



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 08:16 PM EST

PDB ID : 8URV  
BMRB ID : 31122  
Title : Solution NMR structure of pro-IL-18  
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Deposited on : 2023-10-26

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

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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

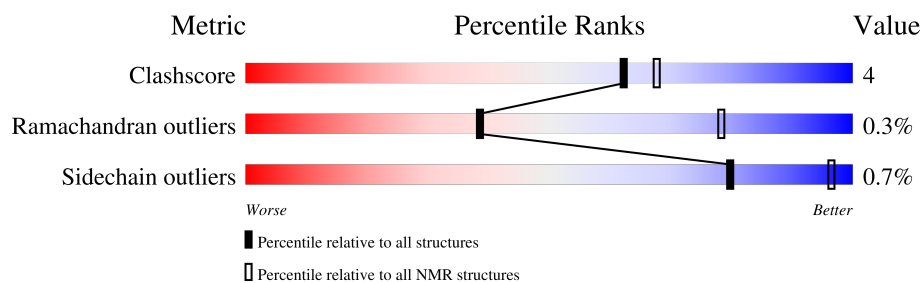
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 94%.

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	193	91% . . .

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:9-A:193 (185)	1.33	5

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

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

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

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

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

There is only 1 type of molecule in this entry. The entry contains 3079 atoms, of which 1517 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interleukin-18.

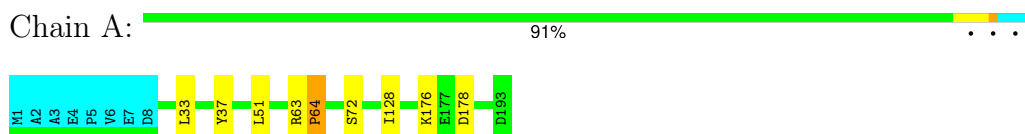
Mol	Chain	Residues	Atoms						Trace
1	A	193	Total	C	H	N	O	S	0
			3079	981	1517	253	315	13	

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

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

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

- Molecule 1: Interleukin-18

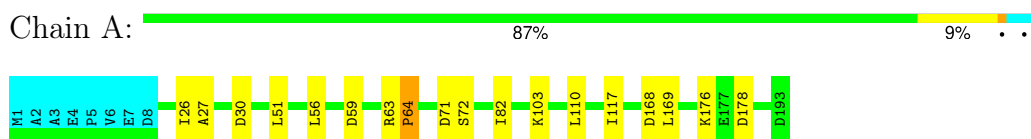


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

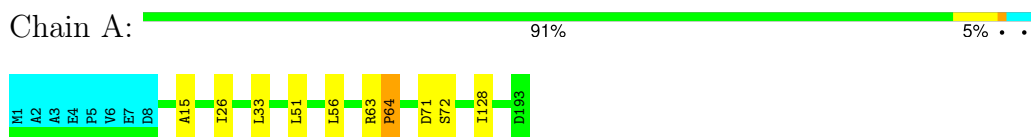
#### 4.2.1 Score per residue for model 1

- Molecule 1: Interleukin-18



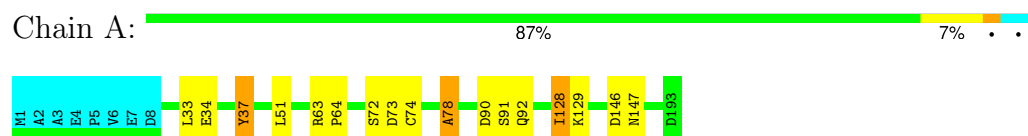
#### 4.2.2 Score per residue for model 2

- Molecule 1: Interleukin-18



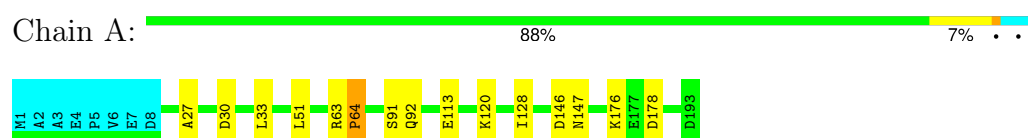
### 4.2.3 Score per residue for model 3

- Molecule 1: Interleukin-18



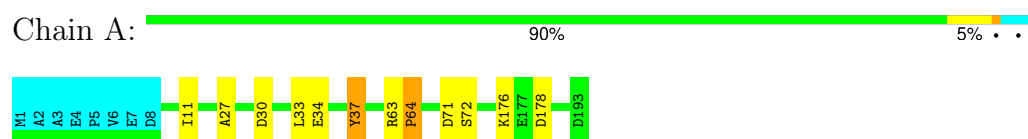
### 4.2.4 Score per residue for model 4

- Molecule 1: Interleukin-18



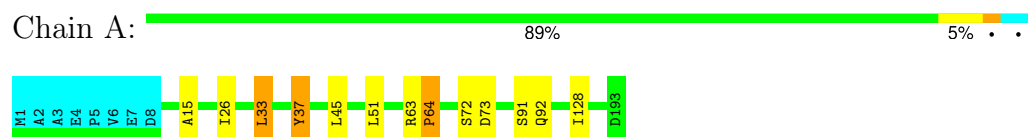
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Interleukin-18



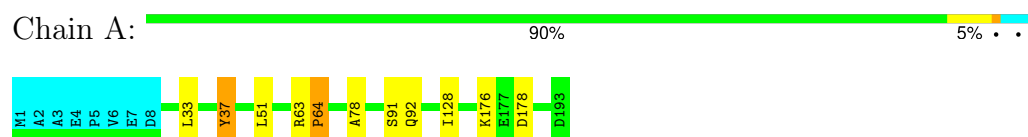
### 4.2.6 Score per residue for model 6

- Molecule 1: Interleukin-18



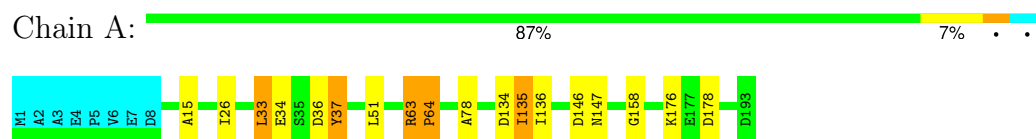
### 4.2.7 Score per residue for model 7

- Molecule 1: Interleukin-18



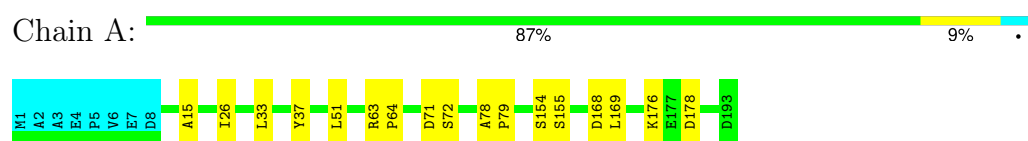
#### 4.2.8 Score per residue for model 8

- Molecule 1: Interleukin-18



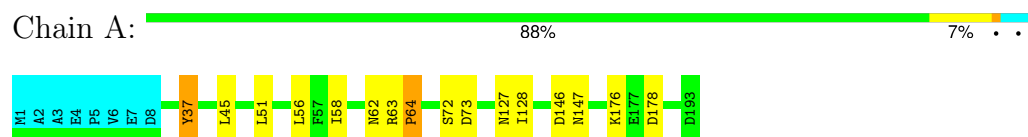
#### 4.2.9 Score per residue for model 9

- Molecule 1: Interleukin-18



#### 4.2.10 Score per residue for model 10

- Molecule 1: Interleukin-18



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.15
Rosetta	refinement	3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2484
Number of shifts mapped to atoms	2484
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%



## 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	0.72±0.01	1±0/1529 ( 0.1± 0.0%)	0.37±0.01	0±0/2052 ( 0.0± 0.0%)
All	All	0.72	8/15290 ( 0.1%)	0.37	0/20520 ( 0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	64	PRO	N-CD	6.41	1.56	1.47	2	8

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	36	ASP	Peptide	1

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1504	1464	1464	12±2
All	All	15040	14640	14640	122

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:ILE:HD13	1:A:128:ILE:H	0.63	1.53	3	1
1:A:110:LEU:HD11	1:A:117:ILE:HG23	0.60	1.74	1	1
1:A:33:LEU:HD12	1:A:33:LEU:C	0.59	2.18	3	6
1:A:134:ASP:O	1:A:136:ILE:N	0.58	2.36	8	1
1:A:37:TYR:N	1:A:37:TYR:CD1	0.57	2.72	3	7
1:A:134:ASP:O	1:A:135:ILE:C	0.57	2.42	8	1
1:A:128:ILE:HG13	1:A:128:ILE:O	0.57	1.99	6	4
1:A:51:LEU:H	1:A:51:LEU:HD23	0.56	1.60	7	9
1:A:33:LEU:HD12	1:A:34:GLU:N	0.55	2.15	3	3
1:A:37:TYR:N	1:A:37:TYR:HD1	0.54	2.01	3	6
1:A:176:LYS:NZ	1:A:178:ASP:OD2	0.54	2.41	5	7
1:A:63:ARG:N	1:A:64:PRO:CD	0.52	2.72	10	9
1:A:27:ALA:HB3	1:A:30:ASP:HB3	0.51	1.82	4	2
1:A:33:LEU:HD13	1:A:37:TYR:CZ	0.51	2.40	8	2
1:A:71:ASP:OD1	1:A:72:SER:N	0.51	2.44	5	4
1:A:63:ARG:H	1:A:64:PRO:HD2	0.51	1.65	8	1
1:A:26:ILE:HD12	1:A:26:ILE:N	0.50	2.20	9	4
1:A:15:ALA:HB3	1:A:26:ILE:HB	0.50	1.83	9	4
1:A:63:ARG:N	1:A:64:PRO:HD2	0.49	2.22	10	8
1:A:74:CYS:O	1:A:78:ALA:N	0.49	2.46	3	1
1:A:91:SER:O	1:A:92:GLN:C	0.48	2.50	4	3
1:A:33:LEU:C	1:A:33:LEU:CD1	0.48	2.81	3	3
1:A:58:ILE:HD12	1:A:62:ASN:O	0.48	2.09	10	1
1:A:56:LEU:HD11	1:A:58:ILE:HD11	0.47	1.84	10	1
1:A:90:ASP:OD2	1:A:129:LYS:NZ	0.46	2.45	3	1
1:A:27:ALA:HB3	1:A:30:ASP:CG	0.45	2.30	5	1
1:A:51:LEU:H	1:A:51:LEU:CD2	0.44	2.25	9	6
1:A:33:LEU:O	1:A:37:TYR:CD1	0.44	2.70	3	2
1:A:37:TYR:H	1:A:37:TYR:HD1	0.44	1.54	7	1
1:A:33:LEU:HD13	1:A:37:TYR:CD2	0.44	2.47	3	1
1:A:127:ASN:O	1:A:128:ILE:C	0.44	2.56	10	1
1:A:154:SER:OG	1:A:155:SER:N	0.44	2.50	9	1
1:A:56:LEU:HD13	1:A:56:LEU:C	0.44	2.33	1	1
1:A:78:ALA:HB1	1:A:79:PRO:HD2	0.43	1.90	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:HD13	1:A:37:TYR:CE2	0.43	2.49	5	1
1:A:146:ASP:OD1	1:A:147:ASN:N	0.42	2.53	4	4
1:A:72:SER:OG	1:A:73:ASP:N	0.42	2.53	6	3
1:A:135:ILE:O	1:A:135:ILE:HG13	0.42	2.15	8	1
1:A:113:GLU:OE2	1:A:120:LYS:NZ	0.41	2.48	4	1
1:A:168:ASP:OD1	1:A:169:LEU:N	0.41	2.54	1	2
1:A:82:ILE:HD13	1:A:103:LYS:HE2	0.40	1.92	1	1
1:A:11:ILE:HD12	1:A:11:ILE:N	0.40	2.30	5	1
1:A:91:SER:O	1:A:92:GLN:HB2	0.40	2.16	7	1
1:A:27:ALA:HB3	1:A:30:ASP:CB	0.40	2.47	4	1
1:A:59:ASP:N	1:A:59:ASP:OD1	0.40	2.55	1	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/193 (95%)	170±3 (92±2%)	14±3 (7±2%)	1±1 (0±1%)	38	78
All	All	1840/1930 (95%)	1697 (92%)	137 (7%)	6 (0%)	38	78

