	0	1	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	0	0	0	0	0	29	72.5
0	0	0	0	0	0	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	0	1	0	0	1	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	0	0	0	0	0	37	92.5
0	0	0	0	0	0	38	95.0
0	0	0	0	0	0	39	97.5
0	0	0	0	0	0	40	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

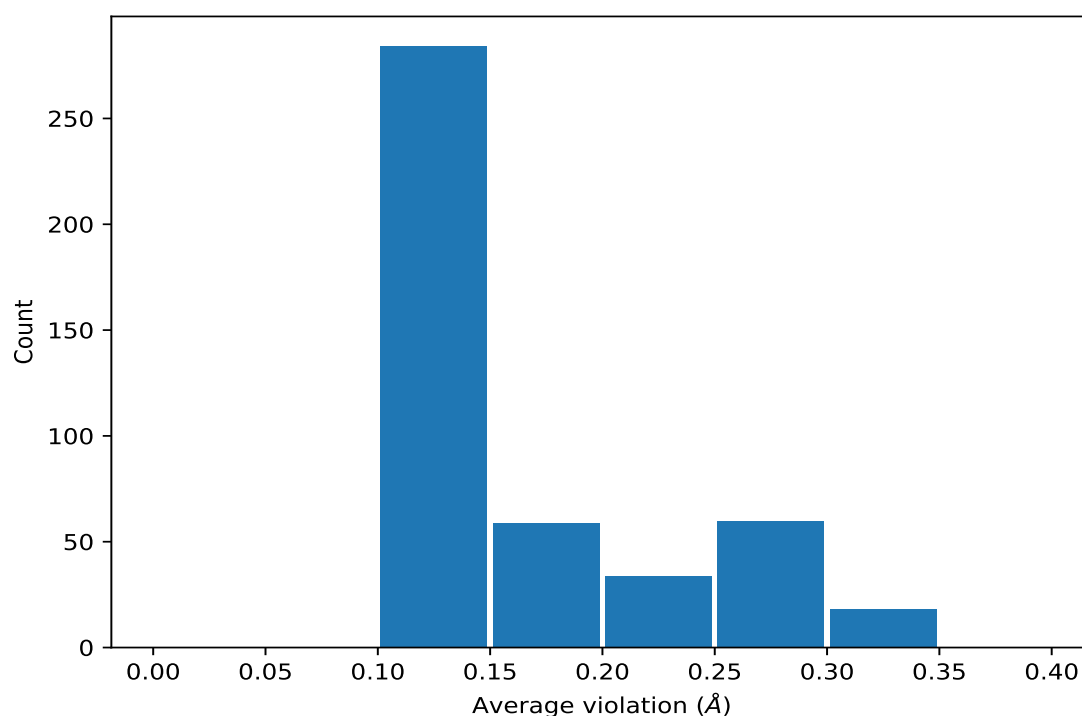
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	33	0.16	0.04	0.15
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	33	0.16	0.04	0.15
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	33	0.16	0.04	0.15
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	33	0.16	0.04	0.15
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	33	0.16	0.04	0.15
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	33	0.16	0.04	0.15
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	25	0.27	0.11	0.27
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	25	0.27	0.11	0.27
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	24	0.3	0.1	0.3

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	24	0.3	0.1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	24	0.3	0.1	0.3
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	15	0.2	0.05	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	15	0.2	0.05	0.2
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	15	0.15	0.06	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	15	0.15	0.06	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	14	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)
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	14	0.14	0.03	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	14	0.14	0.03	0.14
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	12	0.14	0.03	0.14
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	12	0.14	0.03	0.14
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	12	0.14	0.03	0.14
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	12	0.14	0.03	0.14
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	12	0.14	0.03	0.14
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	12	0.14	0.03	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	11	0.14	0.04	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	11	0.14	0.04	0.14
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	10	0.14	0.02	0.14
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	10	0.14	0.02	0.14
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	10	0.14	0.02	0.14
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	10	0.14	0.02	0.14
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	10	0.14	0.02	0.14
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	10	0.14	0.02	0.14
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	9	0.25	0.12	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	9	0.25	0.12	0.2
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	9	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	9	0.15	0.03	0.15
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	9	0.15	0.03	0.15
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	9	0.15	0.03	0.14
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	9	0.15	0.03	0.14
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	9	0.15	0.03	0.14
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	8	0.21	0.06	0.21
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	8	0.21	0.06	0.21
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	8	0.21	0.06	0.21
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	8	0.21	0.06	0.21
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	8	0.21	0.06	0.21
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	8	0.21	0.06	0.21
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	8	0.15	0.04	0.14
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	8	0.15	0.04	0.14
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	8	0.15	0.03	0.16
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	8	0.15	0.03	0.16
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	7	0.21	0.1	0.18
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	7	0.21	0.1	0.18
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	7	0.21	0.1	0.18
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	7	0.21	0.1	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	7	0.19	0.06	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	7	0.19	0.06	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	7	0.19	0.06	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	7	0.19	0.06	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	7	0.19	0.06	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	7	0.19	0.06	0.17
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	7	0.14	0.04	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	7	0.14	0.04	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	7	0.14	0.04	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	7	0.14	0.04	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	7	0.14	0.04	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	7	0.14	0.04	0.13
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	7	0.14	0.03	0.14
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	7	0.14	0.03	0.14
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	7	0.14	0.03	0.14
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	7	0.12	0.02	0.12
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	7	0.12	0.02	0.12
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	7	0.12	0.02	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	7	0.12	0.02	0.11
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	7	0.12	0.02	0.11
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	7	0.12	0.02	0.11
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	7	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	7	0.12	0.02	0.11
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	7	0.12	0.02	0.11
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	6	0.17	0.04	0.16
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	6	0.17	0.04	0.16
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	6	0.14	0.02	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	6	0.14	0.02	0.12
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG11	5	0.17	0.08	0.13
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG12	5	0.17	0.08	0.13
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG13	5	0.17	0.08	0.13
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG11	5	0.17	0.08	0.13
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG12	5	0.17	0.08	0.13
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG13	5	0.17	0.08	0.13
(1,2128)	1:465:A:LEU:HD11	1:466:A:GLN:H	5	0.14	0.02	0.14
(1,2128)	1:465:A:LEU:HD12	1:466:A:GLN:H	5	0.14	0.02	0.14
(1,2128)	1:465:A:LEU:HD13	1:466:A:GLN:H	5	0.14	0.02	0.14
(1,2128)	1:465:A:LEU:HD21	1:466:A:GLN:H	5	0.14	0.02	0.14
(1,2128)	1:465:A:LEU:HD22	1:466:A:GLN:H	5	0.14	0.02	0.14
(1,2128)	1:465:A:LEU:HD23	1:466:A:GLN:H	5	0.14	0.02	0.14
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE1	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE2	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE1	4	0.25	0.09	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE2	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE1	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE2	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE1	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE2	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE1	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE2	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE1	4	0.25	0.09	0.2
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE2	4	0.25	0.09	0.2
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG21	4	0.16	0.05	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG22	4	0.16	0.05	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG23	4	0.16	0.05	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG21	4	0.16	0.05	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG22	4	0.16	0.05	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG23	4	0.16	0.05	0.15
(1,1571)	1:352:A:LEU:HD11	1:380:A:LEU:HA	4	0.16	0.04	0.15
(1,1571)	1:352:A:LEU:HD12	1:380:A:LEU:HA	4	0.16	0.04	0.15
(1,1571)	1:352:A:LEU:HD13	1:380:A:LEU:HA	4	0.16	0.04	0.15
(1,1571)	1:352:A:LEU:HD21	1:380:A:LEU:HA	4	0.16	0.04	0.15
(1,1571)	1:352:A:LEU:HD22	1:380:A:LEU:HA	4	0.16	0.04	0.15
(1,1571)	1:352:A:LEU:HD23	1:380:A:LEU:HA	4	0.16	0.04	0.15
(1,97)	1:436:A:ILE:HD11	1:437:A:THR:HA	4	0.15	0.04	0.14
(1,97)	1:436:A:ILE:HD12	1:437:A:THR:HA	4	0.15	0.04	0.14
(1,97)	1:436:A:ILE:HD13	1:437:A:THR:HA	4	0.15	0.04	0.14
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD21	4	0.13	0.01	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD22	4	0.13	0.01	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD23	4	0.13	0.01	0.12
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB1	4	0.12	0.02	0.12
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB2	4	0.12	0.02	0.12
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB3	4	0.12	0.02	0.12
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB1	4	0.12	0.02	0.12
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB2	4	0.12	0.02	0.12
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB3	4	0.12	0.02	0.12
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE1	4	0.12	0.02	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE2	4	0.12	0.02	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE3	4	0.12	0.02	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE1	4	0.12	0.02	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE2	4	0.12	0.02	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE3	4	0.12	0.02	0.11
(1,1975)	1:408:A:VAL:HG11	1:409:A:SER:H	4	0.11	0.0	0.11
(1,1975)	1:408:A:VAL:HG12	1:409:A:SER:H	4	0.11	0.0	0.11
(1,1975)	1:408:A:VAL:HG13	1:409:A:SER:H	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1975)	1:408:A:VAL:HG21	1:409:A:SER:H	4	0.11	0.0	0.11
(1,1975)	1:408:A:VAL:HG22	1:409:A:SER:H	4	0.11	0.0	0.11
(1,1975)	1:408:A:VAL:HG23	1:409:A:SER:H	4	0.11	0.0	0.11
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD11	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD12	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD13	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD21	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD22	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD23	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD11	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD12	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD13	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD21	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD22	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD23	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD11	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD12	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD13	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD21	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD22	3	0.32	0.13	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD23	3	0.32	0.13	0.25
(1,1455)	1:463:A:ALA:HB1	1:464:A:ALA:H	3	0.26	0.07	0.23
(1,1455)	1:463:A:ALA:HB2	1:464:A:ALA:H	3	0.26	0.07	0.23
(1,1455)	1:463:A:ALA:HB3	1:464:A:ALA:H	3	0.26	0.07	0.23
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD11	3	0.25	0.06	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD12	3	0.25	0.06	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD13	3	0.25	0.06	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD21	3	0.25	0.06	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD22	3	0.25	0.06	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD23	3	0.25	0.06	0.29
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD2	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD3	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD2	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD3	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD2	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD3	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD2	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD3	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD2	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD3	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD2	3	0.21	0.04	0.19
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD3	3	0.21	0.04	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD2	3	0.19	0.06	0.16
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD3	3	0.19	0.06	0.16
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD2	3	0.19	0.06	0.16
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD3	3	0.19	0.06	0.16
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD2	3	0.19	0.06	0.16
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD3	3	0.19	0.06	0.16
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD11	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD12	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD13	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD21	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD22	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD23	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD11	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD12	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD13	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD21	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD22	3	0.15	0.02	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD23	3	0.15	0.02	0.15
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA2	3	0.13	0.04	0.11
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA3	3	0.13	0.04	0.11
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA2	3	0.13	0.04	0.11
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA3	3	0.13	0.04	0.11
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA2	3	0.13	0.04	0.11
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA3	3	0.13	0.04	0.11
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB1	3	0.13	0.02	0.12
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB2	3	0.13	0.02	0.12
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB3	3	0.13	0.02	0.12
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB1	3	0.13	0.02	0.12
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB2	3	0.13	0.02	0.12
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB3	3	0.13	0.02	0.12
(1,521)	1:387:A:MET:HE1	1:391:A:GLN:H	3	0.12	0.01	0.13
(1,521)	1:387:A:MET:HE2	1:391:A:GLN:H	3	0.12	0.01	0.13
(1,521)	1:387:A:MET:HE3	1:391:A:GLN:H	3	0.12	0.01	0.13
(1,1287)	1:397:A:ILE:HD11	1:398:A:THR:H	3	0.12	0.01	0.13
(1,1287)	1:397:A:ILE:HD12	1:398:A:THR:H	3	0.12	0.01	0.13
(1,1287)	1:397:A:ILE:HD13	1:398:A:THR:H	3	0.12	0.01	0.13
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD11	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD12	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD13	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD21	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD22	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD23	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD11	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD12	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD13	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD21	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD22	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD23	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD11	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD12	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD13	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD21	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD22	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD23	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD11	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD12	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD13	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD21	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD22	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD23	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD11	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD12	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD13	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD21	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD22	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD23	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD11	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD12	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD13	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD21	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD22	3	0.11	0.0	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD23	3	0.11	0.0	0.11
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE2	3	0.11	0.01	0.11
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE3	3	0.11	0.01	0.11
(1,389)	1:398:A:THR:HG21	1:481:A:VAL:HB	3	0.11	0.0	0.11
(1,389)	1:398:A:THR:HG22	1:481:A:VAL:HB	3	0.11	0.0	0.11
(1,389)	1:398:A:THR:HG23	1:481:A:VAL:HB	3	0.11	0.0	0.11
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG21	2	0.18	0.0	0.18
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG22	2	0.18	0.0	0.18
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG23	2	0.18	0.0	0.18
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG21	2	0.18	0.0	0.18
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG22	2	0.18	0.0	0.18
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG23	2	0.18	0.0	0.18
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD11	2	0.17	0.0	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD12	2	0.17	0.0	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD13	2	0.17	0.0	0.17
(1,2164)	1:495:A:GLU:H	1:495:A:GLU:HB2	2	0.16	0.02	0.16
(1,2164)	1:495:A:GLU:H	1:495:A:GLU:HB3	2	0.16	0.02	0.16
(1,720)	1:365:A:ILE:HG21	1:366:A:ASP:HB3	2	0.15	0.03	0.15
(1,720)	1:365:A:ILE:HG22	1:366:A:ASP:HB3	2	0.15	0.03	0.15
(1,720)	1:365:A:ILE:HG23	1:366:A:ASP:HB3	2	0.15	0.03	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD11	2	0.15	0.0	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD12	2	0.15	0.0	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD13	2	0.15	0.0	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD21	2	0.15	0.0	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD22	2	0.15	0.0	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD23	2	0.15	0.0	0.15
(1,1534)	1:348:A:MET:HE1	1:351:A:ARG:H	2	0.14	0.02	0.14
(1,1534)	1:348:A:MET:HE2	1:351:A:ARG:H	2	0.14	0.02	0.14
(1,1534)	1:348:A:MET:HE3	1:351:A:ARG:H	2	0.14	0.02	0.14
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE1	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE2	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE3	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE1	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE2	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE3	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE1	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE2	2	0.12	0.01	0.12
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE3	2	0.12	0.01	0.12
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG21	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG22	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG23	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG21	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG22	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG23	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG21	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG22	2	0.12	0.02	0.12
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG23	2	0.12	0.02	0.12
(1,935)	1:363:A:LEU:HD11	1:406:A:PHE:HE1	2	0.12	0.01	0.12
(1,935)	1:363:A:LEU:HD11	1:406:A:PHE:HE2	2	0.12	0.01	0.12
(1,935)	1:363:A:LEU:HD12	1:406:A:PHE:HE1	2	0.12	0.01	0.12
(1,935)	1:363:A:LEU:HD12	1:406:A:PHE:HE2	2	0.12	0.01	0.12
(1,935)	1:363:A:LEU:HD13	1:406:A:PHE:HE1	2	0.12	0.01	0.12
(1,935)	1:363:A:LEU:HD13	1:406:A:PHE:HE2	2	0.12	0.01	0.12
(1,2051)	1:419:A:LEU:HD11	1:422:A:LYS:HE2	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD11	1:422:A:LYS:HE3	2	0.12	0.02	0.12