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	78	ALA	3
1	A	63	ARG	1
1	A	135	ILE	1
1	A	158	GLY	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/180 (97%)	173±1 (99±1%)	1±1 (1±1%)	80	96
All	All	1740/1800 (97%)	1727 (99%)	13 (1%)	80	96

All 5 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	37	TYR	6
1	A	33	LEU	3
1	A	45	LEU	2
1	A	56	LEU	1
1	A	128	ILE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 94% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	2484
Number of shifts mapped to atoms	2484
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	191	$0.07 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	184	$0.04 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	192	$0.44 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	184	$-0.41 \pm 0.31$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 2396 atoms were assigned a chemical shift out of a possible 2551. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	912/919 (99%)	367/370 (99%)	367/370 (99%)	178/179 (99%)
Sidechain	1304/1440 (91%)	873/923 (95%)	412/459 (90%)	19/58 (33%)

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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	180/192 (94%)	90/94 (96%)	90/97 (93%)	0/1 (0%)
Overall	2396/2551 (94%)	1330/1387 (96%)	869/926 (94%)	197/238 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 2484 atoms were assigned a chemical shift out of a possible 2644. 0 out of 21 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	948/957 (99%)	381/385 (99%)	383/386 (99%)	184/186 (99%)
Sidechain	1356/1495 (91%)	909/959 (95%)	428/478 (90%)	19/58 (33%)
Aromatic	180/192 (94%)	90/94 (96%)	90/97 (93%)	0/1 (0%)
Overall	2484/2644 (94%)	1380/1438 (96%)	901/961 (94%)	203/245 (83%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

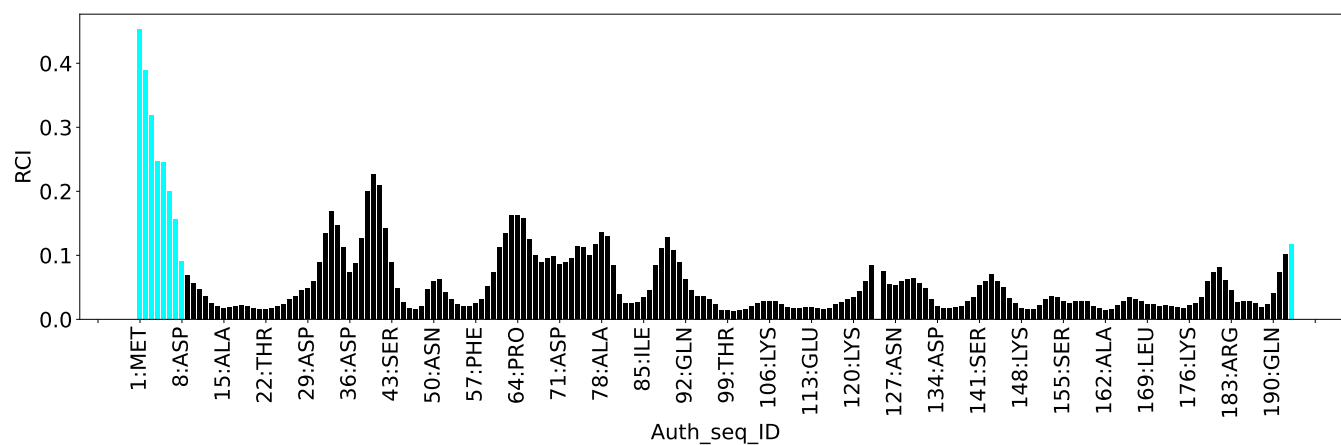
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	115	LYS	HG3	-0.46	0.04 – 2.67	-6.9
1	A	115	LYS	HG2	-0.15	0.13 – 2.61	-6.2

#### 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	3977
Intra-residue ( $ i-j =0$ )	916
Sequential ( $ i-j =1$ )	985
Medium range ( $ i-j >1$ and $ i-j <5$ )	488
Long range ( $ i-j \geq 5$ )	1588
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	136
Number of unmapped restraints	0
Number of restraints per residue	21.3
Number of long range restraints per residue <sup>1</sup>	8.2

<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)	16.1	0.2
0.2-0.5 (Medium)	22.9	0.5
>0.5 (Large)	33.2	2.34



### 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)	None	None
10.0-20.0 (Medium)	None	None
>20.0 (Large)	136.0	178.52

## 9 Distance violation analysis ⓘ

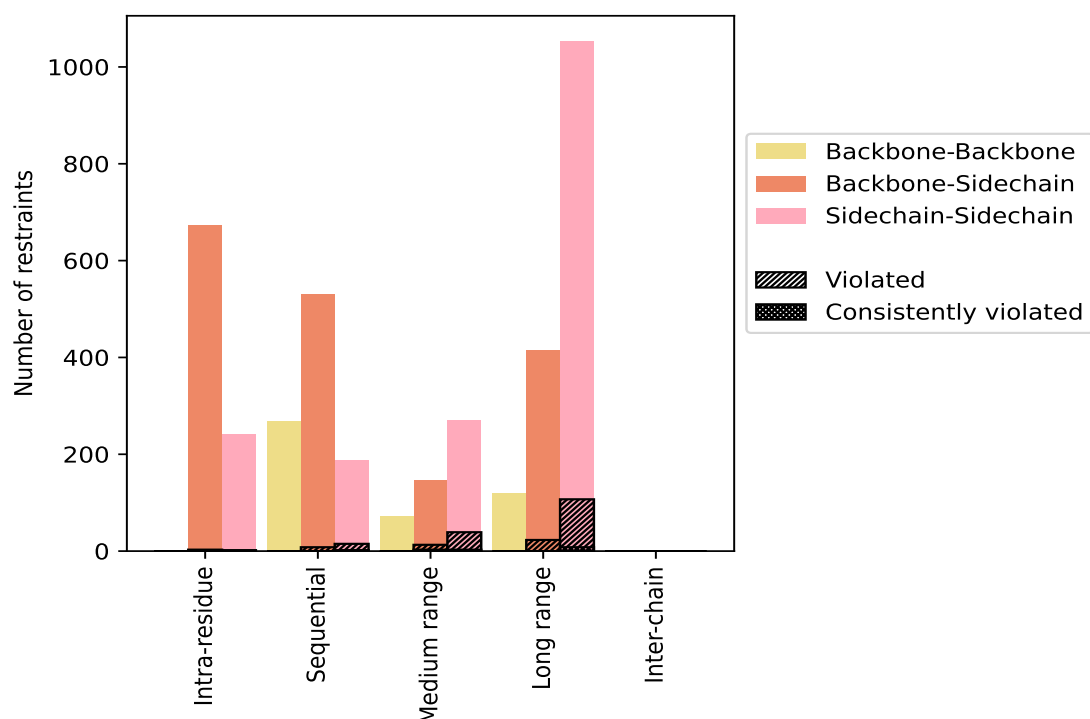
### 9.1 Summary of distance violations ⓘ

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>916</b>	<b>23.0</b>	<b>5</b>	<b>0.5</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	672	16.9	3	0.4	0.1	0	0.0	0.0
Sidechain-Sidechain	242	6.1	2	0.8	0.1	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>985</b>	<b>24.8</b>	<b>23</b>	<b>2.3</b>	<b>0.6</b>	<b>2</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	268	6.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	530	13.3	8	1.5	0.2	0	0.0	0.0
Sidechain-Sidechain	187	4.7	15	8.0	0.4	2	1.1	0.1
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>488</b>	<b>12.3</b>	<b>52</b>	<b>10.7</b>	<b>1.3</b>	<b>6</b>	<b>1.2</b>	<b>0.2</b>
Backbone-Backbone	71	1.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	147	3.7	13	8.8	0.3	3	2.0	0.1
Sidechain-Sidechain	270	6.8	39	14.4	1.0	3	1.1	0.1
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>1588</b>	<b>39.9</b>	<b>130</b>	<b>8.2</b>	<b>3.3</b>	<b>8</b>	<b>0.5</b>	<b>0.2</b>
Backbone-Backbone	120	3.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	415	10.4	23	5.5	0.6	0	0.0	0.0
Sidechain-Sidechain	1053	26.5	107	10.2	2.7	8	0.8	0.2
<b>Inter-chain</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Hydrogen bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>3977</b>	<b>100.0</b>	<b>210</b>	<b>5.3</b>	<b>5.3</b>	<b>16</b>	<b>0.4</b>	<b>0.4</b>
Backbone-Backbone	461	11.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1764	44.4	47	2.7	1.2	3	0.2	0.1
Sidechain-Sidechain	1752	44.1	163	9.3	4.1	13	0.7	0.3

<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 disulfide bonds are counted in their appropriate category on the x-axis

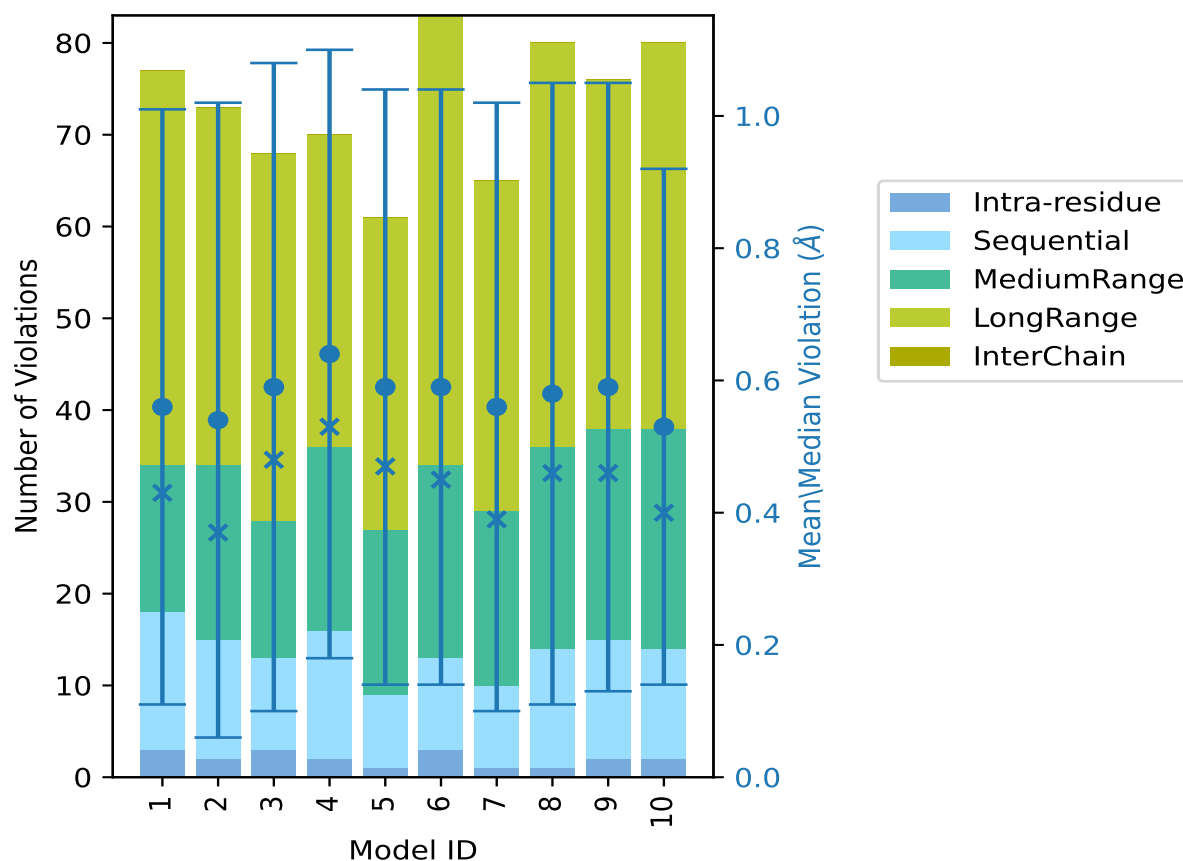
## 9.2 Distance violation statistics for each model [i](#)

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	3	15	16	43	0	77	0.56	1.92	0.45	0.43
2	2	13	19	39	0	73	0.54	2.34	0.48	0.37
3	3	10	15	40	0	68	0.59	2.24	0.49	0.48
4	2	14	20	34	0	70	0.64	1.99	0.46	0.53
5	1	8	18	34	0	61	0.59	2.04	0.45	0.47
6	3	10	21	49	0	83	0.59	2.17	0.45	0.45
7	1	9	19	36	0	65	0.56	2.05	0.46	0.39
8	1	13	22	44	0	80	0.58	2.17	0.47	0.46
9	2	13	23	38	0	76	0.59	2.0	0.46	0.46
10	2	12	24	42	0	80	0.53	2.04	0.39	0.4

<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, 3767(IR:911, SQ:962, MR:436, LR:1458, 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>	%
0	3	17	68	0	88	1	10.0
3	5	9	9	0	26	2	20.0
0	2	1	8	0	11	3	30.0

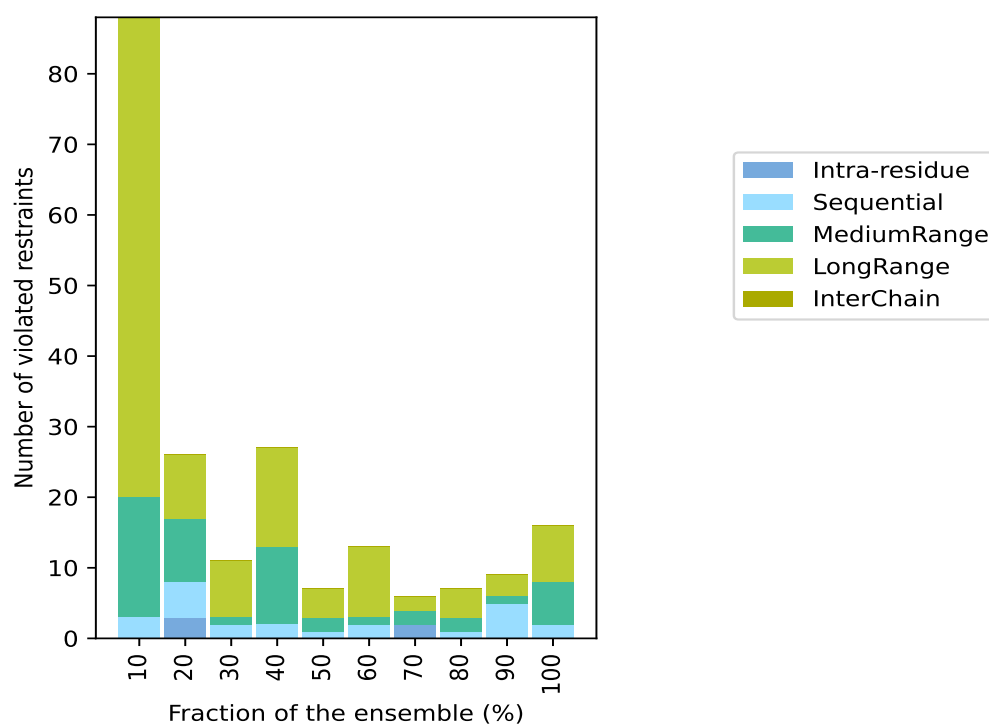
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	2	11	14	0	27	4	40.0
0	1	2	4	0	7	5	50.0
0	2	1	10	0	13	6	60.0
2	0	2	2	0	6	7	70.0
0	1	2	4	0	7	8	80.0
0	5	1	3	0	9	9	90.0
0	2	6	8	0	16	10	100.0

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

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

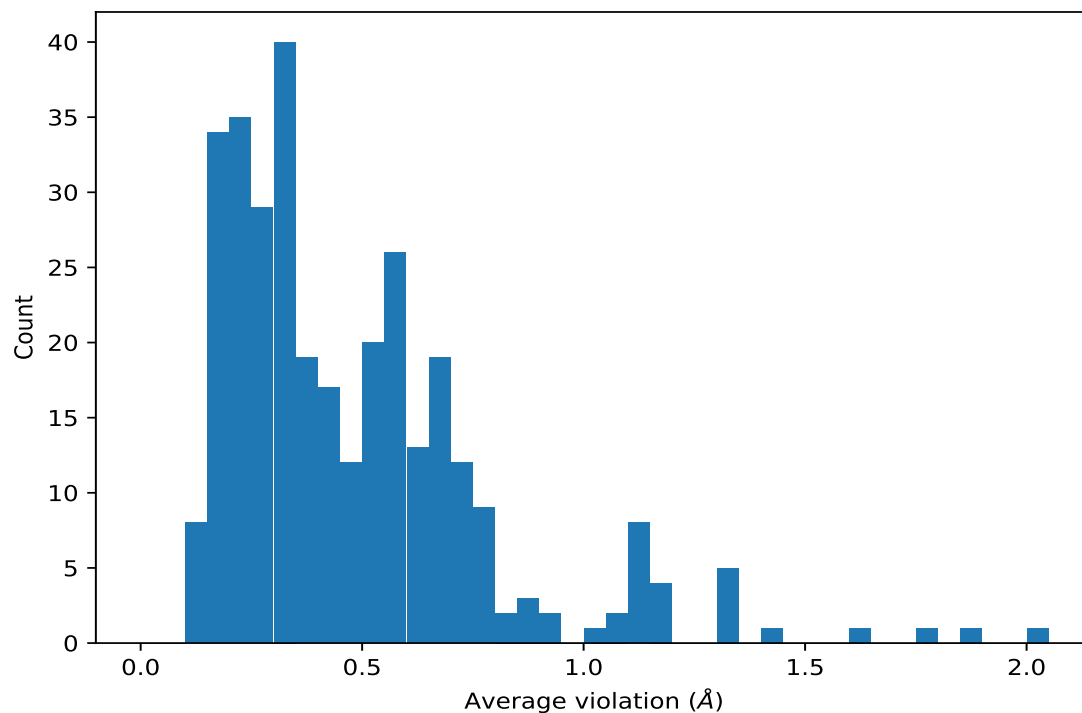


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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)
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	10	2.0	0.11	2.02
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	10	1.89	0.32	1.97
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	10	1.79	0.29	1.87
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	10	1.64	0.14	1.65
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	10	1.1	0.2	1.02
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	10	1.1	0.2	1.02
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	10	1.1	0.2	1.02
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	10	0.89	0.16	0.84
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	10	0.89	0.16	0.84
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	10	0.89	0.16	0.84
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	10	0.8	0.22	0.8
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	10	0.76	0.16	0.74
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	10	0.76	0.16	0.74
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	10	0.76	0.16	0.74
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	10	0.75	0.15	0.71

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	10	0.75	0.15	0.71
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	10	0.75	0.15	0.71
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	10	0.73	0.16	0.66
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	10	0.71	0.33	0.55
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	10	0.63	0.08	0.65
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	10	0.52	0.1	0.51
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	10	0.44	0.11	0.42
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	10	0.44	0.11	0.42
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	10	0.44	0.11	0.42
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	10	0.36	0.14	0.31
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	10	0.36	0.14	0.31
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	10	0.36	0.14	0.31
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	10	0.23	0.17	0.16
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	9	1.19	0.16	1.21
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	9	1.15	0.46	1.51
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	9	1.15	0.46	1.51
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	9	1.15	0.46	1.51
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	9	1.13	0.09	1.11
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	9	1.13	0.09	1.11
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	9	1.13	0.09	1.11
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	9	0.67	0.18	0.74
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	9	0.67	0.18	0.74
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	9	0.67	0.18	0.74
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	9	0.67	0.18	0.74
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	9	0.67	0.18	0.74
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	9	0.67	0.18	0.74
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	9	0.67	0.64	0.36
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	9	0.5	0.07	0.46
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	9	0.45	0.19	0.42
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	9	0.45	0.19	0.42
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	9	0.45	0.19	0.42
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	9	0.45	0.19	0.42
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	9	0.34	0.14	0.29
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	9	0.34	0.14	0.29
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	9	0.34	0.14	0.29
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	9	0.16	0.03	0.17
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	8	0.73	0.12	0.68
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	8	0.72	0.29	0.74
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	8	0.72	0.29	0.74
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	8	0.56	0.22	0.5
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	8	0.45	0.2	0.47
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	8	0.45	0.2	0.47