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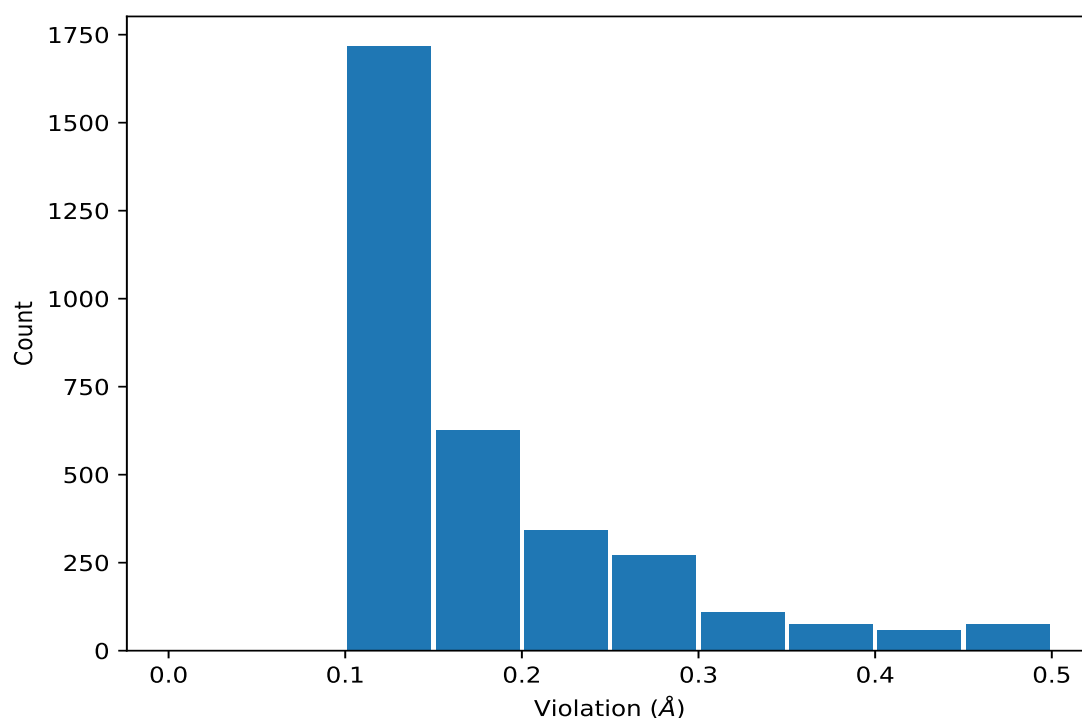
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2051)	1:419:A:LEU:HD12	1:422:A:LYS:HE2	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD12	1:422:A:LYS:HE3	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD13	1:422:A:LYS:HE2	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD13	1:422:A:LYS:HE3	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD21	1:422:A:LYS:HE2	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD21	1:422:A:LYS:HE3	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD22	1:422:A:LYS:HE2	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD22	1:422:A:LYS:HE3	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD23	1:422:A:LYS:HE2	2	0.12	0.02	0.12
(1,2051)	1:419:A:LEU:HD23	1:422:A:LYS:HE3	2	0.12	0.02	0.12
(1,1016)	1:364:A:LYS:HD2	1:365:A:ILE:H	2	0.11	0.01	0.11
(1,1016)	1:364:A:LYS:HD3	1:365:A:ILE:H	2	0.11	0.01	0.11
(1,1682)	1:365:A:ILE:HD11	1:501:A:GLY:HA2	2	0.11	0.0	0.11
(1,1682)	1:365:A:ILE:HD11	1:501:A:GLY:HA3	2	0.11	0.0	0.11
(1,1682)	1:365:A:ILE:HD12	1:501:A:GLY:HA2	2	0.11	0.0	0.11
(1,1682)	1:365:A:ILE:HD12	1:501:A:GLY:HA3	2	0.11	0.0	0.11
(1,1682)	1:365:A:ILE:HD13	1:501:A:GLY:HA2	2	0.11	0.0	0.11
(1,1682)	1:365:A:ILE:HD13	1:501:A:GLY:HA3	2	0.11	0.0	0.11
(1,1047)	1:506:A:VAL:H	1:507:A:ARG:H	2	0.11	0.0	0.11

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	30	0.5
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	30	0.5
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	30	0.5
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	30	0.5
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	30	0.5
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	30	0.5
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	30	0.5
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	30	0.5
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	30	0.5
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	30	0.5
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	30	0.5
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	30	0.5
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	30	0.5
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	30	0.5
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	30	0.5
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	30	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	30	0.5
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	30	0.5
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD11	35	0.5
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD12	35	0.5
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD13	35	0.5
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD21	35	0.5
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD22	35	0.5
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD23	35	0.5
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD11	35	0.5
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD12	35	0.5
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD13	35	0.5
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD21	35	0.5
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD22	35	0.5
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD23	35	0.5
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD11	35	0.5
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD12	35	0.5
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD13	35	0.5
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD21	35	0.5
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD22	35	0.5
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD23	35	0.5
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	7	0.49
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	7	0.49
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	7	0.49
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	7	0.49
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	7	0.49
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	7	0.49
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	7	0.49
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	7	0.49
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	7	0.49
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	7	0.49
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	7	0.49
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	7	0.49
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	40	0.48
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	40	0.48
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	40	0.48
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	40	0.48
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	40	0.48
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	40	0.48
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	40	0.48
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	40	0.48
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	40	0.48
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	27	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	27	0.46
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	27	0.46
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	27	0.46
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	27	0.46
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	27	0.46
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	27	0.46
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	27	0.46
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	27	0.46
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	22	0.45
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	22	0.45
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	22	0.45
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	22	0.45
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	22	0.45
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	22	0.45
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	22	0.45
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	22	0.45
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	22	0.45
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	40	0.44
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	40	0.44
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	40	0.44
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	40	0.44
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	27	0.41
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	27	0.41
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	27	0.41
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	27	0.41
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	27	0.41
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	27	0.41
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	27	0.41
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	27	0.41
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	27	0.41
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	27	0.41
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	27	0.41
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	27	0.41
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE1	22	0.41
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE2	22	0.41
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE1	22	0.41
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE2	22	0.41
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE1	22	0.41
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE2	22	0.41
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE1	22	0.41
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE2	22	0.41
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE1	22	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE2	22	0.41
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE1	22	0.41
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE2	22	0.41
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	29	0.4
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	29	0.4
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	29	0.4
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	29	0.4
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	29	0.4
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	29	0.4
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	29	0.4
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	29	0.4
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	29	0.4
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	29	0.4
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	29	0.4
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	29	0.4
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	29	0.4
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	29	0.4
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	29	0.4
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	29	0.4
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	29	0.4
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	29	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	22	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	22	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	22	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	22	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	22	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	22	0.4
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	22	0.4
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	22	0.4
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	22	0.4
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	22	0.4
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	22	0.4
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	22	0.4
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	20	0.39
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	20	0.39
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	20	0.39
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	20	0.39
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	20	0.39
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	20	0.39
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	20	0.39
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	20	0.39
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	20	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	20	0.39
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	20	0.39
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	20	0.39
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	9	0.39
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	9	0.39
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	9	0.39
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	9	0.39
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	9	0.39
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	9	0.39
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	9	0.39
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	9	0.39
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	9	0.39
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	28	0.39
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	28	0.39
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	28	0.39
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	28	0.39
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	28	0.39
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	28	0.39
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	28	0.39
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	28	0.39
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	28	0.39
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	14	0.38
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	14	0.38
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	14	0.38
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	14	0.38
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	14	0.38
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	14	0.38
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	14	0.38
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	14	0.38
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	14	0.38
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	14	0.38
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	14	0.38
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	14	0.38
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	29	0.38
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	29	0.38
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	29	0.38
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	29	0.38
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	29	0.38
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	29	0.38
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	29	0.38
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	29	0.38
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	29	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	11	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	11	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	11	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	11	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	11	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	11	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	11	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	11	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	11	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	11	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	11	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	11	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	30	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	30	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	30	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	30	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	30	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	30	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	30	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	30	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	30	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	30	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	30	0.37
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	30	0.37
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	12	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	12	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	12	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	12	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	12	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	12	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	12	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	12	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	12	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	12	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	12	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	12	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	16	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	16	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	16	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	16	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	16	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	16	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	16	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	16	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	16	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	16	0.35
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	16	0.35
(1,1455)	1:463:A:ALA:HB1	1:464:A:ALA:H	28	0.35
(1,1455)	1:463:A:ALA:HB2	1:464:A:ALA:H	28	0.35
(1,1455)	1:463:A:ALA:HB3	1:464:A:ALA:H	28	0.35
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	2	0.35
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	2	0.35
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	2	0.35
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	2	0.35
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	2	0.35
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	2	0.35
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	2	0.35
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	2	0.35
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	2	0.35
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	36	0.35
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	36	0.35
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	36	0.35
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	36	0.35
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	36	0.35
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	36	0.35
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	36	0.35
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	36	0.35
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	36	0.35
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	37	0.34
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	37	0.34
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	37	0.34
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	37	0.34
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	37	0.34
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	37	0.34
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	37	0.34
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	37	0.34
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	37	0.34
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	37	0.34
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	37	0.34
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	37	0.34
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG11	40	0.33
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG12	40	0.33
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG13	40	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG11	40	0.33
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG12	40	0.33
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG13	40	0.33
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	13	0.32
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	13	0.32
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	13	0.32
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	13	0.32
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	13	0.32
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	13	0.32
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	13	0.32
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	13	0.32
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	13	0.32
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	13	0.32
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	13	0.32
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	13	0.32
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	9	0.31
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	9	0.31
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	9	0.31
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	9	0.31
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	9	0.31
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	9	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	1	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	1	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	1	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	1	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	1	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	1	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	1	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	1	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	1	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	5	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	5	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	5	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	5	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	5	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	5	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	5	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	5	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	5	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	20	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	20	0.31
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	20	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	20	0.31
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	20	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	20	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	20	0.31
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	20	0.31
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD11	2	0.3
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD12	2	0.3
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD13	2	0.3
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD21	2	0.3
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD22	2	0.3
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD23	2	0.3
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	2	0.3
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	2	0.3
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	2	0.3
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	2	0.3
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	2	0.3
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	2	0.3
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	2	0.3
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	2	0.3
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	2	0.3
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	2	0.3
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	2	0.3
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	2	0.3
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	2	0.3
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	2	0.3
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	2	0.3
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	2	0.3
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	2	0.3
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	2	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	1	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	1	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	10	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	10	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	10	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	10	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	10	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	10	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	10	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	10	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	10	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	10	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	10	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	10	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	35	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	35	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	35	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	35	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	35	0.3
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	35	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	35	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	35	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	35	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	35	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	35	0.3
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	35	0.3
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	3	0.3
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	3	0.3
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	3	0.3
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	3	0.3
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	3	0.3
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	3	0.3
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	3	0.3
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	3	0.3
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	3	0.3
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	27	0.3
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	27	0.3
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	27	0.3
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	27	0.3
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	27	0.3
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	27	0.3
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD11	31	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD12	31	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD13	31	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD21	31	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD22	31	0.29
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD23	31	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	8	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	8	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	8	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	8	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	8	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	8	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	8	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	8	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	8	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	8	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	8	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	8	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	38	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	38	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	38	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	38	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	38	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	38	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	38	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	38	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	38	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	38	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	38	0.29
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	38	0.29
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	34	0.29
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	34	0.29
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	34	0.29
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	34	0.29
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	34	0.29
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	34	0.29
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	34	0.29
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	34	0.29
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	34	0.29
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	34	0.29
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	34	0.29
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	34	0.29
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	28	0.28
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	28	0.28
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	28	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	28	0.28
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	28	0.28
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	28	0.28
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	28	0.28
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	28	0.28
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	28	0.28
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	28	0.28
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	28	0.28
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	28	0.28
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD2	40	0.28
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD3	40	0.28
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD2	40	0.28
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD3	40	0.28
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD2	40	0.28
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD3	40	0.28
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	2	0.28
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	2	0.28
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	2	0.28
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	2	0.28
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	2	0.28
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	2	0.28
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	2	0.28
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	2	0.28
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	2	0.28
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	2	0.28
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	2	0.28
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	2	0.28
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	35	0.27
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	35	0.27
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	35	0.27
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	35	0.27
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	35	0.27
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	35	0.27
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	35	0.27
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	35	0.27
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	35	0.27
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	35	0.27
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	35	0.27
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	35	0.27
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD2	39	0.27
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD3	39	0.27
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD2	39	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD3	39	0.27
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD2	39	0.27
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD3	39	0.27
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD2	39	0.27
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD3	39	0.27
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD2	39	0.27
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD3	39	0.27
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD2	39	0.27
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD3	39	0.27
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	10	0.27
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	10	0.27
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	10	0.27
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	10	0.27
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	10	0.27
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	10	0.27
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	10	0.27
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	10	0.27
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	10	0.27
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	3	0.27
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	3	0.27
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	3	0.27
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	3	0.27
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	3	0.27
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	3	0.27
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	2	0.26
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	2	0.26
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	2	0.26
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	2	0.26
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	2	0.26
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	2	0.26
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	2	0.26
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	2	0.26
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	2	0.26
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	2	0.26
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	2	0.26
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	2	0.26
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	33	0.26
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	33	0.26
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	33	0.26
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	33	0.26
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	33	0.26
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	33	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	33	0.26
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	33	0.26
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	33	0.26
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	33	0.26
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	33	0.26
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	33	0.26
(1,1547)	1:348:A:MET:HG2	1:352:A:LEU:HD11	29	0.26
(1,1547)	1:348:A:MET:HG2	1:352:A:LEU:HD12	29	0.26
(1,1547)	1:348:A:MET:HG2	1:352:A:LEU:HD13	29	0.26
(1,1547)	1:348:A:MET:HG2	1:352:A:LEU:HD21	29	0.26
(1,1547)	1:348:A:MET:HG2	1:352:A:LEU:HD22	29	0.26
(1,1547)	1:348:A:MET:HG2	1:352:A:LEU:HD23	29	0.26
(1,1547)	1:348:A:MET:HG3	1:352:A:LEU:HD11	29	0.26
(1,1547)	1:348:A:MET:HG3	1:352:A:LEU:HD12	29	0.26
(1,1547)	1:348:A:MET:HG3	1:352:A:LEU:HD13	29	0.26
(1,1547)	1:348:A:MET:HG3	1:352:A:LEU:HD21	29	0.26
(1,1547)	1:348:A:MET:HG3	1:352:A:LEU:HD22	29	0.26
(1,1547)	1:348:A:MET:HG3	1:352:A:LEU:HD23	29	0.26
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	9	0.25
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	9	0.25
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	9	0.25
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	9	0.25
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	9	0.25
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	9	0.25
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	9	0.25
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	9	0.25
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	9	0.25
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	9	0.25
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	9	0.25
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	9	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD11	23	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD12	23	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD13	23	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD21	23	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD22	23	0.25
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD23	23	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD11	23	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD12	23	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD13	23	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD21	23	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD22	23	0.25
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD23	23	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD11	23	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD12	23	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD13	23	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD21	23	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD22	23	0.25
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD23	23	0.25
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG21	3	0.25
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG22	3	0.25
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG23	3	0.25
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG21	3	0.25
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG22	3	0.25
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG23	3	0.25
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	32	0.25
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	32	0.25
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	32	0.25
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	32	0.25
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	32	0.25
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	32	0.25
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	32	0.25
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	32	0.25
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	32	0.25
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	32	0.25
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	32	0.25
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	32	0.25
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	34	0.24
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	34	0.24
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	34	0.24
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	34	0.24
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	34	0.24
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	34	0.24
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	34	0.24
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	34	0.24
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	34	0.24
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	34	0.24
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	34	0.24
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	34	0.24
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	4	0.24
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	4	0.24
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	4	0.24
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	4	0.24
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	4	0.24
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	27	0.24
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	27	0.24
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	27	0.24
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	27	0.24
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	27	0.24
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	27	0.24
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	40	0.24
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	40	0.24
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	40	0.24
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	40	0.24
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	40	0.24
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	40	0.24
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	36	0.24
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	36	0.24
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	36	0.24
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	36	0.24
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	36	0.24
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	36	0.24
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	36	0.24
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	36	0.24
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	36	0.24
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	36	0.24
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	36	0.24
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	36	0.24
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	16	0.24
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	16	0.24
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	16	0.24
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	16	0.24
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	16	0.24
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	16	0.24
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	16	0.24
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	16	0.24
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	16	0.24
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	19	0.23
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	19	0.23
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	19	0.23
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	19	0.23
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	19	0.23
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	19	0.23
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	19	0.23
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	19	0.23
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	19	0.23
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	19	0.23
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	19	0.23
(1,1455)	1:463:A:ALA:HB1	1:464:A:ALA:H	38	0.23
(1,1455)	1:463:A:ALA:HB2	1:464:A:ALA:H	38	0.23
(1,1455)	1:463:A:ALA:HB3	1:464:A:ALA:H	38	0.23
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	3	0.23
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	3	0.23
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	3	0.23
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	3	0.23
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	3	0.23
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	3	0.23
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	3	0.23
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	3	0.23
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	3	0.23
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	28	0.22
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	28	0.22
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	28	0.22
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	28	0.22
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	28	0.22
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	28	0.22
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	17	0.22
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	17	0.22
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	17	0.22
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	17	0.22
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	17	0.22
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	17	0.22
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	17	0.22
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	17	0.22
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	17	0.22
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	17	0.22
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	17	0.22
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	17	0.22
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	17	0.22
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	17	0.22
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	17	0.22
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	17	0.22
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	17	0.22
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	17	0.22
(1,1571)	1:352:A:LEU:HD11	1:380:A:LEU:HA	40	0.22
(1,1571)	1:352:A:LEU:HD12	1:380:A:LEU:HA	40	0.22
(1,1571)	1:352:A:LEU:HD13	1:380:A:LEU:HA	40	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1571)	1:352:A:LEU:HD21	1:380:A:LEU:HA	40	0.22
(1,1571)	1:352:A:LEU:HD22	1:380:A:LEU:HA	40	0.22
(1,1571)	1:352:A:LEU:HD23	1:380:A:LEU:HA	40	0.22
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	23	0.22
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	23	0.22
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	23	0.22
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	23	0.22
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	23	0.22
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	23	0.22
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	23	0.22
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	23	0.22
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	23	0.22
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	23	0.22
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	23	0.22
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	23	0.22
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	4	0.22
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	4	0.22
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	4	0.22
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	4	0.22
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	4	0.22
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	4	0.22
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	4	0.22
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	4	0.22
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	4	0.22
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	40	0.22
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	40	0.22
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	40	0.22
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	40	0.22
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	40	0.22
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	40	0.22
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	40	0.22
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	40	0.22
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	40	0.22
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	10	0.22
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	10	0.22
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	10	0.22
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	10	0.22
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	10	0.22
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	10	0.22
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	40	0.21
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	40	0.21
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	40	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	40	0.21
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	40	0.21
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	40	0.21
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD11	34	0.21
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD12	34	0.21
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD13	34	0.21
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD21	34	0.21
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD22	34	0.21
(1,1846)	1:387:A:MET:HE1	1:475:A:LEU:HD23	34	0.21
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD11	34	0.21
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD12	34	0.21
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD13	34	0.21
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD21	34	0.21
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD22	34	0.21
(1,1846)	1:387:A:MET:HE2	1:475:A:LEU:HD23	34	0.21
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD11	34	0.21
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD12	34	0.21
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD13	34	0.21
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD21	34	0.21
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD22	34	0.21
(1,1846)	1:387:A:MET:HE3	1:475:A:LEU:HD23	34	0.21
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE1	38	0.21
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE2	38	0.21
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE1	38	0.21
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE2	38	0.21
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE1	38	0.21
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE2	38	0.21
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE1	38	0.21
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE2	38	0.21
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE1	38	0.21
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE2	38	0.21
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE1	38	0.21
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE2	38	0.21
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	9	0.21
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	9	0.21
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	9	0.21
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	9	0.21
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	9	0.21
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	9	0.21
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	19	0.21
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	19	0.21
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	19	0.21
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	19	0.21
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	19	0.21
(1,1432)	1:436:A:ILE:HA	1:437:A:THR:H	40	0.21
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	3	0.21
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	3	0.21
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	3	0.21
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	9	0.21
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	9	0.21
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	9	0.21
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	9	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	19	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	19	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	19	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	19	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	19	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	19	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	31	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	31	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	31	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	31	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	31	0.21
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	31	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	29	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	29	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	29	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	29	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	29	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	29	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	29	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	29	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	29	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	29	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	29	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	29	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	30	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	30	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	30	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	30	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	30	0.21