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	8	0.45	0.2	0.47
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	8	0.42	0.14	0.43
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	8	0.42	0.14	0.43
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	8	0.42	0.14	0.43
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	8	0.34	0.21	0.32
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	8	0.34	0.21	0.32
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	8	0.34	0.21	0.32
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	8	0.34	0.21	0.32
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	8	0.34	0.21	0.32
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	8	0.34	0.21	0.32
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	8	0.2	0.06	0.21
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	8	0.2	0.06	0.21
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	8	0.2	0.06	0.21
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	7	1.3	0.08	1.32
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	7	1.3	0.08	1.32
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	7	0.59	0.21	0.67
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	7	0.59	0.21	0.67
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	7	0.59	0.21	0.67
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	7	0.59	0.21	0.67
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	7	0.59	0.21	0.67
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	7	0.59	0.21	0.67
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	7	0.32	0.05	0.35
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	7	0.32	0.05	0.35
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	7	0.32	0.0	0.32
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	7	0.27	0.01	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	7	0.27	0.01	0.28
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	7	0.22	0.1	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	7	0.22	0.1	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	7	0.22	0.1	0.23
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	6	0.66	0.15	0.68
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	6	0.66	0.15	0.68
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	6	0.66	0.15	0.68
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	6	0.61	0.64	0.18
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	6	0.59	0.2	0.56
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	6	0.59	0.2	0.56

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	6	0.59	0.2	0.56
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	6	0.5	0.27	0.44
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	6	0.5	0.27	0.44
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	6	0.5	0.03	0.5
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	6	0.5	0.03	0.5
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	6	0.47	0.21	0.48
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	6	0.47	0.21	0.48
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	6	0.44	0.22	0.54
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	6	0.44	0.22	0.54
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	6	0.44	0.22	0.54
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	6	0.44	0.22	0.54
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	6	0.32	0.14	0.32
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	6	0.32	0.14	0.32
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	6	0.32	0.14	0.32
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	6	0.31	0.05	0.32
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	6	0.25	0.14	0.2
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	6	0.25	0.14	0.2
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	6	0.25	0.14	0.2
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	6	0.23	0.15	0.15
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	6	0.23	0.15	0.15
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	6	0.18	0.03	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	6	0.18	0.03	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	6	0.18	0.03	0.18
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	6	0.17	0.03	0.16
(1,178)	1:12:A:ASN:HA	1:49:A:ARG:HD2	5	0.48	0.27	0.6
(2,365)	1:31:A:GLU:HB3	1:33:A:LEU:HG	5	0.44	0.1	0.41
(1,599)	1:55:A:VAL:HG11	1:83:A:PHE:HB2	5	0.38	0.09	0.35
(1,599)	1:55:A:VAL:HG12	1:83:A:PHE:HB2	5	0.38	0.09	0.35
(1,599)	1:55:A:VAL:HG13	1:83:A:PHE:HB2	5	0.38	0.09	0.35
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD11	5	0.3	0.19	0.21
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD12	5	0.3	0.19	0.21
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD13	5	0.3	0.19	0.21
(1,1154)	1:114:A:ASN:HB2	1:116:A:ILE:HG12	5	0.27	0.07	0.27
(1,1935)	1:108:A:SER:HB2	1:120:A:LYS:H	5	0.26	0.07	0.29
(1,93)	1:47:A:VAL:HG21	1:148:A:LYS:HE2	5	0.19	0.05	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,93)	1:47:A:VAL:HG22	1:148:A:LYS:HE2	5	0.19	0.05	0.18
(1,93)	1:47:A:VAL:HG23	1:148:A:LYS:HE2	5	0.19	0.05	0.18
(1,703)	1:148:A:LYS:HD3	1:190:A:GLN:HA	4	1.44	0.15	1.46
(1,741)	1:15:A:ALA:HB1	1:17:A:LYS:HG3	4	1.31	0.06	1.32
(1,741)	1:15:A:ALA:HB2	1:17:A:LYS:HG3	4	1.31	0.06	1.32
(1,741)	1:15:A:ALA:HB3	1:17:A:LYS:HG3	4	1.31	0.06	1.32
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE1	4	1.07	0.06	1.1
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE2	4	1.07	0.06	1.1
(1,288)	1:17:A:LYS:HB3	1:19:A:ILE:HG12	4	1.03	0.08	1.04
(2,99)	1:17:A:LYS:HB3	1:19:A:ILE:HB	4	0.83	0.06	0.83
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE1	4	0.72	0.38	0.7
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE2	4	0.72	0.38	0.7
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE2	4	0.72	0.08	0.68
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE3	4	0.72	0.08	0.68
(2,161)	1:34:A:GLU:HA	1:38:A:PHE:HB3	4	0.69	0.25	0.78
(2,467)	1:63:A:ARG:HB2	1:66:A:PHE:HZ	4	0.69	0.43	0.67
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG21	4	0.67	0.18	0.76
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG22	4	0.67	0.18	0.76
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG23	4	0.67	0.18	0.76
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG21	4	0.67	0.18	0.76
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG22	4	0.67	0.18	0.76
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG23	4	0.67	0.18	0.76
(1,653)	1:59:A:ASP:HA	1:87:A:MET:HB3	4	0.66	0.11	0.66
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD1	4	0.63	0.04	0.64
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD2	4	0.63	0.04	0.64
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD11	4	0.57	0.01	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD12	4	0.57	0.01	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD13	4	0.57	0.01	0.56
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE1	4	0.56	0.3	0.58
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE2	4	0.56	0.3	0.58
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE3	4	0.56	0.3	0.58
(1,817)	1:128:A:ILE:HD11	1:136:A:ILE:HG12	4	0.53	0.29	0.56
(1,817)	1:128:A:ILE:HD12	1:136:A:ILE:HG12	4	0.53	0.29	0.56
(1,817)	1:128:A:ILE:HD13	1:136:A:ILE:HG12	4	0.53	0.29	0.56
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG2	4	0.46	0.01	0.46
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG3	4	0.46	0.01	0.46
(1,252)	1:17:A:LYS:HB3	1:24:A:TYR:HB3	4	0.38	0.07	0.38
(1,245)	1:17:A:LYS:HB2	1:24:A:TYR:HB3	4	0.37	0.1	0.34
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG21	4	0.32	0.01	0.32
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG22	4	0.32	0.01	0.32
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG23	4	0.32	0.01	0.32
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD11	4	0.32	0.27	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD12	4	0.32	0.27	0.19
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD13	4	0.32	0.27	0.19
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD11	4	0.32	0.27	0.19
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD12	4	0.32	0.27	0.19
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD13	4	0.32	0.27	0.19
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG2	4	0.3	0.05	0.31
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG3	4	0.3	0.05	0.31
(1,468)	1:47:A:VAL:HG21	1:148:A:LYS:HD3	4	0.3	0.11	0.29
(1,468)	1:47:A:VAL:HG22	1:148:A:LYS:HD3	4	0.3	0.11	0.29
(1,468)	1:47:A:VAL:HG23	1:148:A:LYS:HD3	4	0.3	0.11	0.29
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD11	4	0.22	0.07	0.2
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD12	4	0.22	0.07	0.2
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD13	4	0.22	0.07	0.2
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD11	4	0.2	0.05	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD12	4	0.2	0.05	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD13	4	0.2	0.05	0.22
(1,524)	1:49:A:ARG:HB2	1:51:A:LEU:HB2	4	0.18	0.06	0.18
(2,106)	1:26:A:ILE:HG12	1:169:A:LEU:HB2	4	0.17	0.04	0.18
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD21	4	0.16	0.01	0.16
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD22	4	0.16	0.01	0.16
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD23	4	0.16	0.01	0.16
(2,157)	1:37:A:TYR:HE1	1:38:A:PHE:HA	3	1.1	0.03	1.09
(2,157)	1:37:A:TYR:HE2	1:38:A:PHE:HA	3	1.1	0.03	1.09
(2,170)	1:58:A:ILE:HD11	1:65:A:LEU:HB3	3	0.72	0.4	0.44
(2,170)	1:58:A:ILE:HD12	1:65:A:LEU:HB3	3	0.72	0.4	0.44
(2,170)	1:58:A:ILE:HD13	1:65:A:LEU:HB3	3	0.72	0.4	0.44
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD2	3	0.64	0.05	0.62
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD3	3	0.64	0.05	0.62
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD2	3	0.64	0.05	0.62
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD3	3	0.64	0.05	0.62
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD2	3	0.64	0.05	0.62
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD3	3	0.64	0.05	0.62
(1,719)	1:100:A:ILE:HD11	1:110:A:LEU:HB2	3	0.51	0.17	0.57
(1,719)	1:100:A:ILE:HD12	1:110:A:LEU:HB2	3	0.51	0.17	0.57
(1,719)	1:100:A:ILE:HD13	1:110:A:LEU:HB2	3	0.51	0.17	0.57
(1,531)	1:47:A:VAL:HG11	1:49:A:ARG:HD2	3	0.41	0.28	0.23
(1,531)	1:47:A:VAL:HG12	1:49:A:ARG:HD2	3	0.41	0.28	0.23
(1,531)	1:47:A:VAL:HG13	1:49:A:ARG:HD2	3	0.41	0.28	0.23
(2,12)	1:37:A:TYR:HE1	1:38:A:PHE:HZ	3	0.39	0.19	0.26
(2,12)	1:37:A:TYR:HE2	1:38:A:PHE:HZ	3	0.39	0.19	0.26
(1,2141)	1:49:A:ARG:HD3	1:190:A:GLN:HE21	3	0.36	0.07	0.36
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB1	3	0.27	0.14	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB2	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB3	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB1	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB2	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB3	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB1	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB2	3	0.27	0.14	0.22
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB3	3	0.27	0.14	0.22
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG21	3	0.27	0.09	0.23
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG22	3	0.27	0.09	0.23
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG23	3	0.27	0.09	0.23
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD11	3	0.23	0.07	0.22
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD12	3	0.23	0.07	0.22
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD13	3	0.23	0.07	0.22
(1,186)	1:14:A:VAL:HA	1:49:A:ARG:HB3	3	0.16	0.01	0.16
(1,2714)	1:144:A:GLY:HA2	1:145:A:HIS:HD2	2	0.92	0.08	0.92
(1,2714)	1:144:A:GLY:HA3	1:145:A:HIS:HD2	2	0.92	0.08	0.92
(1,2840)	1:176:A:LYS:HD2	1:179:A:GLU:HB3	2	0.78	0.11	0.78
(1,2840)	1:176:A:LYS:HD3	1:179:A:GLU:HB3	2	0.78	0.11	0.78
(1,1972)	1:145:A:HIS:H	1:145:A:HIS:HD2	2	0.78	0.02	0.78
(1,1264)	1:142:A:VAL:HG11	1:145:A:HIS:HD2	2	0.6	0.05	0.6
(1,1264)	1:142:A:VAL:HG12	1:145:A:HIS:HD2	2	0.6	0.05	0.6
(1,1264)	1:142:A:VAL:HG13	1:145:A:HIS:HD2	2	0.6	0.05	0.6
(1,1177)	1:176:A:LYS:HB2	1:179:A:GLU:HB3	2	0.56	0.13	0.56
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD11	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD12	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD13	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD11	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD12	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD13	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD11	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD12	2	0.56	0.31	0.56
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD13	2	0.56	0.31	0.56
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD11	2	0.54	0.06	0.54
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD12	2	0.54	0.06	0.54
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD13	2	0.54	0.06	0.54
(1,526)	1:49:A:ARG:HA	1:49:A:ARG:HD3	2	0.54	0.42	0.54
(1,2043)	1:178:A:ASP:H	1:179:A:GLU:HB3	2	0.53	0.02	0.53
(1,173)	1:11:A:ILE:HG21	1:46:A:SER:HB3	2	0.5	0.08	0.5
(1,173)	1:11:A:ILE:HG22	1:46:A:SER:HB3	2	0.5	0.08	0.5
(1,173)	1:11:A:ILE:HG23	1:46:A:SER:HB3	2	0.5	0.08	0.5
(1,1373)	1:142:A:VAL:HG21	1:145:A:HIS:HD2	2	0.42	0.09	0.42