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	30	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	30	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	30	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	30	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	30	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	30	0.21
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	30	0.21
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	30	0.21
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	30	0.21
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	30	0.21
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	30	0.21
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	30	0.21
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	30	0.21
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	30	0.21
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	30	0.21
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	30	0.21
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	35	0.21
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	35	0.21
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	35	0.21
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	35	0.21
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	35	0.21
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	35	0.21
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	35	0.21
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	35	0.21
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	35	0.21
(1,97)	1:436:A:ILE:HD11	1:437:A:THR:HA	3	0.21
(1,97)	1:436:A:ILE:HD12	1:437:A:THR:HA	3	0.21
(1,97)	1:436:A:ILE:HD13	1:437:A:THR:HA	3	0.21
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	4	0.21
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	4	0.21
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	4	0.21
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	4	0.21
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	4	0.21
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	4	0.21
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	40	0.21
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	40	0.21
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	40	0.21
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	40	0.21
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	40	0.21
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	40	0.21
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	23	0.2
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	23	0.2
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	23	0.2
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	23	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	23	0.2
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	23	0.2
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	23	0.2
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	23	0.2
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	23	0.2
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	23	0.2
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	23	0.2
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	23	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	31	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	31	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	31	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	31	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	31	0.2
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	31	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	31	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	31	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	31	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	31	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	31	0.2
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	31	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	31	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	31	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	31	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	31	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	31	0.2
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	31	0.2
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE1	5	0.2
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE2	5	0.2
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE1	5	0.2
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE2	5	0.2
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE1	5	0.2
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE2	5	0.2
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE1	5	0.2
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE2	5	0.2
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE1	5	0.2
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE2	5	0.2
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE1	5	0.2
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE2	5	0.2
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	3	0.2
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	3	0.2
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	3	0.2
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	3	0.2
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	3	0.2
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	12	0.2
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	12	0.2
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	12	0.2
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	27	0.2
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	27	0.2
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	27	0.2
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	27	0.2
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	27	0.2
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	27	0.2
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	27	0.2
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	27	0.2
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	27	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	11	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	11	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	11	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	11	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	11	0.2
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	11	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	11	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	11	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	11	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	11	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	11	0.2
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	11	0.2
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	3	0.2
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	3	0.2
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	3	0.2
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	2	0.19
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	2	0.19
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	2	0.19
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	2	0.19
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	2	0.19
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	2	0.19
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	2	0.19
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	2	0.19
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	2	0.19
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	2	0.19
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	2	0.19
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	2	0.19
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA3	4	0.19
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA2	4	0.19
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA3	4	0.19
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA2	4	0.19
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA3	4	0.19
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	40	0.19
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	40	0.19
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	40	0.19
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	40	0.19
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	40	0.19
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	40	0.19
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	40	0.19
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	40	0.19
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	40	0.19
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	40	0.19
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	40	0.19
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	40	0.19
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	40	0.19
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	40	0.19
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	40	0.19
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	40	0.19
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	40	0.19
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	40	0.19
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	28	0.19
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	28	0.19
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	28	0.19
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	28	0.19
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	28	0.19
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	28	0.19
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD2	4	0.19
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD3	4	0.19
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD2	4	0.19
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD3	4	0.19
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD2	4	0.19
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD3	4	0.19
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD2	4	0.19
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD3	4	0.19
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD2	4	0.19
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD3	4	0.19
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD2	4	0.19
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD3	4	0.19
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	5	0.19
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	5	0.19
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	5	0.19
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	5	0.19
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	5	0.19
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	20	0.19
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	20	0.19
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	20	0.19
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	20	0.19
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	20	0.19
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	20	0.19
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	9	0.19
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	9	0.19
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	9	0.19
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	9	0.19
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	9	0.19
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	9	0.19
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	9	0.19
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	9	0.19
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	9	0.19
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	9	0.19
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	9	0.19
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	9	0.19
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	9	0.19
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	9	0.19
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	9	0.19
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	9	0.19
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	9	0.19
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	9	0.19
(1,1455)	1:463:A:ALA:HB1	1:464:A:ALA:H	17	0.19
(1,1455)	1:463:A:ALA:HB2	1:464:A:ALA:H	17	0.19
(1,1455)	1:463:A:ALA:HB3	1:464:A:ALA:H	17	0.19
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	29	0.19
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	29	0.19
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	29	0.19
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	29	0.19
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	29	0.19
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	29	0.19
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	29	0.19
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	29	0.19
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	29	0.19
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	9	0.19
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	9	0.19
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	9	0.19
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	9	0.19
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	9	0.19
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	9	0.19
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	9	0.19
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	9	0.19
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	20	0.19
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	20	0.19
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	20	0.19
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	20	0.19
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	20	0.19
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	20	0.19
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	20	0.19
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	20	0.19
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	20	0.19
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	20	0.19
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	20	0.19
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	20	0.19
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	19	0.19
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	19	0.19
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	19	0.19
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	19	0.19
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	19	0.19
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	19	0.19
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	19	0.19
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	19	0.19
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	19	0.19
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	38	0.19
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	38	0.19
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	38	0.19
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	38	0.19
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	38	0.19
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	38	0.19
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	38	0.19
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	38	0.19
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	38	0.19
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	13	0.18
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	13	0.18
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	13	0.18
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	13	0.18
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	13	0.18
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	13	0.18
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	13	0.18
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	13	0.18
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	13	0.18
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	13	0.18
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	13	0.18
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	3	0.18
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	3	0.18
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	3	0.18
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	3	0.18
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	3	0.18
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	3	0.18
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	9	0.18
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	9	0.18
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	9	0.18
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	9	0.18
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	9	0.18
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	9	0.18
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	9	0.18
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	9	0.18
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	9	0.18
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	9	0.18
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	9	0.18
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	9	0.18
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD11	22	0.18
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD12	22	0.18
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD13	22	0.18
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD21	22	0.18
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD22	22	0.18
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD23	22	0.18
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD11	22	0.18
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD12	22	0.18
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD13	22	0.18
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD21	22	0.18
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD22	22	0.18
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD23	22	0.18
(1,2007)	1:411:A:VAL:HG11	1:415:A:LYS:HD2	39	0.18
(1,2007)	1:411:A:VAL:HG11	1:415:A:LYS:HD3	39	0.18
(1,2007)	1:411:A:VAL:HG12	1:415:A:LYS:HD2	39	0.18
(1,2007)	1:411:A:VAL:HG12	1:415:A:LYS:HD3	39	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2007)	1:411:A:VAL:HG13	1:415:A:LYS:HD2	39	0.18
(1,2007)	1:411:A:VAL:HG13	1:415:A:LYS:HD3	39	0.18
(1,2007)	1:411:A:VAL:HG21	1:415:A:LYS:HD2	39	0.18
(1,2007)	1:411:A:VAL:HG21	1:415:A:LYS:HD3	39	0.18
(1,2007)	1:411:A:VAL:HG22	1:415:A:LYS:HD2	39	0.18
(1,2007)	1:411:A:VAL:HG22	1:415:A:LYS:HD3	39	0.18
(1,2007)	1:411:A:VAL:HG23	1:415:A:LYS:HD2	39	0.18
(1,2007)	1:411:A:VAL:HG23	1:415:A:LYS:HD3	39	0.18
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	2	0.18
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	2	0.18
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	2	0.18
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	2	0.18
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	2	0.18
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	2	0.18
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	22	0.18
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	22	0.18
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	22	0.18
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	22	0.18
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	22	0.18
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	22	0.18
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG21	20	0.18
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG22	20	0.18
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG23	20	0.18
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG21	20	0.18
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG22	20	0.18
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG23	20	0.18
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	34	0.18
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	34	0.18
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	34	0.18
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	34	0.18
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	34	0.18
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	34	0.18
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	34	0.18
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	34	0.18
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	34	0.18
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	34	0.18
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	34	0.18
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	34	0.18
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	34	0.18
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	34	0.18
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	34	0.18
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	34	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	34	0.18
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	34	0.18
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	19	0.18
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	19	0.18
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	19	0.18
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	28	0.18
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	28	0.18
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	28	0.18
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	28	0.18
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	29	0.18
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	29	0.18
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	29	0.18
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	29	0.18
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	16	0.18
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	16	0.18
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	16	0.18
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	16	0.18
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	16	0.18
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	16	0.18
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	16	0.18
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	16	0.18
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	16	0.18
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	16	0.18
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	16	0.18
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	16	0.18
(1,720)	1:365:A:ILE:HG21	1:366:A:ASP:HB3	40	0.18
(1,720)	1:365:A:ILE:HG22	1:366:A:ASP:HB3	40	0.18
(1,720)	1:365:A:ILE:HG23	1:366:A:ASP:HB3	40	0.18
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	34	0.18
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	34	0.18
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	34	0.18
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	34	0.18
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	34	0.18
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	34	0.18
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	34	0.18
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	34	0.18
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	34	0.18
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	19	0.18
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	19	0.18
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	19	0.18
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	19	0.18
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	19	0.18
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	19	0.18
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	19	0.18
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	19	0.18
(1,244)	1:348:A:MET:HE1	1:351:A:ARG:HD2	40	0.18
(1,244)	1:348:A:MET:HE1	1:351:A:ARG:HD3	40	0.18
(1,244)	1:348:A:MET:HE2	1:351:A:ARG:HD2	40	0.18
(1,244)	1:348:A:MET:HE2	1:351:A:ARG:HD3	40	0.18
(1,244)	1:348:A:MET:HE3	1:351:A:ARG:HD2	40	0.18
(1,244)	1:348:A:MET:HE3	1:351:A:ARG:HD3	40	0.18
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	8	0.18
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	8	0.18
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	8	0.18
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	8	0.18
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	8	0.18
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	8	0.18
(1,2164)	1:495:A:GLU:H	1:495:A:GLU:HB2	29	0.17
(1,2164)	1:495:A:GLU:H	1:495:A:GLU:HB3	29	0.17
(1,2128)	1:465:A:LEU:HD11	1:466:A:GLN:H	5	0.17
(1,2128)	1:465:A:LEU:HD12	1:466:A:GLN:H	5	0.17
(1,2128)	1:465:A:LEU:HD13	1:466:A:GLN:H	5	0.17
(1,2128)	1:465:A:LEU:HD21	1:466:A:GLN:H	5	0.17
(1,2128)	1:465:A:LEU:HD22	1:466:A:GLN:H	5	0.17
(1,2128)	1:465:A:LEU:HD23	1:466:A:GLN:H	5	0.17
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD11	18	0.17
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD12	18	0.17
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD13	18	0.17
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD21	18	0.17
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD22	18	0.17
(1,2125)	1:465:A:LEU:HA	1:465:A:LEU:HD23	18	0.17
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	23	0.17
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	23	0.17
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	23	0.17
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	23	0.17
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	23	0.17
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	23	0.17
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	23	0.17
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	23	0.17
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	23	0.17
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	23	0.17
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	23	0.17
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	23	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	23	0.17
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	23	0.17
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	23	0.17
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	23	0.17
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	23	0.17
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	23	0.17
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	40	0.17
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	40	0.17
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	40	0.17
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	40	0.17
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	40	0.17
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	40	0.17
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	40	0.17
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	40	0.17
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	40	0.17
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	40	0.17
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	40	0.17
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	40	0.17
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	23	0.17
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	23	0.17
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	23	0.17
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	23	0.17
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	23	0.17
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	23	0.17
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE1	15	0.17
(1,1767)	1:377:A:LEU:HD11	1:423:A:PHE:HE2	15	0.17
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE1	15	0.17
(1,1767)	1:377:A:LEU:HD12	1:423:A:PHE:HE2	15	0.17
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE1	15	0.17
(1,1767)	1:377:A:LEU:HD13	1:423:A:PHE:HE2	15	0.17
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE1	15	0.17
(1,1767)	1:377:A:LEU:HD21	1:423:A:PHE:HE2	15	0.17
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE1	15	0.17
(1,1767)	1:377:A:LEU:HD22	1:423:A:PHE:HE2	15	0.17
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE1	15	0.17
(1,1767)	1:377:A:LEU:HD23	1:423:A:PHE:HE2	15	0.17
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD2	19	0.17
(1,1760)	1:377:A:LEU:HD11	1:415:A:LYS:HD3	19	0.17
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD2	19	0.17
(1,1760)	1:377:A:LEU:HD12	1:415:A:LYS:HD3	19	0.17
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD2	19	0.17
(1,1760)	1:377:A:LEU:HD13	1:415:A:LYS:HD3	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD2	19	0.17
(1,1760)	1:377:A:LEU:HD21	1:415:A:LYS:HD3	19	0.17
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD2	19	0.17
(1,1760)	1:377:A:LEU:HD22	1:415:A:LYS:HD3	19	0.17
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD2	19	0.17
(1,1760)	1:377:A:LEU:HD23	1:415:A:LYS:HD3	19	0.17
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	7	0.17
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	7	0.17
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	7	0.17
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	7	0.17
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	7	0.17
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	7	0.17
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	28	0.17
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	28	0.17
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	28	0.17
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	28	0.17
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	28	0.17
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	28	0.17
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG21	32	0.17
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG22	32	0.17
(1,1639)	1:360:A:LYS:HE2	1:399:A:THR:HG23	32	0.17
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG21	32	0.17
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG22	32	0.17
(1,1639)	1:360:A:LYS:HE3	1:399:A:THR:HG23	32	0.17
(1,1571)	1:352:A:LEU:HD11	1:380:A:LEU:HA	2	0.17
(1,1571)	1:352:A:LEU:HD12	1:380:A:LEU:HA	2	0.17
(1,1571)	1:352:A:LEU:HD13	1:380:A:LEU:HA	2	0.17
(1,1571)	1:352:A:LEU:HD21	1:380:A:LEU:HA	2	0.17
(1,1571)	1:352:A:LEU:HD22	1:380:A:LEU:HA	2	0.17
(1,1571)	1:352:A:LEU:HD23	1:380:A:LEU:HA	2	0.17
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	16	0.17
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	16	0.17
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	16	0.17
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	16	0.17
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	16	0.17
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	16	0.17
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	16	0.17
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	16	0.17
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	16	0.17
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	16	0.17
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	16	0.17
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	16	0.17
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	16	0.17
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	16	0.17
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	16	0.17
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	16	0.17
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	16	0.17
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	27	0.17
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	27	0.17
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	27	0.17
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	27	0.17
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	27	0.17
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	27	0.17
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	27	0.17
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	27	0.17
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	27	0.17
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	27	0.17
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	27	0.17
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	27	0.17
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	27	0.17
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	27	0.17
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	27	0.17
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	27	0.17
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	27	0.17
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	27	0.17
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	37	0.17
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	37	0.17
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	37	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD11	28	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD12	28	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD13	28	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD11	40	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD12	40	0.17
(1,1474)	1:471:A:ILE:H	1:471:A:ILE:HD13	40	0.17
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	22	0.17
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	22	0.17
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	22	0.17
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	22	0.17
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	22	0.17
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	22	0.17
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	22	0.17
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	22	0.17
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	22	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	22	0.17
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	22	0.17
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	22	0.17
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	22	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	32	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	32	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	32	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	32	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	32	0.17
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	32	0.17
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	5	0.17
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	5	0.17
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	5	0.17
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	5	0.17
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	5	0.17
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	5	0.17
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	5	0.17
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	5	0.17
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	5	0.17
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	2	0.17
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	2	0.17
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	2	0.17
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	2	0.17
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	2	0.17
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	2	0.17
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	2	0.17
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	2	0.17
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	2	0.17
(1,2173)	1:496:A:GLN:HE21	1:498:A:LEU:HD11	20	0.16
(1,2173)	1:496:A:GLN:HE21	1:498:A:LEU:HD12	20	0.16
(1,2173)	1:496:A:GLN:HE21	1:498:A:LEU:HD13	20	0.16
(1,2173)	1:496:A:GLN:HE21	1:498:A:LEU:HD21	20	0.16
(1,2173)	1:496:A:GLN:HE21	1:498:A:LEU:HD22	20	0.16
(1,2173)	1:496:A:GLN:HE21	1:498:A:LEU:HD23	20	0.16
(1,2173)	1:496:A:GLN:HE22	1:498:A:LEU:HD11	20	0.16
(1,2173)	1:496:A:GLN:HE22	1:498:A:LEU:HD12	20	0.16
(1,2173)	1:496:A:GLN:HE22	1:498:A:LEU:HD13	20	0.16
(1,2173)	1:496:A:GLN:HE22	1:498:A:LEU:HD21	20	0.16
(1,2173)	1:496:A:GLN:HE22	1:498:A:LEU:HD22	20	0.16
(1,2173)	1:496:A:GLN:HE22	1:498:A:LEU:HD23	20	0.16
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	15	0.16
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	15	0.16
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	15	0.16
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	15	0.16
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	15	0.16
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	15	0.16
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	15	0.16
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	15	0.16
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	15	0.16
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	15	0.16
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	15	0.16
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	7	0.16
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	7	0.16
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	7	0.16
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	7	0.16
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	7	0.16
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	7	0.16
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	7	0.16
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	7	0.16
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	7	0.16
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	7	0.16
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	7	0.16
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	7	0.16
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	36	0.16
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	36	0.16
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	36	0.16
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	36	0.16
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	36	0.16
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	36	0.16
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	8	0.16
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	8	0.16
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	8	0.16
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	8	0.16
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	8	0.16
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	8	0.16
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	10	0.16
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	10	0.16
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	10	0.16
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	10	0.16
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	10	0.16
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	10	0.16
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	12	0.16
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	12	0.16
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	12	0.16
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	12	0.16
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	12	0.16
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	13	0.16
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	13	0.16
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	13	0.16
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	13	0.16
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	13	0.16
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	13	0.16
(1,1534)	1:348:A:MET:HE1	1:351:A:ARG:H	19	0.16
(1,1534)	1:348:A:MET:HE2	1:351:A:ARG:H	19	0.16
(1,1534)	1:348:A:MET:HE3	1:351:A:ARG:H	19	0.16
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	4	0.16
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	4	0.16
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	4	0.16
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	9	0.16
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	9	0.16
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	9	0.16
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	27	0.16
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	27	0.16
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	27	0.16
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD2	4	0.16
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD3	4	0.16
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD2	4	0.16
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD3	4	0.16
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD2	4	0.16
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD3	4	0.16
(1,1000)	1:436:A:ILE:HG21	1:438:A:GLN:HA	40	0.16
(1,1000)	1:436:A:ILE:HG22	1:438:A:GLN:HA	40	0.16
(1,1000)	1:436:A:ILE:HG23	1:438:A:GLN:HA	40	0.16
(1,977)	1:403:A:ILE:HD11	1:404:A:ARG:H	40	0.16
(1,977)	1:403:A:ILE:HD12	1:404:A:ARG:H	40	0.16
(1,977)	1:403:A:ILE:HD13	1:404:A:ARG:H	40	0.16
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	21	0.16
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	21	0.16
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	21	0.16
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	21	0.16
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	28	0.16
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	28	0.16
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	28	0.16
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	28	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	28	0.16
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	28	0.16
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	28	0.16
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	28	0.16
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	28	0.16
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	5	0.16
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	5	0.16
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	5	0.16
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	5	0.16
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	5	0.16
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	5	0.16
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	5	0.16
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	5	0.16
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	5	0.16
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	40	0.16
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	40	0.16
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	40	0.16
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	40	0.16
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	40	0.16
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	40	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	13	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	13	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	13	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	13	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	13	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	13	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	13	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	13	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	13	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	13	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	13	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	13	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	31	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	31	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	31	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	31	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	31	0.16
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	31	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	31	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	31	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	31	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	31	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	31	0.16
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	31	0.16
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	20	0.16
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	20	0.16
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	20	0.16
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	28	0.16
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	28	0.16
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	28	0.16
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	28	0.16
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	28	0.16
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	28	0.16
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	28	0.16
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	28	0.16
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	28	0.16
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	26	0.16
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	26	0.16
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	26	0.16
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	26	0.16
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	26	0.16
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	26	0.16
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	26	0.16
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	26	0.16
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	26	0.16
(1,97)	1:436:A:ILE:HD11	1:437:A:THR:HA	2	0.16
(1,97)	1:436:A:ILE:HD12	1:437:A:THR:HA	2	0.16
(1,97)	1:436:A:ILE:HD13	1:437:A:THR:HA	2	0.16
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	19	0.15
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	19	0.15
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	19	0.15
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	19	0.15
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	19	0.15
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	19	0.15
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	19	0.15
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	19	0.15
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	19	0.15
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	19	0.15
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	19	0.15
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	19	0.15
(1,2128)	1:465:A:LEU:HD11	1:466:A:GLN:H	13	0.15
(1,2128)	1:465:A:LEU:HD12	1:466:A:GLN:H	13	0.15
(1,2128)	1:465:A:LEU:HD13	1:466:A:GLN:H	13	0.15
(1,2128)	1:465:A:LEU:HD21	1:466:A:GLN:H	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2128)	1:465:A:LEU:HD22	1:466:A:GLN:H	13	0.15
(1,2128)	1:465:A:LEU:HD23	1:466:A:GLN:H	13	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD11	7	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD12	7	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD13	7	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD21	7	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD22	7	0.15
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD23	7	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD11	7	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD12	7	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD13	7	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD21	7	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD22	7	0.15
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD23	7	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD11	15	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD12	15	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD13	15	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD21	15	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD22	15	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD23	15	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD11	40	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD12	40	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD13	40	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD21	40	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD22	40	0.15
(1,2081)	1:425:A:ASN:HA	1:428:A:LEU:HD23	40	0.15
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	3	0.15
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	3	0.15
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	3	0.15
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	3	0.15
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	3	0.15
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	3	0.15
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	19	0.15
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	19	0.15
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	19	0.15
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	19	0.15
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	19	0.15
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	19	0.15
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	22	0.15
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	22	0.15
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	22	0.15
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	22	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	22	0.15
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	22	0.15
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	11	0.15
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	11	0.15
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	11	0.15
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	11	0.15
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	11	0.15