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1373)	1:142:A:VAL:HG22	1:145:A:HIS:HD2	2	0.42	0.09	0.42
(1,1373)	1:142:A:VAL:HG23	1:145:A:HIS:HD2	2	0.42	0.09	0.42
(1,2363)	1:32:A:ASN:H	1:34:A:GLU:HG2	2	0.38	0.21	0.38
(1,2363)	1:32:A:ASN:H	1:34:A:GLU:HG3	2	0.38	0.21	0.38
(1,2383)	1:41:A:LEU:HD11	1:44:A:LYS:HD2	2	0.38	0.26	0.38
(1,2383)	1:41:A:LEU:HD11	1:44:A:LYS:HD3	2	0.38	0.26	0.38
(1,2383)	1:41:A:LEU:HD12	1:44:A:LYS:HD2	2	0.38	0.26	0.38
(1,2383)	1:41:A:LEU:HD12	1:44:A:LYS:HD3	2	0.38	0.26	0.38
(1,2383)	1:41:A:LEU:HD13	1:44:A:LYS:HD2	2	0.38	0.26	0.38
(1,2383)	1:41:A:LEU:HD13	1:44:A:LYS:HD3	2	0.38	0.26	0.38
(2,407)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	2	0.28	0.18	0.28
(2,407)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	2	0.28	0.18	0.28
(1,2789)	1:165:A:LYS:HA	1:165:A:LYS:HE2	2	0.28	0.0	0.28
(1,2789)	1:165:A:LYS:HA	1:165:A:LYS:HE3	2	0.28	0.0	0.28
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD11	2	0.26	0.08	0.26
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD12	2	0.26	0.08	0.26
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD13	2	0.26	0.08	0.26
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD11	2	0.25	0.12	0.25
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD12	2	0.25	0.12	0.25
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD13	2	0.25	0.12	0.25
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG21	2	0.24	0.1	0.24
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG22	2	0.24	0.1	0.24
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG23	2	0.24	0.1	0.24
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	2	0.24	0.1	0.24
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	2	0.24	0.1	0.24
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	2	0.24	0.1	0.24
(1,2499)	1:82:A:ILE:HG12	1:103:A:LYS:HE2	2	0.22	0.02	0.22
(1,2499)	1:82:A:ILE:HG12	1:103:A:LYS:HE3	2	0.22	0.02	0.22
(1,2499)	1:82:A:ILE:HG13	1:103:A:LYS:HE2	2	0.22	0.02	0.22
(1,2499)	1:82:A:ILE:HG13	1:103:A:LYS:HE3	2	0.22	0.02	0.22
(1,300)	1:21:A:ASN:HB2	1:119:A:PHE:HD1	2	0.18	0.02	0.18
(1,300)	1:21:A:ASN:HB2	1:119:A:PHE:HD2	2	0.18	0.02	0.18
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE1	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE2	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE3	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE1	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE2	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE3	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE1	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE2	2	0.18	0.06	0.18
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE3	2	0.18	0.06	0.18
(1,2435)	1:58:A:ILE:HG21	1:63:A:ARG:HD2	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2435)	1:58:A:ILE:HG21	1:63:A:ARG:HD3	2	0.16	0.02	0.16
(1,2435)	1:58:A:ILE:HG22	1:63:A:ARG:HD2	2	0.16	0.02	0.16
(1,2435)	1:58:A:ILE:HG22	1:63:A:ARG:HD3	2	0.16	0.02	0.16
(1,2435)	1:58:A:ILE:HG23	1:63:A:ARG:HD2	2	0.16	0.02	0.16
(1,2435)	1:58:A:ILE:HG23	1:63:A:ARG:HD3	2	0.16	0.02	0.16
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD11	2	0.16	0.04	0.16
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD12	2	0.16	0.04	0.16
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD13	2	0.16	0.04	0.16
(1,299)	1:21:A:ASN:HB3	1:119:A:PHE:HB3	2	0.14	0.01	0.14
(1,2475)	1:75:A:ARG:HG2	1:76:A:ASP:HB2	2	0.14	0.04	0.14
(1,2475)	1:75:A:ARG:HG2	1:76:A:ASP:HB3	2	0.14	0.04	0.14
(1,2475)	1:75:A:ARG:HG3	1:76:A:ASP:HB2	2	0.14	0.04	0.14
(1,2475)	1:75:A:ARG:HG3	1:76:A:ASP:HB3	2	0.14	0.04	0.14
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD11	2	0.12	0.01	0.12
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD12	2	0.12	0.01	0.12
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD13	2	0.12	0.01	0.12