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	11	0.15
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	3	0.15
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	3	0.15
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	3	0.15
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	3	0.15
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	3	0.15
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	3	0.15
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	3	0.15
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	3	0.15
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	3	0.15
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	3	0.15
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	3	0.15
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	3	0.15
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	7	0.15
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	7	0.15
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	7	0.15
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	7	0.15
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	7	0.15
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	7	0.15
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	7	0.15
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	7	0.15
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	7	0.15
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	7	0.15
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	7	0.15
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	7	0.15
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	15	0.15
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	15	0.15
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	15	0.15
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	15	0.15
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	15	0.15
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	15	0.15
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	16	0.15
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	16	0.15
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	16	0.15
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	16	0.15
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	16	0.15
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	31	0.15
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	31	0.15
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	31	0.15
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	31	0.15
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	31	0.15
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	31	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG21	10	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG22	10	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG23	10	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG21	10	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG22	10	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG23	10	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG21	31	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG22	31	0.15
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG23	31	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG21	31	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG22	31	0.15
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG23	31	0.15
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	35	0.15
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	35	0.15
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	35	0.15
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	35	0.15
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	35	0.15
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	35	0.15
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	35	0.15
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	35	0.15
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	35	0.15
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	35	0.15
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	35	0.15
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	35	0.15
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	35	0.15
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	35	0.15
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	35	0.15
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	35	0.15
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	35	0.15
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	35	0.15
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD21	9	0.15
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD22	9	0.15
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD23	9	0.15
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	33	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	33	0.15
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	33	0.15
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	35	0.15
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	35	0.15
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	35	0.15
(1,1252)	1:386:A:THR:HG1	1:389:A:GLN:H	40	0.15
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	11	0.15
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	11	0.15
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	11	0.15
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	11	0.15
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	11	0.15
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	11	0.15
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	11	0.15
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	11	0.15
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	11	0.15
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	12	0.15
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	12	0.15
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	12	0.15
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	12	0.15
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	12	0.15
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	12	0.15
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	12	0.15
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	12	0.15
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	12	0.15
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	28	0.15
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	28	0.15
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	28	0.15
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	28	0.15
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	28	0.15
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	28	0.15
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	28	0.15
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	28	0.15
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	28	0.15
(1,881)	1:428:A:LEU:HA	1:429:A:VAL:HG11	35	0.15
(1,881)	1:428:A:LEU:HA	1:429:A:VAL:HG12	35	0.15
(1,881)	1:428:A:LEU:HA	1:429:A:VAL:HG13	35	0.15
(1,881)	1:428:A:LEU:HA	1:429:A:VAL:HG21	35	0.15
(1,881)	1:428:A:LEU:HA	1:429:A:VAL:HG22	35	0.15
(1,881)	1:428:A:LEU:HA	1:429:A:VAL:HG23	35	0.15
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	40	0.15
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	40	0.15
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	40	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:380:A:LEU:HG	1:419:A:LEU:HD21	8	0.15
(1,599)	1:380:A:LEU:HG	1:419:A:LEU:HD22	8	0.15
(1,599)	1:380:A:LEU:HG	1:419:A:LEU:HD23	8	0.15
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	33	0.15
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	33	0.15
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	33	0.15
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	33	0.15
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	33	0.15
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	33	0.15
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	33	0.15
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	33	0.15
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	33	0.15
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	2	0.15
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	2	0.15
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	2	0.15
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	2	0.15
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	2	0.15
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	2	0.15
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	2	0.15
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	2	0.15
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	2	0.15
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG11	3	0.15
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG12	3	0.15
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG13	3	0.15
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG11	3	0.15
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG12	3	0.15
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG13	3	0.15
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB1	23	0.15
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB2	23	0.15
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB3	23	0.15
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB1	23	0.15
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB2	23	0.15
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB3	23	0.15
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB1	5	0.15
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB2	5	0.15
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB3	5	0.15
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB1	5	0.15
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB2	5	0.15
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB3	5	0.15
(1,24)	1:498:A:LEU:HA	1:498:A:LEU:HD11	36	0.15
(1,24)	1:498:A:LEU:HA	1:498:A:LEU:HD12	36	0.15
(1,24)	1:498:A:LEU:HA	1:498:A:LEU:HD13	36	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2164)	1:495:A:GLU:H	1:495:A:GLU:HB2	22	0.14
(1,2164)	1:495:A:GLU:H	1:495:A:GLU:HB3	22	0.14
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	21	0.14
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	21	0.14
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	21	0.14
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	21	0.14
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	21	0.14
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	21	0.14
(1,2128)	1:465:A:LEU:HD11	1:466:A:GLN:H	8	0.14
(1,2128)	1:465:A:LEU:HD12	1:466:A:GLN:H	8	0.14
(1,2128)	1:465:A:LEU:HD13	1:466:A:GLN:H	8	0.14
(1,2128)	1:465:A:LEU:HD21	1:466:A:GLN:H	8	0.14
(1,2128)	1:465:A:LEU:HD22	1:466:A:GLN:H	8	0.14
(1,2128)	1:465:A:LEU:HD23	1:466:A:GLN:H	8	0.14
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	27	0.14
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	27	0.14
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	27	0.14
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	27	0.14
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	27	0.14
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	27	0.14
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	28	0.14
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	28	0.14
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	28	0.14
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	28	0.14
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	28	0.14
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	28	0.14
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	17	0.14
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	17	0.14
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	17	0.14
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	17	0.14
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	17	0.14
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	17	0.14
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	17	0.14
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	17	0.14
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	17	0.14
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	17	0.14
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	17	0.14
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	17	0.14
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	29	0.14
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	29	0.14
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	29	0.14
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	29	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	29	0.14
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	29	0.14
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	32	0.14
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	32	0.14
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	32	0.14
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	32	0.14
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	32	0.14
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	32	0.14
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	33	0.14
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	33	0.14
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	33	0.14
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	33	0.14
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	33	0.14
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	33	0.14
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	36	0.14
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	36	0.14
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	36	0.14
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	36	0.14
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	36	0.14
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	36	0.14
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	24	0.14
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	24	0.14
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	24	0.14
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	19	0.14
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	19	0.14
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	19	0.14
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	40	0.14
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	40	0.14
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	40	0.14
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD2	29	0.14
(1,1013)	1:475:A:LEU:HD21	1:476:A:ARG:HD3	29	0.14
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD2	29	0.14
(1,1013)	1:475:A:LEU:HD22	1:476:A:ARG:HD3	29	0.14
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD2	29	0.14
(1,1013)	1:475:A:LEU:HD23	1:476:A:ARG:HD3	29	0.14
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	34	0.14
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	34	0.14
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	34	0.14
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	34	0.14
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	34	0.14
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	34	0.14
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	34	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	34	0.14
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	34	0.14
(1,990)	1:428:A:LEU:HD21	1:482:A:PHE:HD1	3	0.14
(1,990)	1:428:A:LEU:HD21	1:482:A:PHE:HD2	3	0.14
(1,990)	1:428:A:LEU:HD22	1:482:A:PHE:HD1	3	0.14
(1,990)	1:428:A:LEU:HD22	1:482:A:PHE:HD2	3	0.14
(1,990)	1:428:A:LEU:HD23	1:482:A:PHE:HD1	3	0.14
(1,990)	1:428:A:LEU:HD23	1:482:A:PHE:HD2	3	0.14
(1,959)	1:391:A:GLN:H	1:426:A:MET:HE1	20	0.14
(1,959)	1:391:A:GLN:H	1:426:A:MET:HE2	20	0.14
(1,959)	1:391:A:GLN:H	1:426:A:MET:HE3	20	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	2	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	2	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	2	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	2	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	2	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	2	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	2	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	2	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	2	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	19	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	19	0.14
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	19	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	19	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	19	0.14
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	19	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	19	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	19	0.14
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	19	0.14
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE1	40	0.14
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE2	40	0.14
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE3	40	0.14
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE1	40	0.14
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE2	40	0.14
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE3	40	0.14
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	26	0.14
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	26	0.14
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	26	0.14
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	26	0.14
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	26	0.14
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	26	0.14
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	26	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	26	0.14
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	26	0.14
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	26	0.14
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	26	0.14
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	26	0.14
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG21	27	0.14
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG22	27	0.14
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG23	27	0.14
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG21	27	0.14
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG22	27	0.14
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG23	27	0.14
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG21	27	0.14
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG22	27	0.14
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG23	27	0.14
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	4	0.14
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	4	0.14
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	4	0.14
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	40	0.14
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	40	0.14
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	40	0.14
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	37	0.14
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	37	0.14
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	37	0.14
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	37	0.14
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	37	0.14
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	37	0.14
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	37	0.14
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	37	0.14
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	37	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	15	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	15	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	15	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	15	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	15	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	15	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	15	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	15	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	15	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	37	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	37	0.14
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	37	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	37	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	37	0.14
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	37	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	37	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	37	0.14
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	37	0.14
(1,361)	1:399:A:THR:HB	1:403:A:ILE:HG21	40	0.14
(1,361)	1:399:A:THR:HB	1:403:A:ILE:HG22	40	0.14
(1,361)	1:399:A:THR:HB	1:403:A:ILE:HG23	40	0.14
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	9	0.14
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	9	0.14
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	9	0.14
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	9	0.14
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	9	0.14
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	9	0.14
(1,21)	1:498:A:LEU:HA	1:498:A:LEU:HD21	20	0.14
(1,21)	1:498:A:LEU:HA	1:498:A:LEU:HD22	20	0.14
(1,21)	1:498:A:LEU:HA	1:498:A:LEU:HD23	20	0.14
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	13	0.13
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	13	0.13
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	13	0.13
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	13	0.13
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	13	0.13
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	13	0.13
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	13	0.13
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	13	0.13
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	13	0.13
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	13	0.13
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	13	0.13
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	13	0.13
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	23	0.13
(1,2145)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	23	0.13
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	23	0.13
(1,2145)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	23	0.13
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	23	0.13
(1,2145)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	23	0.13
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB2	23	0.13
(1,2145)	1:475:A:LEU:HD21	1:478:A:PHE:HB3	23	0.13
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB2	23	0.13
(1,2145)	1:475:A:LEU:HD22	1:478:A:PHE:HB3	23	0.13
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB2	23	0.13
(1,2145)	1:475:A:LEU:HD23	1:478:A:PHE:HB3	23	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	38	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	38	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	38	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	38	0.13
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	38	0.13
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	13	0.13
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	13	0.13
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	13	0.13
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	13	0.13
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	13	0.13
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	13	0.13
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	13	0.13
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	13	0.13
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	13	0.13
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	13	0.13
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	13	0.13
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	13	0.13
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	13	0.13
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	13	0.13
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	13	0.13
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	13	0.13
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	13	0.13
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	13	0.13
(1,2108)	1:436:A:ILE:HG21	1:438:A:GLN:HB2	4	0.13
(1,2108)	1:436:A:ILE:HG21	1:438:A:GLN:HB3	4	0.13
(1,2108)	1:436:A:ILE:HG22	1:438:A:GLN:HB2	4	0.13
(1,2108)	1:436:A:ILE:HG22	1:438:A:GLN:HB3	4	0.13
(1,2108)	1:436:A:ILE:HG23	1:438:A:GLN:HB2	4	0.13
(1,2108)	1:436:A:ILE:HG23	1:438:A:GLN:HB3	4	0.13
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	6	0.13
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	6	0.13
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	6	0.13
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	6	0.13
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	6	0.13
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	6	0.13
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	6	0.13
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	6	0.13
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	6	0.13
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	6	0.13
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	6	0.13
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	6	0.13
(1,2051)	1:419:A:LEU:HD11	1:422:A:LYS:HE2	38	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:419:A:LEU:HD11	1:422:A:LYS:HE3	38	0.13
(1,2051)	1:419:A:LEU:HD12	1:422:A:LYS:HE2	38	0.13
(1,2051)	1:419:A:LEU:HD12	1:422:A:LYS:HE3	38	0.13
(1,2051)	1:419:A:LEU:HD13	1:422:A:LYS:HE2	38	0.13
(1,2051)	1:419:A:LEU:HD13	1:422:A:LYS:HE3	38	0.13
(1,2051)	1:419:A:LEU:HD21	1:422:A:LYS:HE2	38	0.13
(1,2051)	1:419:A:LEU:HD21	1:422:A:LYS:HE3	38	0.13
(1,2051)	1:419:A:LEU:HD22	1:422:A:LYS:HE2	38	0.13
(1,2051)	1:419:A:LEU:HD22	1:422:A:LYS:HE3	38	0.13
(1,2051)	1:419:A:LEU:HD23	1:422:A:LYS:HE2	38	0.13
(1,2051)	1:419:A:LEU:HD23	1:422:A:LYS:HE3	38	0.13
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	4	0.13
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	4	0.13
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	4	0.13
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	4	0.13
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	4	0.13
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	4	0.13
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	5	0.13
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	5	0.13
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	5	0.13
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	5	0.13
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	5	0.13
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	5	0.13
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	7	0.13
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	7	0.13
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	7	0.13
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	7	0.13
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	7	0.13
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	7	0.13
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	6	0.13
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	6	0.13
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	6	0.13
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	6	0.13
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	6	0.13
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	6	0.13
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	21	0.13
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	21	0.13
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	21	0.13
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	21	0.13
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	21	0.13
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	21	0.13
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	23	0.13
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	23	0.13
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	23	0.13
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	23	0.13
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	23	0.13
(1,1571)	1:352:A:LEU:HD11	1:380:A:LEU:HA	20	0.13
(1,1571)	1:352:A:LEU:HD12	1:380:A:LEU:HA	20	0.13
(1,1571)	1:352:A:LEU:HD13	1:380:A:LEU:HA	20	0.13
(1,1571)	1:352:A:LEU:HD21	1:380:A:LEU:HA	20	0.13
(1,1571)	1:352:A:LEU:HD22	1:380:A:LEU:HA	20	0.13
(1,1571)	1:352:A:LEU:HD23	1:380:A:LEU:HA	20	0.13
(1,1571)	1:352:A:LEU:HD11	1:380:A:LEU:HA	27	0.13
(1,1571)	1:352:A:LEU:HD12	1:380:A:LEU:HA	27	0.13
(1,1571)	1:352:A:LEU:HD13	1:380:A:LEU:HA	27	0.13
(1,1571)	1:352:A:LEU:HD21	1:380:A:LEU:HA	27	0.13
(1,1571)	1:352:A:LEU:HD22	1:380:A:LEU:HA	27	0.13
(1,1571)	1:352:A:LEU:HD23	1:380:A:LEU:HA	27	0.13
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	20	0.13
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	20	0.13
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	20	0.13
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	20	0.13
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	20	0.13
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	20	0.13
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	20	0.13
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	20	0.13
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	20	0.13
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	20	0.13
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	20	0.13
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	20	0.13
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	20	0.13
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	20	0.13
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	20	0.13
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	20	0.13
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	20	0.13
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	20	0.13
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	8	0.13
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	8	0.13
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	8	0.13
(1,1426)	1:495:A:GLU:H	1:496:A:GLN:H	20	0.13
(1,1287)	1:397:A:ILE:HD11	1:398:A:THR:H	27	0.13
(1,1287)	1:397:A:ILE:HD12	1:398:A:THR:H	27	0.13
(1,1287)	1:397:A:ILE:HD13	1:398:A:THR:H	27	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1287)	1:397:A:ILE:HD11	1:398:A:THR:H	28	0.13
(1,1287)	1:397:A:ILE:HD12	1:398:A:THR:H	28	0.13
(1,1287)	1:397:A:ILE:HD13	1:398:A:THR:H	28	0.13
(1,1023)	1:404:A:ARG:HA	1:405:A:ARG:HD2	5	0.13
(1,1023)	1:404:A:ARG:HA	1:405:A:ARG:HD3	5	0.13
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	22	0.13
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	22	0.13
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	22	0.13
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	22	0.13
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	22	0.13
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	22	0.13
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	22	0.13
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	22	0.13
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	22	0.13
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD1	11	0.13
(1,953)	1:427:A:PHE:HE1	1:482:A:PHE:HD2	11	0.13
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD1	11	0.13
(1,953)	1:427:A:PHE:HE2	1:482:A:PHE:HD2	11	0.13
(1,935)	1:363:A:LEU:HD11	1:406:A:PHE:HE1	3	0.13
(1,935)	1:363:A:LEU:HD11	1:406:A:PHE:HE2	3	0.13
(1,935)	1:363:A:LEU:HD12	1:406:A:PHE:HE1	3	0.13
(1,935)	1:363:A:LEU:HD12	1:406:A:PHE:HE2	3	0.13
(1,935)	1:363:A:LEU:HD13	1:406:A:PHE:HE1	3	0.13
(1,935)	1:363:A:LEU:HD13	1:406:A:PHE:HE2	3	0.13
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	21	0.13
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	21	0.13
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	21	0.13
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	21	0.13
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	21	0.13
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	21	0.13
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	21	0.13
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	21	0.13
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	21	0.13
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	29	0.13
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	29	0.13
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	29	0.13
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	29	0.13
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	29	0.13
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	29	0.13
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	29	0.13
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	29	0.13
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	29	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	5	0.13
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	5	0.13
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	5	0.13
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	5	0.13
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	5	0.13
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	5	0.13
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	5	0.13
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	5	0.13
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	5	0.13
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	5	0.13
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	5	0.13
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	5	0.13
(1,714)	1:365:A:ILE:H	1:365:A:ILE:HD11	20	0.13
(1,714)	1:365:A:ILE:H	1:365:A:ILE:HD12	20	0.13
(1,714)	1:365:A:ILE:H	1:365:A:ILE:HD13	20	0.13
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	2	0.13
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	2	0.13
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	2	0.13
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	4	0.13
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	4	0.13
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	4	0.13
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	12	0.13
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	12	0.13
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	12	0.13
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	12	0.13
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	12	0.13
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	12	0.13
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	12	0.13
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	12	0.13
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	12	0.13
(1,521)	1:387:A:MET:HE1	1:391:A:GLN:H	2	0.13
(1,521)	1:387:A:MET:HE2	1:391:A:GLN:H	2	0.13
(1,521)	1:387:A:MET:HE3	1:391:A:GLN:H	2	0.13
(1,521)	1:387:A:MET:HE1	1:391:A:GLN:H	40	0.13
(1,521)	1:387:A:MET:HE2	1:391:A:GLN:H	40	0.13
(1,521)	1:387:A:MET:HE3	1:391:A:GLN:H	40	0.13
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	22	0.13
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	22	0.13
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	22	0.13
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	22	0.13
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	22	0.13
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	22	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	22	0.13
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	22	0.13
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	22	0.13
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE1	33	0.13
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE2	33	0.13
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE3	33	0.13
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE1	33	0.13
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE2	33	0.13
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE3	33	0.13
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE1	33	0.13
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE2	33	0.13
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE3	33	0.13
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	7	0.13
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	7	0.13
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	7	0.13
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	7	0.13
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	7	0.13
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	7	0.13
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	7	0.13
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	7	0.13
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	7	0.13
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG11	20	0.13
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG12	20	0.13
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG13	20	0.13
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG11	20	0.13
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG12	20	0.13
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG13	20	0.13
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	15	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	15	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	15	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	15	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	15	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	15	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	15	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	15	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	15	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	15	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	15	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	15	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	22	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	22	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	22	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	22	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	22	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	22	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	22	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	22	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	22	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	22	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	22	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	30	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	30	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	30	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	30	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	30	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	30	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	30	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	30	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	30	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	30	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	30	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	30	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	32	0.12
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	32	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	32	0.12
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	32	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	32	0.12
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	32	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	32	0.12
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	32	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	32	0.12
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	32	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	32	0.12
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	32	0.12
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	36	0.12
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	36	0.12
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	36	0.12
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	36	0.12
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	36	0.12
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	36	0.12
(1,2128)	1:465:A:LEU:HD11	1:466:A:GLN:H	20	0.12
(1,2128)	1:465:A:LEU:HD12	1:466:A:GLN:H	20	0.12
(1,2128)	1:465:A:LEU:HD13	1:466:A:GLN:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2128)	1:465:A:LEU:HD21	1:466:A:GLN:H	20	0.12
(1,2128)	1:465:A:LEU:HD22	1:466:A:GLN:H	20	0.12
(1,2128)	1:465:A:LEU:HD23	1:466:A:GLN:H	20	0.12
(1,2110)	1:436:A:ILE:HG12	1:437:A:THR:HA	40	0.12
(1,2110)	1:436:A:ILE:HG13	1:437:A:THR:HA	40	0.12
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD11	27	0.12
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD12	27	0.12
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD13	27	0.12
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD21	27	0.12
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD22	27	0.12
(1,2094)	1:427:A:PHE:HD1	1:428:A:LEU:HD23	27	0.12
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD11	27	0.12
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD12	27	0.12
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD13	27	0.12
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD21	27	0.12
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD22	27	0.12
(1,2094)	1:427:A:PHE:HD2	1:428:A:LEU:HD23	27	0.12
(1,1996)	1:411:A:VAL:HA	1:414:A:GLU:HB2	40	0.12
(1,1996)	1:411:A:VAL:HA	1:414:A:GLU:HB3	40	0.12
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	5	0.12
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	5	0.12
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	5	0.12
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	5	0.12
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	5	0.12
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	5	0.12
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	19	0.12
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	19	0.12
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	19	0.12
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	19	0.12
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	19	0.12
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	19	0.12
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	36	0.12
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	36	0.12
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	36	0.12
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	36	0.12
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	36	0.12
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	36	0.12
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE2	3	0.12
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE3	3	0.12
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	37	0.12
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	37	0.12
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	37	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	37	0.12
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	37	0.12
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	37	0.12
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD11	27	0.12
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD12	27	0.12
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD13	27	0.12
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD21	27	0.12
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD22	27	0.12
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD23	27	0.12
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD11	27	0.12
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD12	27	0.12
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD13	27	0.12
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD21	27	0.12
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD22	27	0.12
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD23	27	0.12
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD11	27	0.12
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD12	27	0.12
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD13	27	0.12
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD21	27	0.12
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD22	27	0.12
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD23	27	0.12
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD11	27	0.12
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD12	27	0.12
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD13	27	0.12
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD21	27	0.12
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD22	27	0.12
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD23	27	0.12
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD11	27	0.12
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD12	27	0.12
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD13	27	0.12
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD21	27	0.12
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD22	27	0.12
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD23	27	0.12
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD11	27	0.12
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD12	27	0.12
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD13	27	0.12
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD21	27	0.12
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD22	27	0.12
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD23	27	0.12
(1,1534)	1:348:A:MET:HE1	1:351:A:ARG:H	9	0.12
(1,1534)	1:348:A:MET:HE2	1:351:A:ARG:H	9	0.12
(1,1534)	1:348:A:MET:HE3	1:351:A:ARG:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD21	21	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD22	21	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD23	21	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD21	23	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD22	23	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD23	23	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD21	40	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD22	40	0.12
(1,1533)	1:351:A:ARG:H	1:383:A:LEU:HD23	40	0.12
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	26	0.12
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	26	0.12
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	26	0.12
(1,1468)	1:466:A:GLN:HA	1:467:A:VAL:H	5	0.12
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	2	0.12
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	2	0.12
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	2	0.12
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	28	0.12
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	28	0.12
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	28	0.12
(1,1016)	1:364:A:LYS:HD2	1:365:A:ILE:H	40	0.12
(1,1016)	1:364:A:LYS:HD3	1:365:A:ILE:H	40	0.12
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	19	0.12
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	19	0.12
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	19	0.12
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	19	0.12
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	19	0.12
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	19	0.12
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	19	0.12
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	19	0.12
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	19	0.12
(1,935)	1:363:A:LEU:HD11	1:406:A:PHE:HE1	7	0.12
(1,935)	1:363:A:LEU:HD11	1:406:A:PHE:HE2	7	0.12
(1,935)	1:363:A:LEU:HD12	1:406:A:PHE:HE1	7	0.12
(1,935)	1:363:A:LEU:HD12	1:406:A:PHE:HE2	7	0.12
(1,935)	1:363:A:LEU:HD13	1:406:A:PHE:HE1	7	0.12
(1,935)	1:363:A:LEU:HD13	1:406:A:PHE:HE2	7	0.12
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	37	0.12
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	37	0.12
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	37	0.12
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	37	0.12
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	37	0.12
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	37	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	37	0.12
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	37	0.12
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	37	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	4	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	4	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	4	0.12
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	4	0.12
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	4	0.12
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	4	0.12
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	4	0.12
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	4	0.12
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	4	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	12	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	12	0.12
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	12	0.12
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	12	0.12
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	12	0.12
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	12	0.12
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	12	0.12
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	12	0.12
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	12	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	4	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	4	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	4	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	4	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	4	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	4	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG11	15	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG12	15	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG13	15	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG21	15	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG22	15	0.12
(1,878)	1:425:A:ASN:HA	1:429:A:VAL:HG23	15	0.12
(1,720)	1:365:A:ILE:HG21	1:366:A:ASP:HB3	3	0.12
(1,720)	1:365:A:ILE:HG22	1:366:A:ASP:HB3	3	0.12
(1,720)	1:365:A:ILE:HG23	1:366:A:ASP:HB3	3	0.12
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	3	0.12
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	3	0.12
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	3	0.12
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	3	0.12
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	3	0.12
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	3	0.12
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	3	0.12
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	3	0.12
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	11	0.12
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	11	0.12
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	11	0.12
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	11	0.12
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	11	0.12
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	11	0.12
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	11	0.12
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	11	0.12
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	11	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	13	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	13	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	13	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	13	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	13	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	13	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	13	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	13	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	13	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	36	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	36	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	36	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	36	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	36	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	36	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	36	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	36	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	36	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB1	40	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB2	40	0.12
(1,489)	1:385:A:VAL:HG21	1:390:A:ALA:HB3	40	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB1	40	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB2	40	0.12
(1,489)	1:385:A:VAL:HG22	1:390:A:ALA:HB3	40	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB1	40	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB2	40	0.12
(1,489)	1:385:A:VAL:HG23	1:390:A:ALA:HB3	40	0.12
(1,474)	1:394:A:THR:HG21	1:478:A:PHE:HB2	22	0.12
(1,474)	1:394:A:THR:HG21	1:478:A:PHE:HB3	22	0.12
(1,474)	1:394:A:THR:HG22	1:478:A:PHE:HB2	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:394:A:THR:HG22	1:478:A:PHE:HB3	22	0.12
(1,474)	1:394:A:THR:HG23	1:478:A:PHE:HB2	22	0.12
(1,474)	1:394:A:THR:HG23	1:478:A:PHE:HB3	22	0.12
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE1	21	0.12
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE2	21	0.12
(1,458)	1:352:A:LEU:HD21	1:396:A:MET:HE3	21	0.12
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE1	21	0.12
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE2	21	0.12
(1,458)	1:352:A:LEU:HD22	1:396:A:MET:HE3	21	0.12
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE1	21	0.12
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE2	21	0.12
(1,458)	1:352:A:LEU:HD23	1:396:A:MET:HE3	21	0.12
(1,97)	1:436:A:ILE:HD11	1:437:A:THR:HA	31	0.12
(1,97)	1:436:A:ILE:HD12	1:437:A:THR:HA	31	0.12
(1,97)	1:436:A:ILE:HD13	1:437:A:THR:HA	31	0.12
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB1	30	0.12
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB2	30	0.12
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB3	30	0.12
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB1	30	0.12
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB2	30	0.12
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB3	30	0.12
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB1	27	0.12
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB2	27	0.12
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB3	27	0.12
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB1	27	0.12
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB2	27	0.12
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB3	27	0.12
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE1	38	0.12
(1,46)	1:481:A:VAL:HG11	1:482:A:PHE:HE2	38	0.12
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE1	38	0.12
(1,46)	1:481:A:VAL:HG12	1:482:A:PHE:HE2	38	0.12
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE1	38	0.12
(1,46)	1:481:A:VAL:HG13	1:482:A:PHE:HE2	38	0.12
(1,2174)	1:497:A:PHE:HA	1:498:A:LEU:HD11	36	0.11
(1,2174)	1:497:A:PHE:HA	1:498:A:LEU:HD12	36	0.11
(1,2174)	1:497:A:PHE:HA	1:498:A:LEU:HD13	36	0.11
(1,2174)	1:497:A:PHE:HA	1:498:A:LEU:HD21	36	0.11
(1,2174)	1:497:A:PHE:HA	1:498:A:LEU:HD22	36	0.11
(1,2174)	1:497:A:PHE:HA	1:498:A:LEU:HD23	36	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	1	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	1	0.11
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	1	0.11
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	1	0.11
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	1	0.11
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	1	0.11
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	1	0.11
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	1	0.11
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	1	0.11
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	1	0.11
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	1	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	11	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	11	0.11
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	11	0.11
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	11	0.11
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	11	0.11
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	11	0.11
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	11	0.11
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	11	0.11
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	11	0.11
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	11	0.11
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	11	0.11
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	11	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	33	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	33	0.11
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	33	0.11
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	33	0.11
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	33	0.11
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	33	0.11
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	33	0.11
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	33	0.11
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	33	0.11
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	33	0.11
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	33	0.11
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	33	0.11
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA2	7	0.11
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA3	7	0.11
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA2	7	0.11
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA3	7	0.11
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA2	7	0.11
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA3	7	0.11
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	6	0.11
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	6	0.11
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	6	0.11
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	6	0.11
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	6	0.11
(1,2128)	1:465:A:LEU:HD11	1:466:A:GLN:H	29	0.11
(1,2128)	1:465:A:LEU:HD12	1:466:A:GLN:H	29	0.11
(1,2128)	1:465:A:LEU:HD13	1:466:A:GLN:H	29	0.11
(1,2128)	1:465:A:LEU:HD21	1:466:A:GLN:H	29	0.11
(1,2128)	1:465:A:LEU:HD22	1:466:A:GLN:H	29	0.11
(1,2128)	1:465:A:LEU:HD23	1:466:A:GLN:H	29	0.11
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD11	3	0.11
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD12	3	0.11
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD13	3	0.11
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD21	3	0.11
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD22	3	0.11
(1,2122)	1:464:A:ALA:HB1	1:465:A:LEU:HD23	3	0.11
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD11	3	0.11
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD12	3	0.11
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD13	3	0.11
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD21	3	0.11
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD22	3	0.11
(1,2122)	1:464:A:ALA:HB2	1:465:A:LEU:HD23	3	0.11
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD11	3	0.11
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD12	3	0.11
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD13	3	0.11
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD21	3	0.11
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD22	3	0.11
(1,2122)	1:464:A:ALA:HB3	1:465:A:LEU:HD23	3	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	5	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	5	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	5	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	5	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	5	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	5	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	5	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	5	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	5	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	5	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	5	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	5	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD11	39	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD12	39	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD13	39	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD21	39	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD22	39	0.11
(1,2096)	1:427:A:PHE:HE1	1:428:A:LEU:HD23	39	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD11	39	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD12	39	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD13	39	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD21	39	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD22	39	0.11
(1,2096)	1:427:A:PHE:HE2	1:428:A:LEU:HD23	39	0.11
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	7	0.11
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	7	0.11
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	7	0.11
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	7	0.11
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	7	0.11
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	7	0.11
(1,1975)	1:408:A:VAL:HG11	1:409:A:SER:H	3	0.11
(1,1975)	1:408:A:VAL:HG12	1:409:A:SER:H	3	0.11
(1,1975)	1:408:A:VAL:HG13	1:409:A:SER:H	3	0.11
(1,1975)	1:408:A:VAL:HG21	1:409:A:SER:H	3	0.11
(1,1975)	1:408:A:VAL:HG22	1:409:A:SER:H	3	0.11
(1,1975)	1:408:A:VAL:HG23	1:409:A:SER:H	3	0.11
(1,1975)	1:408:A:VAL:HG11	1:409:A:SER:H	5	0.11
(1,1975)	1:408:A:VAL:HG12	1:409:A:SER:H	5	0.11
(1,1975)	1:408:A:VAL:HG13	1:409:A:SER:H	5	0.11
(1,1975)	1:408:A:VAL:HG21	1:409:A:SER:H	5	0.11
(1,1975)	1:408:A:VAL:HG22	1:409:A:SER:H	5	0.11
(1,1975)	1:408:A:VAL:HG23	1:409:A:SER:H	5	0.11
(1,1975)	1:408:A:VAL:HG11	1:409:A:SER:H	29	0.11
(1,1975)	1:408:A:VAL:HG12	1:409:A:SER:H	29	0.11
(1,1975)	1:408:A:VAL:HG13	1:409:A:SER:H	29	0.11
(1,1975)	1:408:A:VAL:HG21	1:409:A:SER:H	29	0.11
(1,1975)	1:408:A:VAL:HG22	1:409:A:SER:H	29	0.11
(1,1975)	1:408:A:VAL:HG23	1:409:A:SER:H	29	0.11
(1,1975)	1:408:A:VAL:HG11	1:409:A:SER:H	40	0.11
(1,1975)	1:408:A:VAL:HG12	1:409:A:SER:H	40	0.11
(1,1975)	1:408:A:VAL:HG13	1:409:A:SER:H	40	0.11
(1,1975)	1:408:A:VAL:HG21	1:409:A:SER:H	40	0.11
(1,1975)	1:408:A:VAL:HG22	1:409:A:SER:H	40	0.11
(1,1975)	1:408:A:VAL:HG23	1:409:A:SER:H	40	0.11
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE1	27	0.11
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE2	27	0.11
(1,1968)	1:407:A:LYS:HG2	1:413:A:MET:HE3	27	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE1	27	0.11
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE2	27	0.11
(1,1968)	1:407:A:LYS:HG3	1:413:A:MET:HE3	27	0.11
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE2	2	0.11
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE3	2	0.11
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	11	0.11
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	11	0.11
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	11	0.11
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	11	0.11
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	11	0.11
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	11	0.11
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	11	0.11
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	11	0.11
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	11	0.11
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	11	0.11
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	11	0.11
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	11	0.11
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	23	0.11
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	23	0.11
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	23	0.11
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	23	0.11
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	23	0.11
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	23	0.11
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	23	0.11
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	23	0.11
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	23	0.11
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	23	0.11
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	23	0.11
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	23	0.11
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	1	0.11
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	1	0.11
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	1	0.11
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	1	0.11
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	1	0.11
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	1	0.11
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	8	0.11
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	8	0.11
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	8	0.11
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	8	0.11
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	8	0.11
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	8	0.11
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	34	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	34	0.11
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	34	0.11
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	34	0.11
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	34	0.11
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	34	0.11
(1,1682)	1:365:A:ILE:HD11	1:501:A:GLY:HA2	28	0.11
(1,1682)	1:365:A:ILE:HD11	1:501:A:GLY:HA3	28	0.11
(1,1682)	1:365:A:ILE:HD12	1:501:A:GLY:HA2	28	0.11
(1,1682)	1:365:A:ILE:HD12	1:501:A:GLY:HA3	28	0.11
(1,1682)	1:365:A:ILE:HD13	1:501:A:GLY:HA2	28	0.11
(1,1682)	1:365:A:ILE:HD13	1:501:A:GLY:HA3	28	0.11
(1,1682)	1:365:A:ILE:HD11	1:501:A:GLY:HA2	40	0.11
(1,1682)	1:365:A:ILE:HD11	1:501:A:GLY:HA3	40	0.11
(1,1682)	1:365:A:ILE:HD12	1:501:A:GLY:HA2	40	0.11
(1,1682)	1:365:A:ILE:HD12	1:501:A:GLY:HA3	40	0.11
(1,1682)	1:365:A:ILE:HD13	1:501:A:GLY:HA2	40	0.11
(1,1682)	1:365:A:ILE:HD13	1:501:A:GLY:HA3	40	0.11
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG21	17	0.11
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG22	17	0.11
(1,1637)	1:360:A:LYS:HD2	1:399:A:THR:HG23	17	0.11
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG21	17	0.11
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG22	17	0.11
(1,1637)	1:360:A:LYS:HD3	1:399:A:THR:HG23	17	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD11	38	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD12	38	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD13	38	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD21	38	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD22	38	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD23	38	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD11	38	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD12	38	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD13	38	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD21	38	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD22	38	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD23	38	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD11	38	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD12	38	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD13	38	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD21	38	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD22	38	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD23	38	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD11	38	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD12	38	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD13	38	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD21	38	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD22	38	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD23	38	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD11	38	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD12	38	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD13	38	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD21	38	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD22	38	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD23	38	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD11	38	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD12	38	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD13	38	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD21	38	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD22	38	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD23	38	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD11	40	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD12	40	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD13	40	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD21	40	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD22	40	0.11
(1,1572)	1:352:A:LEU:HD11	1:380:A:LEU:HD23	40	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD11	40	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD12	40	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD13	40	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD21	40	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD22	40	0.11
(1,1572)	1:352:A:LEU:HD12	1:380:A:LEU:HD23	40	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD11	40	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD12	40	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD13	40	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD21	40	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD22	40	0.11
(1,1572)	1:352:A:LEU:HD13	1:380:A:LEU:HD23	40	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD11	40	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD12	40	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD13	40	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD21	40	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD22	40	0.11
(1,1572)	1:352:A:LEU:HD21	1:380:A:LEU:HD23	40	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD11	40	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD12	40	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD13	40	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD21	40	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD22	40	0.11
(1,1572)	1:352:A:LEU:HD22	1:380:A:LEU:HD23	40	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD11	40	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD12	40	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD13	40	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD21	40	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD22	40	0.11
(1,1572)	1:352:A:LEU:HD23	1:380:A:LEU:HD23	40	0.11
(1,1475)	1:470:A:ALA:HB1	1:471:A:ILE:H	32	0.11
(1,1475)	1:470:A:ALA:HB2	1:471:A:ILE:H	32	0.11
(1,1475)	1:470:A:ALA:HB3	1:471:A:ILE:H	32	0.11
(1,1287)	1:397:A:ILE:HD11	1:398:A:THR:H	20	0.11
(1,1287)	1:397:A:ILE:HD12	1:398:A:THR:H	20	0.11
(1,1287)	1:397:A:ILE:HD13	1:398:A:THR:H	20	0.11
(1,1150)	1:368:A:LEU:HD11	1:369:A:ASP:H	31	0.11
(1,1150)	1:368:A:LEU:HD12	1:369:A:ASP:H	31	0.11
(1,1150)	1:368:A:LEU:HD13	1:369:A:ASP:H	31	0.11
(1,1115)	1:344:A:TRP:HB2	1:345:A:GLU:H	26	0.11
(1,1115)	1:344:A:TRP:HB3	1:345:A:GLU:H	26	0.11
(1,1047)	1:506:A:VAL:H	1:507:A:ARG:H	13	0.11
(1,1012)	1:475:A:LEU:HD11	1:476:A:ARG:HD2	19	0.11
(1,1012)	1:475:A:LEU:HD11	1:476:A:ARG:HD3	19	0.11
(1,1012)	1:475:A:LEU:HD12	1:476:A:ARG:HD2	19	0.11
(1,1012)	1:475:A:LEU:HD12	1:476:A:ARG:HD3	19	0.11
(1,1012)	1:475:A:LEU:HD13	1:476:A:ARG:HD2	19	0.11
(1,1012)	1:475:A:LEU:HD13	1:476:A:ARG:HD3	19	0.11
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	1	0.11
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	1	0.11
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	1	0.11
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	1	0.11
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	1	0.11
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	1	0.11
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	1	0.11
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	1	0.11
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	1	0.11
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	13	0.11
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	13	0.11
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	13	0.11
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	13	0.11
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	13	0.11
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	13	0.11
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	13	0.11
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	13	0.11
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	10	0.11
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	10	0.11
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	10	0.11
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	10	0.11
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	10	0.11
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	10	0.11
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	10	0.11
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	10	0.11
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	10	0.11
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE1	17	0.11
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE2	17	0.11
(1,895)	1:385:A:VAL:HG21	1:426:A:MET:HE3	17	0.11
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE1	17	0.11
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE2	17	0.11
(1,895)	1:385:A:VAL:HG22	1:426:A:MET:HE3	17	0.11
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE1	17	0.11
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE2	17	0.11
(1,895)	1:385:A:VAL:HG23	1:426:A:MET:HE3	17	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	11	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	11	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	11	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	11	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	11	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	11	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	11	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	11	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	11	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	36	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	36	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	36	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	36	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	36	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	36	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	36	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	36	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	36	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	40	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	40	0.11
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	40	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	40	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	40	0.11
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	40	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	40	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	40	0.11
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	40	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE1	7	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE2	7	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE3	7	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE1	7	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE2	7	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE3	7	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE1	27	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE2	27	0.11
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE3	27	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE1	27	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE2	27	0.11
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE3	27	0.11
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG11	6	0.11
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG12	6	0.11
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG13	6	0.11
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG21	6	0.11
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG22	6	0.11
(1,876)	1:466:A:GLN:HG2	1:467:A:VAL:HG23	6	0.11
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG11	6	0.11
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG12	6	0.11
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG13	6	0.11
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG21	6	0.11
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG22	6	0.11
(1,876)	1:466:A:GLN:HG3	1:467:A:VAL:HG23	6	0.11
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG21	33	0.11
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG22	33	0.11
(1,748)	1:363:A:LEU:HD21	1:403:A:ILE:HG23	33	0.11
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG21	33	0.11
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG22	33	0.11
(1,748)	1:363:A:LEU:HD22	1:403:A:ILE:HG23	33	0.11
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG21	33	0.11
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG22	33	0.11
(1,748)	1:363:A:LEU:HD23	1:403:A:ILE:HG23	33	0.11
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	9	0.11
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	9	0.11
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	3	0.11
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	3	0.11
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	3	0.11
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	23	0.11
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	23	0.11
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	23	0.11
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	29	0.11
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	29	0.11
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	29	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	4	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	4	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	4	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	4	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	4	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	4	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	4	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	4	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	4	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	22	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	22	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	22	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	22	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	22	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	22	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	22	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	22	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	22	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	27	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	27	0.11
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	27	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	27	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	27	0.11
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	27	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	27	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	27	0.11
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	27	0.11
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	17	0.11
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	17	0.11
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	17	0.11
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	17	0.11
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	17	0.11
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	17	0.11
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	17	0.11
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	17	0.11
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD21	23	0.11
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD22	23	0.11
(1,547)	1:355:A:ILE:HG21	1:383:A:LEU:HD23	23	0.11
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD21	23	0.11
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD22	23	0.11
(1,547)	1:355:A:ILE:HG22	1:383:A:LEU:HD23	23	0.11
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD21	23	0.11
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD22	23	0.11
(1,547)	1:355:A:ILE:HG23	1:383:A:LEU:HD23	23	0.11
(1,522)	1:387:A:MET:HE1	1:427:A:PHE:H	3	0.11
(1,522)	1:387:A:MET:HE2	1:427:A:PHE:H	3	0.11
(1,522)	1:387:A:MET:HE3	1:427:A:PHE:H	3	0.11
(1,521)	1:387:A:MET:HE1	1:391:A:GLN:H	28	0.11
(1,521)	1:387:A:MET:HE2	1:391:A:GLN:H	28	0.11
(1,521)	1:387:A:MET:HE3	1:391:A:GLN:H	28	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	20	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	20	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	20	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	20	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	20	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	20	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	20	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	20	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	20	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	29	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	29	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	29	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	29	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	29	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	29	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	29	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	29	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	29	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	34	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	34	0.11
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	34	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	34	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	34	0.11
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	34	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	34	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	34	0.11
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	34	0.11
(1,389)	1:398:A:THR:HG21	1:481:A:VAL:HB	5	0.11
(1,389)	1:398:A:THR:HG22	1:481:A:VAL:HB	5	0.11
(1,389)	1:398:A:THR:HG23	1:481:A:VAL:HB	5	0.11
(1,389)	1:398:A:THR:HG21	1:481:A:VAL:HB	6	0.11
(1,389)	1:398:A:THR:HG22	1:481:A:VAL:HB	6	0.11
(1,389)	1:398:A:THR:HG23	1:481:A:VAL:HB	6	0.11
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG11	4	0.11
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG12	4	0.11
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG13	4	0.11
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG11	4	0.11
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG12	4	0.11
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG13	4	0.11
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG11	19	0.11
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG12	19	0.11
(1,320)	1:406:A:PHE:HD1	1:408:A:VAL:HG13	19	0.11
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG11	19	0.11
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG12	19	0.11
(1,320)	1:406:A:PHE:HD2	1:408:A:VAL:HG13	19	0.11
(1,97)	1:436:A:ILE:HD11	1:437:A:THR:HA	40	0.11
(1,97)	1:436:A:ILE:HD12	1:437:A:THR:HA	40	0.11
(1,97)	1:436:A:ILE:HD13	1:437:A:THR:HA	40	0.11
(1,93)	1:470:A:ALA:HA	1:471:A:ILE:HG21	19	0.11
(1,93)	1:470:A:ALA:HA	1:471:A:ILE:HG22	19	0.11
(1,93)	1:470:A:ALA:HA	1:471:A:ILE:HG23	19	0.11
(1,79)	1:475:A:LEU:HD11	1:478:A:PHE:HB2	35	0.11
(1,79)	1:475:A:LEU:HD11	1:478:A:PHE:HB3	35	0.11
(1,79)	1:475:A:LEU:HD12	1:478:A:PHE:HB2	35	0.11
(1,79)	1:475:A:LEU:HD12	1:478:A:PHE:HB3	35	0.11
(1,79)	1:475:A:LEU:HD13	1:478:A:PHE:HB2	35	0.11
(1,79)	1:475:A:LEU:HD13	1:478:A:PHE:HB3	35	0.11
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB1	16	0.11
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB2	16	0.11
(1,56)	1:477:A:ARG:HD2	1:480:A:ALA:HB3	16	0.11
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB1	16	0.11
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB2	16	0.11
(1,56)	1:477:A:ARG:HD3	1:480:A:ALA:HB3	16	0.11
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB1	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB2	19	0.11
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB3	19	0.11
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB1	19	0.11
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB2	19	0.11
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB3	19	0.11
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	27	0.1
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	27	0.1
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	27	0.1
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	27	0.1
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	27	0.1
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	27	0.1
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	27	0.1
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	27	0.1
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	27	0.1
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	27	0.1
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	27	0.1
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	27	0.1
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB2	38	0.1
(1,2142)	1:475:A:LEU:HD11	1:476:A:ARG:HB3	38	0.1
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB2	38	0.1
(1,2142)	1:475:A:LEU:HD12	1:476:A:ARG:HB3	38	0.1
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB2	38	0.1
(1,2142)	1:475:A:LEU:HD13	1:476:A:ARG:HB3	38	0.1
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB2	38	0.1
(1,2142)	1:475:A:LEU:HD21	1:476:A:ARG:HB3	38	0.1
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB2	38	0.1
(1,2142)	1:475:A:LEU:HD22	1:476:A:ARG:HB3	38	0.1
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB2	38	0.1
(1,2142)	1:475:A:LEU:HD23	1:476:A:ARG:HB3	38	0.1
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA2	33	0.1
(1,2136)	1:471:A:ILE:HD11	1:472:A:GLY:HA3	33	0.1
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA2	33	0.1
(1,2136)	1:471:A:ILE:HD12	1:472:A:GLY:HA3	33	0.1
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA2	33	0.1
(1,2136)	1:471:A:ILE:HD13	1:472:A:GLY:HA3	33	0.1
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD11	39	0.1
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD12	39	0.1
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD13	39	0.1
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD21	39	0.1
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD22	39	0.1
(1,2132)	1:470:A:ALA:HA	1:475:A:LEU:HD23	39	0.1
(1,2051)	1:419:A:LEU:HD11	1:422:A:LYS:HE2	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:419:A:LEU:HD11	1:422:A:LYS:HE3	18	0.1
(1,2051)	1:419:A:LEU:HD12	1:422:A:LYS:HE2	18	0.1
(1,2051)	1:419:A:LEU:HD12	1:422:A:LYS:HE3	18	0.1
(1,2051)	1:419:A:LEU:HD13	1:422:A:LYS:HE2	18	0.1
(1,2051)	1:419:A:LEU:HD13	1:422:A:LYS:HE3	18	0.1
(1,2051)	1:419:A:LEU:HD21	1:422:A:LYS:HE2	18	0.1
(1,2051)	1:419:A:LEU:HD21	1:422:A:LYS:HE3	18	0.1
(1,2051)	1:419:A:LEU:HD22	1:422:A:LYS:HE2	18	0.1
(1,2051)	1:419:A:LEU:HD22	1:422:A:LYS:HE3	18	0.1
(1,2051)	1:419:A:LEU:HD23	1:422:A:LYS:HE2	18	0.1
(1,2051)	1:419:A:LEU:HD23	1:422:A:LYS:HE3	18	0.1
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	10	0.1
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	10	0.1
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	10	0.1
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	10	0.1
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	10	0.1
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	10	0.1
(1,1981)	1:408:A:VAL:HG11	1:498:A:LEU:HG	15	0.1
(1,1981)	1:408:A:VAL:HG12	1:498:A:LEU:HG	15	0.1
(1,1981)	1:408:A:VAL:HG13	1:498:A:LEU:HG	15	0.1
(1,1981)	1:408:A:VAL:HG21	1:498:A:LEU:HG	15	0.1
(1,1981)	1:408:A:VAL:HG22	1:498:A:LEU:HG	15	0.1
(1,1981)	1:408:A:VAL:HG23	1:498:A:LEU:HG	15	0.1
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE2	19	0.1
(1,1891)	1:398:A:THR:HA	1:402:A:LYS:HE3	19	0.1
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	6	0.1
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	6	0.1
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	6	0.1
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	6	0.1
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	6	0.1
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	6	0.1
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	6	0.1
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	6	0.1
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	6	0.1
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	6	0.1
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	6	0.1
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	6	0.1
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	13	0.1
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	13	0.1
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	13	0.1
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	13	0.1
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	13	0.1
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	13	0.1
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	13	0.1
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	13	0.1
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	13	0.1
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	13	0.1
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	13	0.1
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE21	35	0.1
(1,1827)	1:385:A:VAL:HG11	1:389:A:GLN:HE22	35	0.1
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE21	35	0.1
(1,1827)	1:385:A:VAL:HG12	1:389:A:GLN:HE22	35	0.1
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE21	35	0.1
(1,1827)	1:385:A:VAL:HG13	1:389:A:GLN:HE22	35	0.1
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE21	35	0.1
(1,1827)	1:385:A:VAL:HG21	1:389:A:GLN:HE22	35	0.1
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE21	35	0.1
(1,1827)	1:385:A:VAL:HG22	1:389:A:GLN:HE22	35	0.1
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE21	35	0.1
(1,1827)	1:385:A:VAL:HG23	1:389:A:GLN:HE22	35	0.1
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	11	0.1
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	11	0.1
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	11	0.1
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	11	0.1
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	11	0.1
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	11	0.1
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	24	0.1
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	24	0.1
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	24	0.1
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	24	0.1
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	24	0.1
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	24	0.1
(1,1701)	1:370:A:VAL:HG11	1:374:A:ILE:HG12	30	0.1
(1,1701)	1:370:A:VAL:HG12	1:374:A:ILE:HG12	30	0.1
(1,1701)	1:370:A:VAL:HG13	1:374:A:ILE:HG12	30	0.1
(1,1701)	1:370:A:VAL:HG21	1:374:A:ILE:HG12	30	0.1
(1,1701)	1:370:A:VAL:HG22	1:374:A:ILE:HG12	30	0.1
(1,1701)	1:370:A:VAL:HG23	1:374:A:ILE:HG12	30	0.1
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	38	0.1
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	38	0.1
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	38	0.1
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	38	0.1
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	38	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	38	0.1
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	38	0.1
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	38	0.1
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	38	0.1
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	38	0.1
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	38	0.1
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	38	0.1
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	38	0.1
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	38	0.1
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	38	0.1
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	38	0.1
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	38	0.1
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	38	0.1
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG21	40	0.1
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG22	40	0.1
(1,1569)	1:352:A:LEU:HD11	1:355:A:ILE:HG23	40	0.1
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG21	40	0.1
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG22	40	0.1
(1,1569)	1:352:A:LEU:HD12	1:355:A:ILE:HG23	40	0.1
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG21	40	0.1
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG22	40	0.1
(1,1569)	1:352:A:LEU:HD13	1:355:A:ILE:HG23	40	0.1
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG21	40	0.1
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG22	40	0.1
(1,1569)	1:352:A:LEU:HD21	1:355:A:ILE:HG23	40	0.1
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG21	40	0.1
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG22	40	0.1
(1,1569)	1:352:A:LEU:HD22	1:355:A:ILE:HG23	40	0.1
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG21	40	0.1
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG22	40	0.1
(1,1569)	1:352:A:LEU:HD23	1:355:A:ILE:HG23	40	0.1
(1,1458)	1:464:A:ALA:HA	1:465:A:LEU:H	15	0.1
(1,1065)	1:350:A:SER:H	1:351:A:ARG:HB2	23	0.1
(1,1065)	1:350:A:SER:H	1:351:A:ARG:HB3	23	0.1
(1,1048)	1:505:A:GLU:HA	1:506:A:VAL:H	2	0.1
(1,1047)	1:506:A:VAL:H	1:507:A:ARG:H	5	0.1
(1,1019)	1:387:A:MET:HE1	1:391:A:GLN:HG3	17	0.1
(1,1019)	1:387:A:MET:HE2	1:391:A:GLN:HG3	17	0.1
(1,1019)	1:387:A:MET:HE3	1:391:A:GLN:HG3	17	0.1
(1,1016)	1:364:A:LYS:HD2	1:365:A:ILE:H	3	0.1
(1,1016)	1:364:A:LYS:HD3	1:365:A:ILE:H	3	0.1
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG11	21	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG12	21	0.1
(1,1004)	1:398:A:THR:HG21	1:481:A:VAL:HG13	21	0.1
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG11	21	0.1
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG12	21	0.1
(1,1004)	1:398:A:THR:HG22	1:481:A:VAL:HG13	21	0.1
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG11	21	0.1
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG12	21	0.1
(1,1004)	1:398:A:THR:HG23	1:481:A:VAL:HG13	21	0.1
(1,924)	1:475:A:LEU:HD11	1:476:A:ARG:H	2	0.1
(1,924)	1:475:A:LEU:HD12	1:476:A:ARG:H	2	0.1
(1,924)	1:475:A:LEU:HD13	1:476:A:ARG:H	2	0.1
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE1	21	0.1
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE2	21	0.1
(1,893)	1:386:A:THR:HG21	1:426:A:MET:HE3	21	0.1
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE1	21	0.1
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE2	21	0.1
(1,893)	1:386:A:THR:HG22	1:426:A:MET:HE3	21	0.1
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE1	21	0.1
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE2	21	0.1
(1,893)	1:386:A:THR:HG23	1:426:A:MET:HE3	21	0.1
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE1	22	0.1
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE2	22	0.1
(1,889)	1:422:A:LYS:HE2	1:426:A:MET:HE3	22	0.1
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE1	22	0.1
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE2	22	0.1
(1,889)	1:422:A:LYS:HE3	1:426:A:MET:HE3	22	0.1
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	11	0.1
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	11	0.1
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	11	0.1
(1,726)	1:365:A:ILE:HG21	1:500:A:PHE:H	22	0.1
(1,726)	1:365:A:ILE:HG22	1:500:A:PHE:H	22	0.1
(1,726)	1:365:A:ILE:HG23	1:500:A:PHE:H	22	0.1
(1,691)	1:368:A:LEU:HD11	1:498:A:LEU:HA	19	0.1
(1,691)	1:368:A:LEU:HD12	1:498:A:LEU:HA	19	0.1
(1,691)	1:368:A:LEU:HD13	1:498:A:LEU:HA	19	0.1
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD21	16	0.1
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD22	16	0.1
(1,626)	1:359:A:ILE:HG21	1:363:A:LEU:HD23	16	0.1
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD21	16	0.1
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD22	16	0.1
(1,626)	1:359:A:ILE:HG22	1:363:A:LEU:HD23	16	0.1
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD21	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD22	16	0.1
(1,626)	1:359:A:ILE:HG23	1:363:A:LEU:HD23	16	0.1
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG21	23	0.1
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG22	23	0.1
(1,410)	1:397:A:ILE:HG21	1:398:A:THR:HG23	23	0.1
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG21	23	0.1
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG22	23	0.1
(1,410)	1:397:A:ILE:HG22	1:398:A:THR:HG23	23	0.1
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG21	23	0.1
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG22	23	0.1
(1,410)	1:397:A:ILE:HG23	1:398:A:THR:HG23	23	0.1
(1,389)	1:398:A:THR:HG21	1:481:A:VAL:HB	12	0.1
(1,389)	1:398:A:THR:HG22	1:481:A:VAL:HB	12	0.1
(1,389)	1:398:A:THR:HG23	1:481:A:VAL:HB	12	0.1
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB1	3	0.1
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB2	3	0.1
(1,55)	1:478:A:PHE:HB2	1:480:A:ALA:HB3	3	0.1
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB1	3	0.1
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB2	3	0.1
(1,55)	1:478:A:PHE:HB3	1:480:A:ALA:HB3	3	0.1