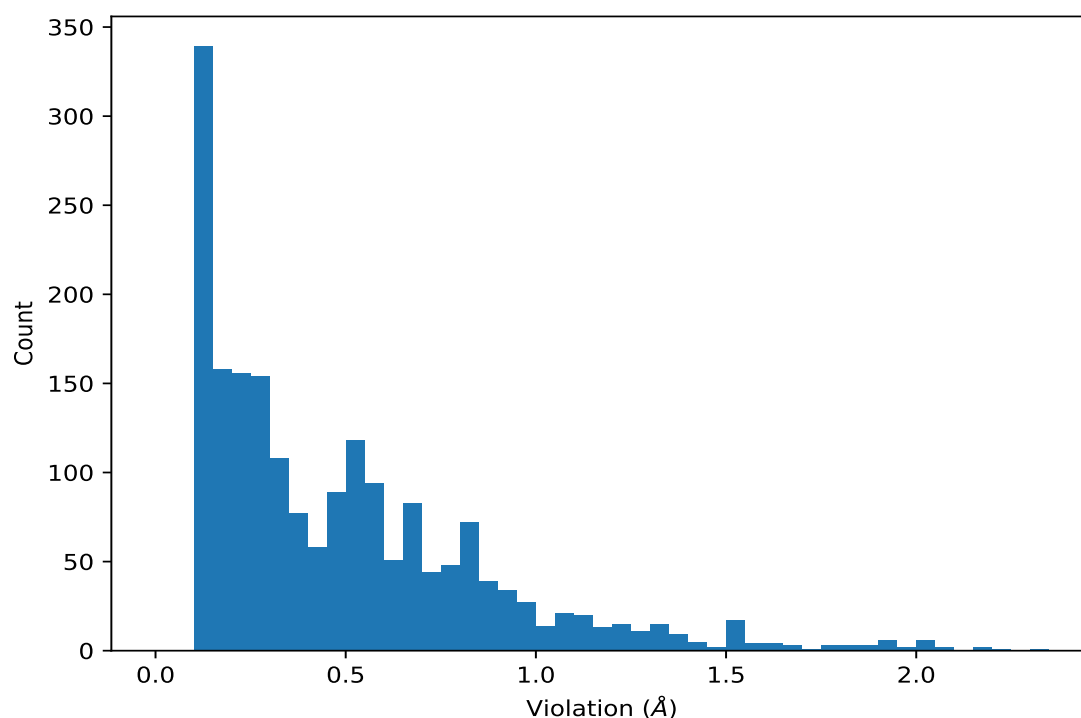
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 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)
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	2	2.34
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	3	2.24
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	6	2.17
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	8	2.17
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	3	2.09
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	8	2.09
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	7	2.05
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	5	2.04
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	10	2.04
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	3	2.04
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	7	2.0
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	9	2.0
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	4	1.99
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	9	1.98
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	6	1.94
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	4	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	6	1.92
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	1	1.92
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	2	1.92
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	4	1.91
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	5	1.9
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	8	1.88
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	9	1.86
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	2	1.83
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	8	1.82
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	1	1.8
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	9	1.77
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	2	1.76
(1,1182)	1:16:A:MET:HG2	1:54:A:GLN:HG2	7	1.75
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	5	1.74
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	10	1.69
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	4	1.69
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	1	1.67
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	7	1.64
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	1	1.62
(1,703)	1:148:A:LYS:HD3	1:190:A:GLN:HA	3	1.61
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	4	1.6
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	6	1.57
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	3	1.57
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	3	1.57
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	3	1.57
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	2	1.54
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	2	1.54
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	2	1.54
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	5	1.54
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	5	1.54
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	5	1.54
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	1	1.53
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	1	1.53
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	1	1.53
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	3	1.53
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	3	1.53
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	3	1.53
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	8	1.51
(1,703)	1:148:A:LYS:HD3	1:190:A:GLN:HA	1	1.51
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	4	1.51
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	4	1.51
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	4	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	3	1.47
(1,1302)	1:175:A:LYS:HB2	1:179:A:GLU:HG3	4	1.46
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	7	1.45
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	6	1.44
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	6	1.44
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	8	1.42
(1,703)	1:148:A:LYS:HD3	1:190:A:GLN:HA	7	1.42
(1,741)	1:15:A:ALA:HB1	1:17:A:LYS:HG3	9	1.4
(1,741)	1:15:A:ALA:HB2	1:17:A:LYS:HG3	9	1.4
(1,741)	1:15:A:ALA:HB3	1:17:A:LYS:HG3	9	1.4
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	5	1.37
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	1	1.36
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	1	1.36
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	9	1.36
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	9	1.36
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	9	1.36
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	5	1.34
(1,741)	1:15:A:ALA:HB1	1:17:A:LYS:HG3	6	1.33
(1,741)	1:15:A:ALA:HB2	1:17:A:LYS:HG3	6	1.33
(1,741)	1:15:A:ALA:HB3	1:17:A:LYS:HG3	6	1.33
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	2	1.32
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	2	1.32
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	7	1.32
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	7	1.32
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	10	1.31
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	10	1.31
(1,741)	1:15:A:ALA:HB1	1:17:A:LYS:HG3	8	1.3
(1,741)	1:15:A:ALA:HB2	1:17:A:LYS:HG3	8	1.3
(1,741)	1:15:A:ALA:HB3	1:17:A:LYS:HG3	8	1.3
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	1	1.3
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	3	1.3
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	1	1.29
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	1	1.29
(2,170)	1:58:A:ILE:HD11	1:65:A:LEU:HB3	2	1.29
(2,170)	1:58:A:ILE:HD12	1:65:A:LEU:HB3	2	1.29
(2,170)	1:58:A:ILE:HD13	1:65:A:LEU:HB3	2	1.29
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	6	1.28
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	6	1.28
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	6	1.28
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	7	1.26
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	7	1.26
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	7	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,467)	1:63:A:ARG:HB2	1:66:A:PHE:HZ	9	1.24
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	1	1.24
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	1	1.24
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	1	1.24
(2,201)	1:49:A:ARG:HD3	1:51:A:LEU:HB2	10	1.22
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	6	1.22
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	6	1.22
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	6	1.22
(1,741)	1:15:A:ALA:HB1	1:17:A:LYS:HG3	10	1.22
(1,741)	1:15:A:ALA:HB2	1:17:A:LYS:HG3	10	1.22
(1,741)	1:15:A:ALA:HB3	1:17:A:LYS:HG3	10	1.22
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	9	1.21
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	9	1.21
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	8	1.21
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	6	1.21
(1,703)	1:148:A:LYS:HD3	1:190:A:GLN:HA	9	1.2
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	4	1.2
(1,421)	1:41:A:LEU:HB2	1:185:A:ILE:HG21	6	1.19
(1,421)	1:41:A:LEU:HB2	1:185:A:ILE:HG22	6	1.19
(1,421)	1:41:A:LEU:HB2	1:185:A:ILE:HG23	6	1.19
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	10	1.19
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	10	1.19
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	10	1.19
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	2	1.18
(1,2831)	1:175:A:LYS:HE2	1:179:A:GLU:HB2	5	1.17
(1,2831)	1:175:A:LYS:HE3	1:179:A:GLU:HB2	5	1.17
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE1	1	1.16
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE2	1	1.16
(2,157)	1:37:A:TYR:HE1	1:38:A:PHE:HA	2	1.14
(2,157)	1:37:A:TYR:HE2	1:38:A:PHE:HA	2	1.14
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	5	1.14
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	5	1.14
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	5	1.14
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE1	8	1.13
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE2	8	1.13
(1,288)	1:17:A:LYS:HB3	1:19:A:ILE:HG12	9	1.13
(1,2611)	1:113:A:GLU:HG2	1:114:A:ASN:HB3	4	1.12
(1,2611)	1:113:A:GLU:HG3	1:114:A:ASN:HB3	4	1.12
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	10	1.12
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	10	1.12
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	3	1.11
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	3	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	3	1.11
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE1	10	1.1
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE2	10	1.1
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	7	1.1
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	7	1.1
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	7	1.1
(2,157)	1:37:A:TYR:HE1	1:38:A:PHE:HA	1	1.09
(2,157)	1:37:A:TYR:HE2	1:38:A:PHE:HA	1	1.09
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE1	6	1.09
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE2	6	1.09
(1,527)	1:12:A:ASN:HB2	1:49:A:ARG:HD2	10	1.09
(1,288)	1:17:A:LYS:HB3	1:19:A:ILE:HG12	10	1.09
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	4	1.08
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	8	1.08
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	8	1.08
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	8	1.08
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	10	1.07
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	9	1.07
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	9	1.07
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	9	1.07
(2,157)	1:37:A:TYR:HE1	1:38:A:PHE:HA	9	1.06
(2,157)	1:37:A:TYR:HE2	1:38:A:PHE:HA	9	1.06
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	4	1.06
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	8	1.06
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	2	1.05
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	2	1.05
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	2	1.05
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	2	1.04
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	2	1.04
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	2	1.04
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE1	9	1.04
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE2	9	1.04
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	1	1.03
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	1	1.03
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	1	1.03
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	6	1.01
(1,2714)	1:144:A:GLY:HA2	1:145:A:HIS:HD2	4	1.0
(1,2714)	1:144:A:GLY:HA3	1:145:A:HIS:HD2	4	1.0
(1,374)	1:27:A:ALA:HB1	1:28:A:GLU:HG3	4	1.0
(1,374)	1:27:A:ALA:HB2	1:28:A:GLU:HG3	4	1.0
(1,374)	1:27:A:ALA:HB3	1:28:A:GLU:HG3	4	1.0
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	5	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	2	0.99
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	4	0.99
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	4	0.99
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	4	0.99
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	3	0.98
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	3	0.98
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	3	0.98
(1,288)	1:17:A:LYS:HB3	1:19:A:ILE:HG12	6	0.98
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	8	0.97
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	8	0.97
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	8	0.97
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE1	9	0.97
(2,67)	1:17:A:LYS:HB3	1:24:A:TYR:HE2	9	0.97
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	8	0.97
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	8	0.97
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	8	0.97
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	5	0.97
(2,467)	1:63:A:ARG:HB2	1:66:A:PHE:HZ	5	0.96
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	7	0.96
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	7	0.96
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	7	0.96
(1,656)	1:45:A:LEU:HA	1:185:A:ILE:HG12	9	0.96
(1,526)	1:49:A:ARG:HA	1:49:A:ARG:HD3	10	0.96
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	8	0.96
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	8	0.96
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	8	0.96
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	5	0.95
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	5	0.95
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	5	0.95
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	4	0.94
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	4	0.94
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	4	0.94
(2,161)	1:34:A:GLU:HA	1:38:A:PHE:HB3	7	0.94
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	10	0.94
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	10	0.94
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	10	0.94
(1,288)	1:17:A:LYS:HB3	1:19:A:ILE:HG12	8	0.94
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	6	0.93
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	6	0.93
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	6	0.93
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	6	0.93
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	6	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	10	0.93
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	10	0.93
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	10	0.93
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	2	0.92
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	2	0.92
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	3	0.91
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	3	0.91
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	3	0.91
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	8	0.91
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	8	0.91
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	8	0.91
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	9	0.91
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	9	0.91
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	9	0.91
(2,99)	1:17:A:LYS:HB3	1:19:A:ILE:HB	8	0.9
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	9	0.9
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	9	0.9
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	9	0.9
(2,99)	1:17:A:LYS:HB3	1:19:A:ILE:HB	6	0.89
(1,2840)	1:176:A:LYS:HD2	1:179:A:GLU:HB3	4	0.89
(1,2840)	1:176:A:LYS:HD3	1:179:A:GLU:HB3	4	0.89
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	6	0.89
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	6	0.89
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	6	0.89
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	9	0.88
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	9	0.88
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	9	0.88
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	9	0.88
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	9	0.88
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	9	0.88
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	9	0.88
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	9	0.88
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	9	0.88
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE1	1	0.88
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE2	1	0.88
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE3	1	0.88
(1,447)	1:45:A:LEU:HD21	1:148:A:LYS:HE3	6	0.88
(1,447)	1:45:A:LEU:HD22	1:148:A:LYS:HE3	6	0.88
(1,447)	1:45:A:LEU:HD23	1:148:A:LYS:HE3	6	0.88
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	9	0.88
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	5	0.87
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD11	9	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD12	9	0.87
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD13	9	0.87
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD11	9	0.87
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD12	9	0.87
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD13	9	0.87
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD11	9	0.87
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD12	9	0.87
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD13	9	0.87
(1,225)	1:14:A:VAL:HG21	1:28:A:GLU:HB2	2	0.87
(1,225)	1:14:A:VAL:HG22	1:28:A:GLU:HB2	2	0.87
(1,225)	1:14:A:VAL:HG23	1:28:A:GLU:HB2	2	0.87
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	8	0.86
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	8	0.86
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	8	0.86
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	8	0.86
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE2	8	0.85
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE3	8	0.85
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	1	0.85
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	1	0.85
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	1	0.85
(1,817)	1:128:A:ILE:HD11	1:136:A:ILE:HG12	3	0.85
(1,817)	1:128:A:ILE:HD12	1:136:A:ILE:HG12	3	0.85
(1,817)	1:128:A:ILE:HD13	1:136:A:ILE:HG12	3	0.85
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	6	0.84
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	6	0.84
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	6	0.84
(1,2714)	1:144:A:GLY:HA2	1:145:A:HIS:HD2	3	0.84