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

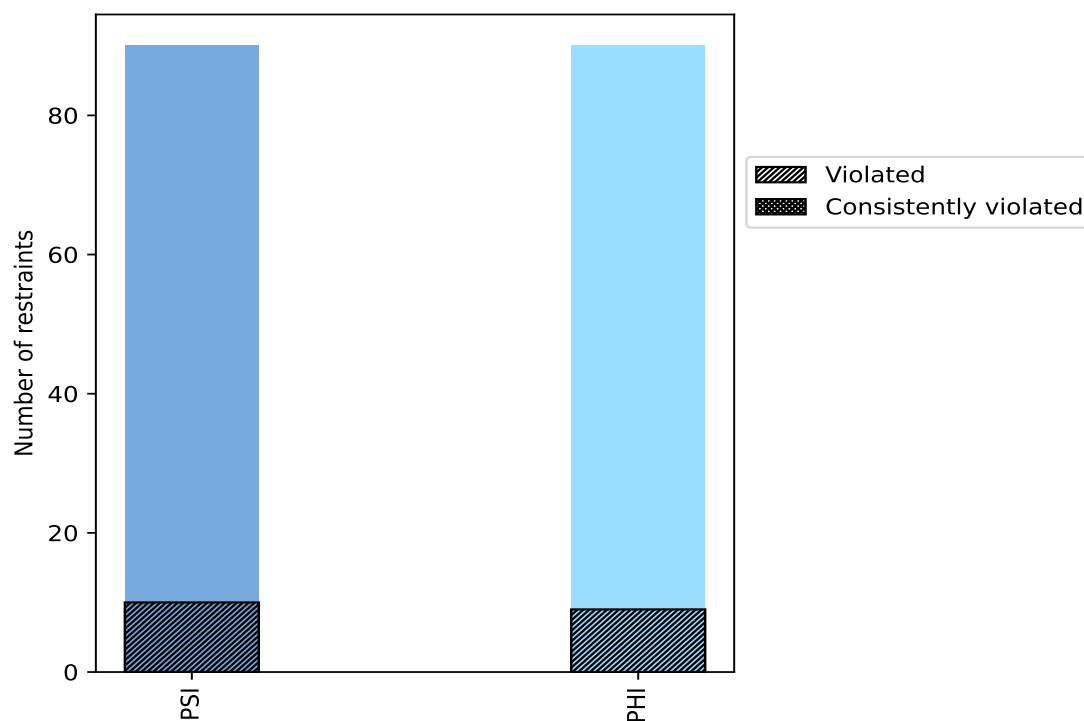
### 10.1 Summary of dihedral-angle violations [i](#)

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	90	50.0	10	11.1	5.6	0	0.0	0.0
PHI	90	50.0	9	10.0	5.0	0	0.0	0.0
Total	180	100.0	19	10.6	10.6	0	0.0	0.0

<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 [i](#)

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.