(1,2714)	1:144:A:GLY:HA3	1:145:A:HIS:HD2	3	0.84
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	4	0.84
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	4	0.84
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	4	0.84
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	4	0.84
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	4	0.84
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	4	0.84
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	2	0.84
(1,44)	1:100:A:ILE:HD11	1:110:A:LEU:HD11	1	0.84
(1,44)	1:100:A:ILE:HD11	1:110:A:LEU:HD12	1	0.84
(1,44)	1:100:A:ILE:HD11	1:110:A:LEU:HD13	1	0.84
(1,44)	1:100:A:ILE:HD12	1:110:A:LEU:HD11	1	0.84
(1,44)	1:100:A:ILE:HD12	1:110:A:LEU:HD12	1	0.84
(1,44)	1:100:A:ILE:HD12	1:110:A:LEU:HD13	1	0.84
(1,44)	1:100:A:ILE:HD13	1:110:A:LEU:HD11	1	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:100:A:ILE:HD13	1:110:A:LEU:HD12	1	0.84
(1,44)	1:100:A:ILE:HD13	1:110:A:LEU:HD13	1	0.84
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	4	0.83
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	4	0.83
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	4	0.83
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	4	0.83
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	1	0.83
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	1	0.83
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	1	0.83
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	1	0.83
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	1	0.83
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	1	0.83
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	6	0.82
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	6	0.82
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	6	0.82
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	6	0.82
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	6	0.82
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	6	0.82
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	8	0.82
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	8	0.82
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	8	0.82
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE1	8	0.82
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE2	8	0.82
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE3	8	0.82
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	5	0.81
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	5	0.81
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	5	0.81
(1,531)	1:47:A:VAL:HG11	1:49:A:ARG:HD2	10	0.81
(1,531)	1:47:A:VAL:HG12	1:49:A:ARG:HD2	10	0.81
(1,531)	1:47:A:VAL:HG13	1:49:A:ARG:HD2	10	0.81
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	3	0.8
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	3	0.8
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	3	0.8
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	3	0.8
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	3	0.8
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	3	0.8
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	9	0.8
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	9	0.8
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	9	0.8
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG21	6	0.8
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG22	6	0.8
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG23	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG21	6	0.8
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG22	6	0.8
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG23	6	0.8
(2,161)	1:34:A:GLU:HA	1:38:A:PHE:HB3	3	0.79
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	6	0.79
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	6	0.79
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	6	0.79
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	6	0.79
(1,1972)	1:145:A:HIS:H	1:145:A:HIS:HD2	3	0.79
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG21	5	0.79
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG22	5	0.79
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG23	5	0.79
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG21	5	0.79
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG22	5	0.79
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG23	5	0.79
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	6	0.79
(1,653)	1:59:A:ASP:HA	1:87:A:MET:HB3	1	0.79
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	3	0.78
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	3	0.78
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	10	0.77
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	10	0.77
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD11	6	0.77
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD12	6	0.77
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD13	6	0.77
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD11	6	0.77
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD12	6	0.77
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD13	6	0.77
(2,161)	1:34:A:GLU:HA	1:38:A:PHE:HB3	5	0.77
(2,99)	1:17:A:LYS:HB3	1:19:A:ILE:HB	9	0.77
(2,99)	1:17:A:LYS:HB3	1:19:A:ILE:HB	10	0.77
(1,817)	1:128:A:ILE:HD11	1:136:A:ILE:HG12	8	0.77
(1,817)	1:128:A:ILE:HD12	1:136:A:ILE:HG12	8	0.77
(1,817)	1:128:A:ILE:HD13	1:136:A:ILE:HG12	8	0.77
(1,433)	1:45:A:LEU:HD11	1:145:A:HIS:HD2	7	0.77
(1,433)	1:45:A:LEU:HD12	1:145:A:HIS:HD2	7	0.77
(1,433)	1:45:A:LEU:HD13	1:145:A:HIS:HD2	7	0.77
(1,1972)	1:145:A:HIS:H	1:145:A:HIS:HD2	4	0.76
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	5	0.76
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	5	0.76
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	5	0.76
(1,178)	1:12:A:ASN:HA	1:49:A:ARG:HD2	7	0.76
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	5	0.76
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	5	0.76
(1,2558)	1:100:A:ILE:HG12	1:110:A:LEU:HD11	6	0.75
(1,2558)	1:100:A:ILE:HG12	1:110:A:LEU:HD12	6	0.75
(1,2558)	1:100:A:ILE:HG12	1:110:A:LEU:HD13	6	0.75
(1,2558)	1:100:A:ILE:HG13	1:110:A:LEU:HD11	6	0.75
(1,2558)	1:100:A:ILE:HG13	1:110:A:LEU:HD12	6	0.75
(1,2558)	1:100:A:ILE:HG13	1:110:A:LEU:HD13	6	0.75
(1,653)	1:59:A:ASP:HA	1:87:A:MET:HB3	6	0.75
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	6	0.74
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	6	0.74
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	6	0.74
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	7	0.74
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	7	0.74
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	7	0.74
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	7	0.74
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	7	0.74
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	7	0.74
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	5	0.73
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	1	0.73
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	1	0.73
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	1	0.73
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	9	0.73
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG21	2	0.73
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG22	2	0.73
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG23	2	0.73
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG21	2	0.73
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG22	2	0.73
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG23	2	0.73
(1,213)	1:14:A:VAL:HG11	1:49:A:ARG:HG2	10	0.73
(1,213)	1:14:A:VAL:HG12	1:49:A:ARG:HG2	10	0.73
(1,213)	1:14:A:VAL:HG13	1:49:A:ARG:HG2	10	0.73
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	5	0.71
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	5	0.71
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE2	2	0.71
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE3	2	0.71
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	1	0.71
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	1	0.71
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	1	0.71
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	1	0.71
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	1	0.71
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	8	0.71
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	8	0.71
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	8	0.71
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	8	0.71
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	8	0.71
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	8	0.71
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	10	0.71
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	10	0.71
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	10	0.71
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	4	0.71
(1,178)	1:12:A:ASN:HA	1:49:A:ARG:HD2	10	0.71
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	4	0.7
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	4	0.7
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	4	0.7
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	4	0.7
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	4	0.7
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	4	0.7
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD2	4	0.7
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD3	4	0.7
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD2	4	0.7
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD3	4	0.7
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD2	4	0.7
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD3	4	0.7
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	1	0.7
(1,1177)	1:176:A:LYS:HB2	1:179:A:GLU:HB3	4	0.7
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	2	0.7
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	1	0.7
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	1	0.7
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	1	0.7
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	6	0.69
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	10	0.69
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	5	0.69
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	5	0.69
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	5	0.69
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	5	0.69
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	7	0.69
(1,719)	1:100:A:ILE:HD11	1:110:A:LEU:HB2	2	0.69
(1,719)	1:100:A:ILE:HD12	1:110:A:LEU:HB2	2	0.69
(1,719)	1:100:A:ILE:HD13	1:110:A:LEU:HB2	2	0.69
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	9	0.68
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	10	0.68
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	10	0.68
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG11	4	0.68
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG12	4	0.68
(1,1390)	1:48:A:ILE:HG13	1:55:A:VAL:HG13	4	0.68
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	4	0.68
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	4	0.68
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	4	0.68
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	3	0.68
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	2	0.67
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	2	0.67
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	2	0.67
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	2	0.67
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	7	0.67
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	7	0.67
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	7	0.67
(1,2840)	1:176:A:LYS:HD2	1:179:A:GLU:HB3	8	0.67
(1,2840)	1:176:A:LYS:HD3	1:179:A:GLU:HB3	8	0.67
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	3	0.67
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	3	0.67
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	3	0.67
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	3	0.67
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	3	0.67
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	3	0.67
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	9	0.67
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	6	0.67
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	6	0.67
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	6	0.67
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD1	8	0.67
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD2	8	0.67
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE2	4	0.66
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE3	4	0.66
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	7	0.66
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	7	0.66
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	7	0.66
(2,12)	1:37:A:TYR:HE1	1:38:A:PHE:HZ	2	0.66
(2,12)	1:37:A:TYR:HE2	1:38:A:PHE:HZ	2	0.66
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	3	0.66
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	7	0.66
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD1	6	0.66
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD2	6	0.66
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	1	0.66
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	1	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	1	0.66
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE2	6	0.65
(2,943)	1:41:A:LEU:HB2	1:44:A:LYS:HE3	6	0.65
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	7	0.65
(1,1264)	1:142:A:VAL:HG11	1:145:A:HIS:HD2	4	0.65
(1,1264)	1:142:A:VAL:HG12	1:145:A:HIS:HD2	4	0.65
(1,1264)	1:142:A:VAL:HG13	1:145:A:HIS:HD2	4	0.65
(1,859)	1:163:A:CYS:HB3	1:185:A:ILE:HD11	6	0.65
(1,859)	1:163:A:CYS:HB3	1:185:A:ILE:HD12	6	0.65
(1,859)	1:163:A:CYS:HB3	1:185:A:ILE:HD13	6	0.65
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	1	0.64
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	1	0.64
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	1	0.64
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	1	0.64
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	6	0.64
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	6	0.64
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	6	0.64
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	6	0.64
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	6	0.64
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	6	0.64
(1,2383)	1:41:A:LEU:HD11	1:44:A:LYS:HD2	10	0.64
(1,2383)	1:41:A:LEU:HD11	1:44:A:LYS:HD3	10	0.64
(1,2383)	1:41:A:LEU:HD12	1:44:A:LYS:HD2	10	0.64
(1,2383)	1:41:A:LEU:HD12	1:44:A:LYS:HD3	10	0.64
(1,2383)	1:41:A:LEU:HD13	1:44:A:LYS:HD2	10	0.64
(1,2383)	1:41:A:LEU:HD13	1:44:A:LYS:HD3	10	0.64
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	6	0.64
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	8	0.63
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	5	0.63
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	1	0.63
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	9	0.63
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	3	0.63
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	3	0.62
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	1	0.62
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	1	0.62
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	1	0.62
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	1	0.62
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD2	6	0.62
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD3	6	0.62
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD2	6	0.62
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD3	6	0.62
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD2	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD3	6	0.62
(1,1179)	1:175:A:LYS:HB2	1:179:A:GLU:HB2	10	0.62
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	8	0.62
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	8	0.62
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	8	0.62
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD1	10	0.62
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD2	10	0.62
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	4	0.62
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	4	0.62
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	4	0.62
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	7	0.61
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD11	10	0.61
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD12	10	0.61
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD13	10	0.61
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	8	0.61
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	8	0.61
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	8	0.61
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	8	0.61
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	7	0.61
(2,365)	1:31:A:GLU:HB3	1:33:A:LEU:HG	9	0.6
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	5	0.6
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	5	0.6
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	5	0.6
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	5	0.6
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	5	0.6
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	5	0.6
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	3	0.6
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	3	0.6
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	3	0.6
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	7	0.6