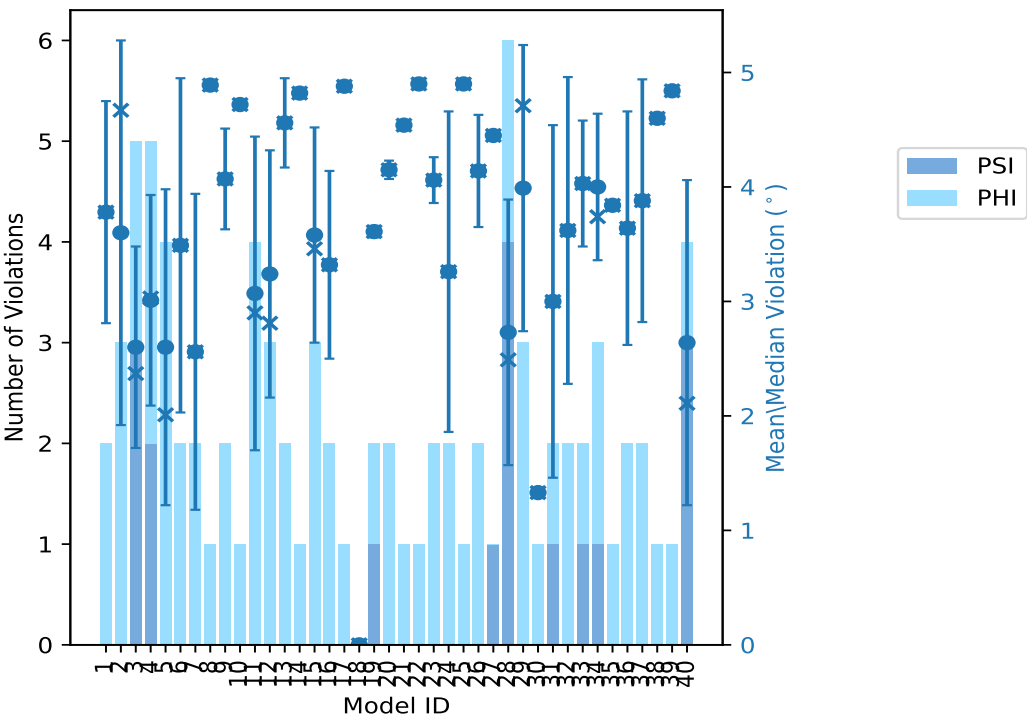
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	2	2	3.78	4.75	0.97	3.78
2	0	3	3	3.6	4.89	1.68	4.67
3	3	2	5	2.6	4.04	0.88	2.37
4	2	3	5	3.01	4.18	0.92	3.03
5	0	4	4	2.6	4.91	1.38	2.01
6	0	2	2	3.49	4.94	1.46	3.49
7	0	2	2	2.56	3.94	1.38	2.56
8	0	1	1	4.89	4.89	0.0	4.89
9	0	2	2	4.07	4.51	0.44	4.07
10	0	1	1	4.72	4.72	0.0	4.72
11	0	4	4	3.07	5.01	1.37	2.9
12	0	3	3	3.24	4.72	1.08	2.81
13	0	2	2	4.56	4.95	0.39	4.56
14	0	1	1	4.82	4.82	0.0	4.82
15	0	3	3	3.58	4.78	0.94	3.46
16	0	2	2	3.32	4.13	0.82	3.32
17	0	1	1	4.88	4.88	0.0	4.88
18	0	0	0	0.0	0.0	0.0	0.0
19	1	1	2	3.61	3.66	0.05	3.61
20	0	2	2	4.15	4.23	0.08	4.15
21	0	1	1	4.54	4.54	0.0	4.54
22	0	1	1	4.9	4.9	0.0	4.9
23	0	2	2	4.06	4.26	0.2	4.06
24	0	2	2	3.26	4.67	1.4	3.26
25	0	1	1	4.9	4.9	0.0	4.9
26	0	2	2	4.14	4.63	0.49	4.14
27	1	0	1	4.45	4.45	0.0	4.45
28	4	2	6	2.73	4.91	1.16	2.49
29	0	3	3	3.99	5.02	1.25	4.71
30	0	1	1	1.33	1.33	0.0	1.33
31	1	1	2	3.0	4.53	1.54	3.0
32	0	2	2	3.62	4.95	1.34	3.62
33	1	1	2	4.03	4.58	0.55	4.03
34	1	2	3	4.0	4.88	0.64	3.74
35	0	1	1	3.84	3.84	0.0	3.84
36	0	2	2	3.64	4.67	1.02	3.64
37	0	2	2	3.88	4.93	1.06	3.88
38	0	1	1	4.6	4.6	0.0	4.6

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	0	1	1	4.84	4.84	0.0	4.84
40	3	1	4	2.64	4.97	1.42	2.11

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 ⓘ

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>	%
5	2	7	1	2.5
4	3	7	2	5.0
0	0	0	3	7.5
1	0	1	4	10.0

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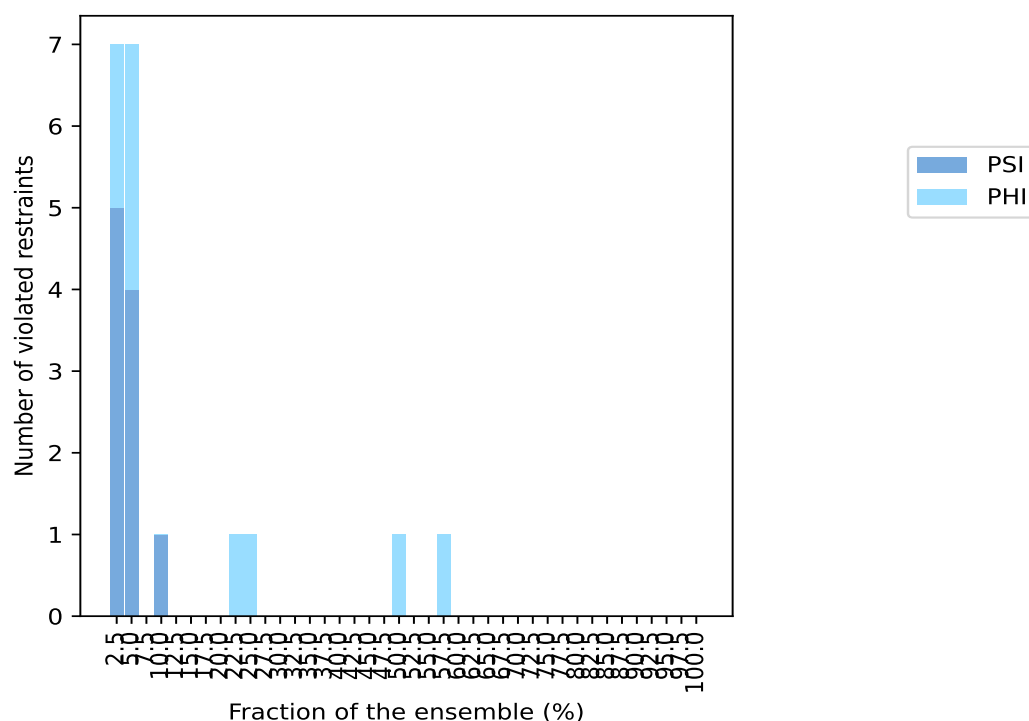


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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	5	12.5
0	0	0	6	15.0
0	0	0	7	17.5
0	0	0	8	20.0
0	1	1	9	22.5
0	1	1	10	25.0
0	0	0	11	27.5
0	0	0	12	30.0
0	0	0	13	32.5
0	0	0	14	35.0
0	0	0	15	37.5
0	0	0	16	40.0
0	0	0	17	42.5
0	0	0	18	45.0
0	0	0	19	47.5
0	1	1	20	50.0
0	0	0	21	52.5
0	0	0	22	55.0
0	1	1	23	57.5
0	0	0	24	60.0
0	0	0	25	62.5
0	0	0	26	65.0
0	0	0	27	67.5
0	0	0	28	70.0
0	0	0	29	72.5
0	0	0	30	75.0
0	0	0	31	77.5
0	0	0	32	80.0
0	0	0	33	82.5
0	0	0	34	85.0
0	0	0	35	87.5
0	0	0	36	90.0
0	0	0	37	92.5
0	0	0	38	95.0
0	0	0	39	97.5
0	0	0	40	100.0

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

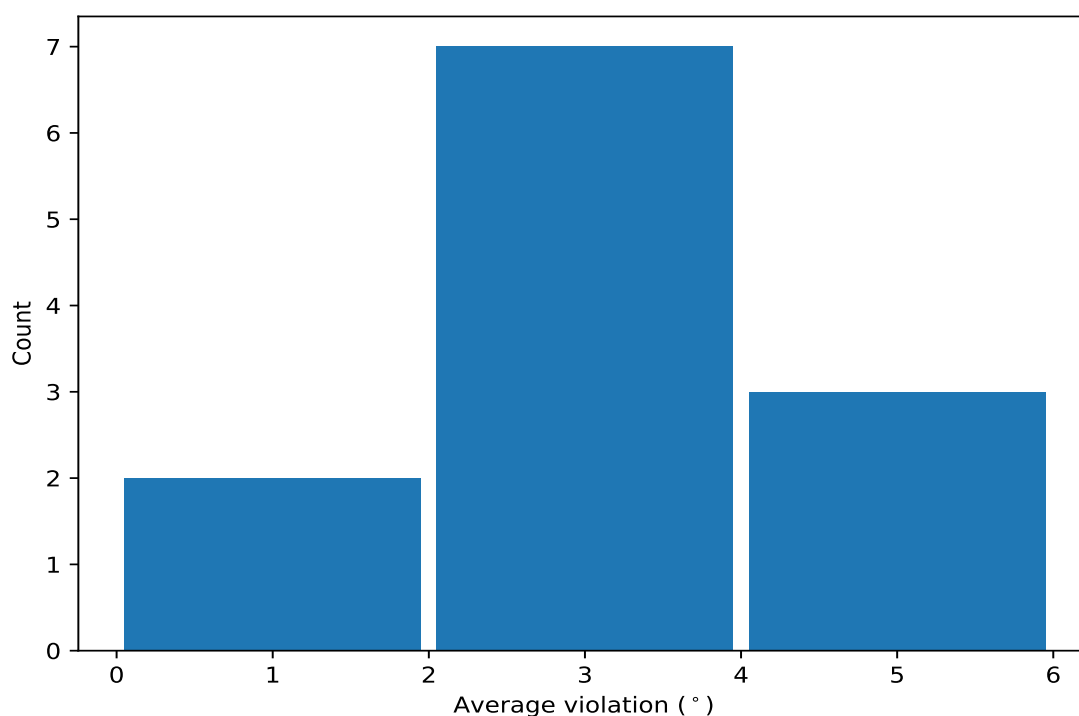
### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

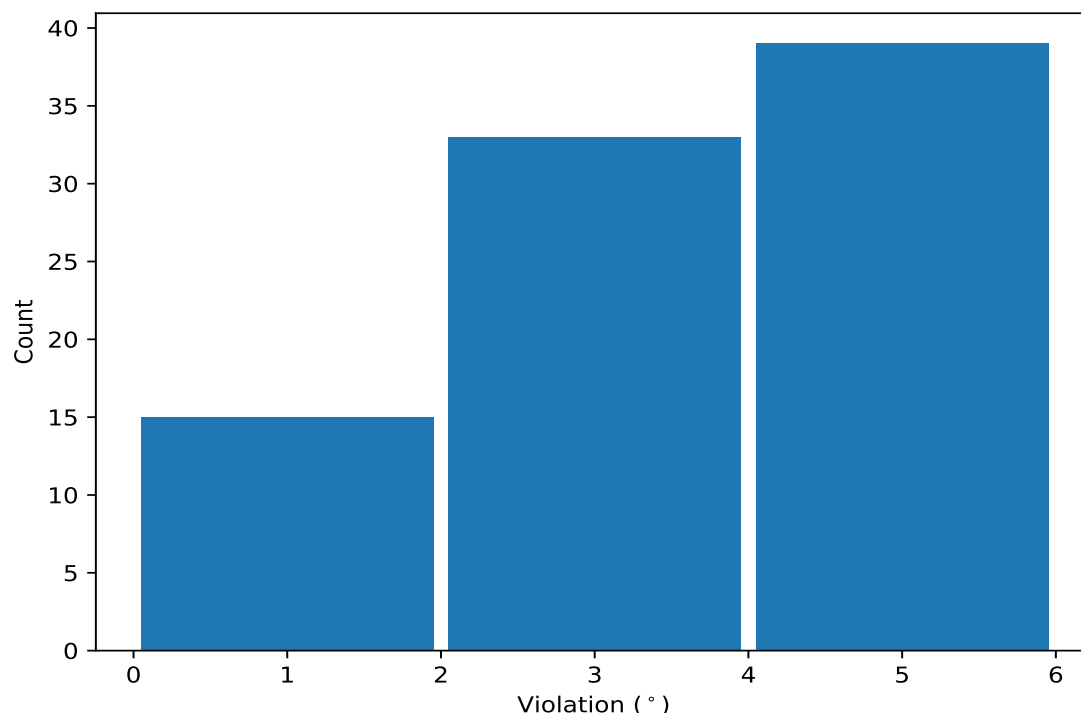
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	23	4.08	0.86	4.51
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	20	3.14	1.24	2.66
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	10	3.8	1.1	3.86
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	9	3.82	1.34	4.53
(1,38)	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	1:364:A:LYS:N	4	4.1	0.75	4.24
(1,13)	1:350:A:SER:C	1:351:A:ARG:N	1:351:A:ARG:CA	1:351:A:ARG:C	2	4.78	0.24	4.78
(1,173)	1:478:A:PHE:C	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	2	3.84	0.87	3.84
(1,174)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:ALA:N	2	3.18	1.72	3.18
(1,180)	1:482:A:PHE:N	1:482:A:PHE:CA	1:482:A:PHE:C	1:483:A:GLY:N	2	3.09	1.09	3.09
(1,164)	1:474:A:ASN:N	1:474:A:ASN:CA	1:474:A:ASN:C	1:475:A:LEU:N	2	2.92	0.55	2.92
(1,151)	1:424:A:LYS:C	1:425:A:ASN:N	1:425:A:ASN:CA	1:425:A:ASN:C	2	1.74	0.28	1.74
(1,92)	1:394:A:THR:N	1:394:A:THR:CA	1:394:A:THR:C	1:395:A:GLU:N	2	1.6	0.04	1.6

<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 (°)
(1,13)	1:350:A:SER:C	1:351:A:ARG:N	1:351:A:ARG:CA	1:351:A:ARG:C	29	5.02
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	11	5.01
(1,38)	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	1:364:A:LYS:N	40	4.97
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	13	4.95
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	32	4.95
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	6	4.94
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	37	4.93
(1,174)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:ALA:N	28	4.91
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	5	4.91
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	22	4.9
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	25	4.9
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	2	4.89
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	8	4.89
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	34	4.88

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	17	4.88
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	39	4.84
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	14	4.82
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	15	4.78
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	1	4.75
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	12	4.72
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	10	4.72
(1,173)	1:478:A:PHE:C	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	29	4.71
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	36	4.67
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	2	4.67
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	24	4.67
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	26	4.63
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	38	4.6
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	33	4.58
(1,13)	1:350:A:SER:C	1:351:A:ARG:N	1:351:A:ARG:CA	1:351:A:ARG:C	21	4.54
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	31	4.53
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	9	4.51
(1,38)	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	1:364:A:LYS:N	27	4.45
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	23	4.26
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	20	4.23
(1,180)	1:482:A:PHE:N	1:482:A:PHE:CA	1:482:A:PHE:C	1:483:A:GLY:N	4	4.18
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	13	4.18
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	16	4.13
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	20	4.07
(1,38)	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	1:364:A:LYS:N	3	4.04
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	7	3.94
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	23	3.85
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	35	3.84
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	34	3.74
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	19	3.66
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	26	3.64
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	11	3.63
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	9	3.63
(1,160)	1:462:A:ASP:N	1:462:A:ASP:CA	1:462:A:ASP:C	1:463:A:ALA:N	19	3.56
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	4	3.51
(1,164)	1:474:A:ASN:N	1:474:A:ASN:CA	1:474:A:ASN:C	1:475:A:LEU:N	33	3.47
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	15	3.46
(1,172)	1:478:A:PHE:N	1:478:A:PHE:CA	1:478:A:PHE:C	1:479:A:ARG:N	34	3.39
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	28	3.23
(1,175)	1:479:A:ARG:C	1:480:A:ALA:N	1:480:A:ALA:CA	1:480:A:ALA:C	3	3.1
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	4	3.03
(1,173)	1:478:A:PHE:C	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	28	2.97
(1,38)	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	1:364:A:LYS:N	4	2.93
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	1	2.82
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	37	2.82
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	12	2.81
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	36	2.62
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	40	2.61
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	16	2.5
(1,155)	1:426:A:MET:C	1:427:A:PHE:N	1:427:A:PHE:CA	1:427:A:PHE:C	15	2.49
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	5	2.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	1:474:A:ASN:N	1:474:A:ASN:CA	1:474:A:ASN:C	1:475:A:LEU:N	3	2.37
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	32	2.28
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	29	2.23
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	12	2.19
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	11	2.17
(1,151)	1:424:A:LYS:C	1:425:A:ASN:N	1:425:A:ASN:CA	1:425:A:ASN:C	6	2.03
(1,180)	1:482:A:PHE:N	1:482:A:PHE:CA	1:482:A:PHE:C	1:483:A:GLY:N	28	2.0
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	24	1.86
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	3	1.83
(1,170)	1:477:A:ARG:N	1:477:A:ARG:CA	1:477:A:ARG:C	1:478:A:PHE:N	28	1.71
(1,92)	1:394:A:THR:N	1:394:A:THR:CA	1:394:A:THR:C	1:395:A:GLU:N	3	1.64
(1,122)	1:410:A:GLN:N	1:410:A:GLN:CA	1:410:A:GLN:C	1:411:A:VAL:N	40	1.61
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	5	1.6
(1,92)	1:394:A:THR:N	1:394:A:THR:CA	1:394:A:THR:C	1:395:A:GLU:N	28	1.55
(1,174)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:ALA:N	31	1.46
(1,151)	1:424:A:LYS:C	1:425:A:ASN:N	1:425:A:ASN:CA	1:425:A:ASN:C	11	1.46
(1,97)	1:396:A:MET:C	1:397:A:ILE:N	1:397:A:ILE:CA	1:397:A:ILE:C	5	1.46
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	4	1.4
(1,110)	1:403:A:ILE:N	1:403:A:ILE:CA	1:403:A:ILE:C	1:404:A:ARG:N	40	1.37
(1,37)	1:362:A:SER:C	1:363:A:LEU:N	1:363:A:LEU:CA	1:363:A:LEU:C	30	1.33
(1,177)	1:480:A:ALA:C	1:481:A:VAL:N	1:481:A:VAL:CA	1:481:A:VAL:C	2	1.23
(1,81)	1:388:A:GLN:C	1:389:A:GLN:N	1:389:A:GLN:CA	1:389:A:GLN:C	7	1.19