(1,178)	1:12:A:ASN:HA	1:49:A:ARG:HD2	5	0.6
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	7	0.6
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	7	0.6
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	7	0.6
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD2	5	0.59
(1,2496)	1:82:A:ILE:HG21	1:103:A:LYS:HD3	5	0.59
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD2	5	0.59
(1,2496)	1:82:A:ILE:HG22	1:103:A:LYS:HD3	5	0.59
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD2	5	0.59
(1,2496)	1:82:A:ILE:HG23	1:103:A:LYS:HD3	5	0.59
(1,2363)	1:32:A:ASN:H	1:34:A:GLU:HG2	4	0.59
(1,2363)	1:32:A:ASN:H	1:34:A:GLU:HG3	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	2	0.59
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	10	0.59
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	10	0.59
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	10	0.59
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	10	0.59
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	10	0.58
(1,653)	1:59:A:ASP:HA	1:87:A:MET:HB3	3	0.58
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	2	0.58
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	2	0.58
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	2	0.58
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD11	8	0.58
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD12	8	0.58
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD13	8	0.58
(1,173)	1:11:A:ILE:HG21	1:46:A:SER:HB3	9	0.58
(1,173)	1:11:A:ILE:HG22	1:46:A:SER:HB3	9	0.58
(1,173)	1:11:A:ILE:HG23	1:46:A:SER:HB3	9	0.58
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	3	0.58
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	3	0.58
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	3	0.58
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	6	0.57
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	6	0.57
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	1	0.57
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	7	0.57
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	7	0.57
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	7	0.57
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	10	0.57
(1,719)	1:100:A:ILE:HD11	1:110:A:LEU:HB2	7	0.57
(1,719)	1:100:A:ILE:HD12	1:110:A:LEU:HB2	7	0.57
(1,719)	1:100:A:ILE:HD13	1:110:A:LEU:HB2	7	0.57
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	8	0.57
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	8	0.57
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	8	0.57
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD11	6	0.57
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD12	6	0.57
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD13	6	0.57
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	3	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD11	9	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD12	9	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD13	9	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD11	10	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD12	10	0.56
(1,283)	1:17:A:LYS:HB3	1:19:A:ILE:HD13	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD1	9	0.56
(1,249)	1:17:A:LYS:HB3	1:24:A:TYR:HD2	9	0.56
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	1	0.56
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD11	2	0.56
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD12	2	0.56
(1,60)	1:17:A:LYS:HD3	1:26:A:ILE:HD13	2	0.56
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	4	0.55
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	4	0.55
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	4	0.55
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	4	0.55
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	6	0.55
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	6	0.55
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	6	0.55
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	6	0.55
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	6	0.55
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	6	0.55
(1,2043)	1:178:A:ASP:H	1:179:A:GLU:HB3	4	0.55
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	4	0.55
(1,1264)	1:142:A:VAL:HG11	1:145:A:HIS:HD2	3	0.55
(1,1264)	1:142:A:VAL:HG12	1:145:A:HIS:HD2	3	0.55
(1,1264)	1:142:A:VAL:HG13	1:145:A:HIS:HD2	3	0.55
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	2	0.55
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	2	0.55
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	2	0.55
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	4	0.55
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	4	0.55
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	4	0.55
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	4	0.55
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	4	0.55
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	3	0.54
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	3	0.54
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	1	0.54
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	1	0.54
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD11	10	0.54
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD12	10	0.54
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD13	10	0.54
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	7	0.54
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	7	0.54
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	7	0.54
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	1	0.54
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	9	0.54
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	5	0.53
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	5	0.53
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	1	0.53
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	1	0.53
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	1	0.53
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	5	0.53
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	5	0.53
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	5	0.53
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	5	0.53
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	5	0.53
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	5	0.53
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	6	0.53
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	6	0.53
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	6	0.53
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	6	0.53
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	6	0.53
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	6	0.53
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	6	0.53
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	6	0.53
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	6	0.53
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	1	0.53
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	1	0.53
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	1	0.53
(1,677)	1:176:A:LYS:HB2	1:179:A:GLU:HA	3	0.53
(1,653)	1:59:A:ASP:HA	1:87:A:MET:HB3	7	0.53
(1,599)	1:55:A:VAL:HG11	1:83:A:PHE:HB2	7	0.53
(1,599)	1:55:A:VAL:HG12	1:83:A:PHE:HB2	7	0.53
(1,599)	1:55:A:VAL:HG13	1:83:A:PHE:HB2	7	0.53
(1,536)	1:12:A:ASN:HB2	1:49:A:ARG:HG2	10	0.53
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	8	0.53
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	8	0.52
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	8	0.52
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	8	0.52
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	8	0.52
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	6	0.52
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	8	0.52
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	8	0.52
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	8	0.52
(1,360)	1:17:A:LYS:HD3	1:26:A:ILE:HG13	2	0.52
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	1	0.52
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	1	0.52
(1,245)	1:17:A:LYS:HB2	1:24:A:TYR:HB3	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	8	0.52
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	8	0.52
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	8	0.52
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	4	0.51
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	2	0.51
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	2	0.51
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	2	0.51
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD11	9	0.51
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD12	9	0.51
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD13	9	0.51
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	4	0.51
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	4	0.51
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	4	0.51
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	4	0.51
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	4	0.51
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	4	0.51
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	4	0.51
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	4	0.51
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	4	0.51
(1,2043)	1:178:A:ASP:H	1:179:A:GLU:HB3	8	0.51
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	3	0.51
(1,1373)	1:142:A:VAL:HG21	1:145:A:HIS:HD2	3	0.51
(1,1373)	1:142:A:VAL:HG22	1:145:A:HIS:HD2	3	0.51
(1,1373)	1:142:A:VAL:HG23	1:145:A:HIS:HD2	3	0.51
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	10	0.51
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	10	0.51
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	10	0.51
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	3	0.51
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	3	0.51
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	3	0.51
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	9	0.51
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	9	0.51
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	9	0.51
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	3	0.5
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	3	0.5
(2,365)	1:31:A:GLU:HB3	1:33:A:LEU:HG	2	0.5
(2,284)	1:99:A:THR:HG21	1:128:A:ILE:HD11	6	0.5
(2,284)	1:99:A:THR:HG21	1:128:A:ILE:HD12	6	0.5
(2,284)	1:99:A:THR:HG21	1:128:A:ILE:HD13	6	0.5
(2,284)	1:99:A:THR:HG22	1:128:A:ILE:HD11	6	0.5
(2,284)	1:99:A:THR:HG22	1:128:A:ILE:HD12	6	0.5
(2,284)	1:99:A:THR:HG22	1:128:A:ILE:HD13	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,284)	1:99:A:THR:HG23	1:128:A:ILE:HD11	6	0.5
(2,284)	1:99:A:THR:HG23	1:128:A:ILE:HD12	6	0.5
(2,284)	1:99:A:THR:HG23	1:128:A:ILE:HD13	6	0.5
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	2	0.5
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	2	0.5
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	2	0.5
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	2	0.5
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	8	0.5
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	5	0.5
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	5	0.5
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	7	0.5
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	7	0.5
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	4	0.5
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	4	0.5
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	4	0.5
(1,124)	1:27:A:ALA:HB1	1:37:A:TYR:HE1	4	0.5
(1,124)	1:27:A:ALA:HB1	1:37:A:TYR:HE2	4	0.5
(1,124)	1:27:A:ALA:HB2	1:37:A:TYR:HE1	4	0.5
(1,124)	1:27:A:ALA:HB2	1:37:A:TYR:HE2	4	0.5
(1,124)	1:27:A:ALA:HB3	1:37:A:TYR:HE1	4	0.5
(1,124)	1:27:A:ALA:HB3	1:37:A:TYR:HE2	4	0.5
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	8	0.49
(2,542)	1:114:A:ASN:HA	1:116:A:ILE:HG12	1	0.48
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD11	9	0.48
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD12	9	0.48
(2,221)	1:64:A:PRO:HG3	1:65:A:LEU:HD13	9	0.48
(1,2727)	1:147:A:ASN:HD21	1:190:A:GLN:HE21	5	0.48
(1,2727)	1:147:A:ASN:HD22	1:190:A:GLN:HE21	5	0.48
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	2	0.48
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	2	0.48
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	2	0.48
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	2	0.48
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	2	0.48
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	2	0.48
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	4	0.48
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	3	0.48
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	7	0.48
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	8	0.47
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	8	0.47
(2,407)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	1	0.47
(2,407)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	1	0.47
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	1	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	1	0.47
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	1	0.47
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	7	0.47
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	7	0.47
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	7	0.47
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG2	1	0.47
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG3	1	0.47
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG2	5	0.47
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG3	5	0.47
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	2	0.47
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	2	0.47
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD1	3	0.47
(1,267)	1:17:A:LYS:HG2	1:24:A:TYR:HD2	3	0.47
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	5	0.47
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	5	0.47
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	5	0.47
(1,252)	1:17:A:LYS:HB3	1:24:A:TYR:HB3	10	0.47
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG2	8	0.46
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG3	8	0.46
(1,2726)	1:147:A:ASN:HD21	1:190:A:GLN:HE22	9	0.46
(1,2726)	1:147:A:ASN:HD22	1:190:A:GLN:HE22	9	0.46
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	5	0.46
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	5	0.46
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	5	0.46
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	5	0.46
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	5	0.46
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	5	0.46
(1,2441)	1:60:A:GLN:HB2	1:88:A:TYR:HA	8	0.46
(1,2441)	1:60:A:GLN:HB3	1:88:A:TYR:HA	8	0.46
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	2	0.46
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	8	0.46
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	9	0.46
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	9	0.46
(1,427)	1:41:A:LEU:HD11	1:185:A:ILE:HD11	1	0.46
(1,427)	1:41:A:LEU:HD11	1:185:A:ILE:HD12	1	0.46
(1,427)	1:41:A:LEU:HD11	1:185:A:ILE:HD13	1	0.46
(1,427)	1:41:A:LEU:HD12	1:185:A:ILE:HD11	1	0.46
(1,427)	1:41:A:LEU:HD12	1:185:A:ILE:HD12	1	0.46
(1,427)	1:41:A:LEU:HD12	1:185:A:ILE:HD13	1	0.46
(1,427)	1:41:A:LEU:HD13	1:185:A:ILE:HD11	1	0.46
(1,427)	1:41:A:LEU:HD13	1:185:A:ILE:HD12	1	0.46
(1,427)	1:41:A:LEU:HD13	1:185:A:ILE:HD13	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB1	8	0.46
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB2	8	0.46
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB3	8	0.46
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB1	8	0.46
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB2	8	0.46
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB3	8	0.46
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB1	8	0.46
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB2	8	0.46
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB3	8	0.46
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	2	0.45
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	2	0.45
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	2	0.45
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	7	0.45
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	7	0.45
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	7	0.45
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	7	0.45
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	7	0.45
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	7	0.45
(1,2141)	1:49:A:ARG:HD3	1:190:A:GLN:HE21	8	0.45
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	6	0.45
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	6	0.45
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	6	0.45
(1,468)	1:47:A:VAL:HG21	1:148:A:LYS:HD3	3	0.45
(1,468)	1:47:A:VAL:HG22	1:148:A:LYS:HD3	3	0.45
(1,468)	1:47:A:VAL:HG23	1:148:A:LYS:HD3	3	0.45
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	10	0.45
(2,170)	1:58:A:ILE:HD11	1:65:A:LEU:HB3	8	0.44
(2,170)	1:58:A:ILE:HD12	1:65:A:LEU:HB3	8	0.44
(2,170)	1:58:A:ILE:HD13	1:65:A:LEU:HB3	8	0.44
(2,170)	1:58:A:ILE:HD11	1:65:A:LEU:HB3	9	0.44
(2,170)	1:58:A:ILE:HD12	1:65:A:LEU:HB3	9	0.44
(2,170)	1:58:A:ILE:HD13	1:65:A:LEU:HB3	9	0.44
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG2	4	0.44
(1,2774)	1:164:A:GLU:HA	1:165:A:LYS:HG3	4	0.44
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	5	0.44
(1,1166)	1:109:A:THR:HG21	1:122:A:MET:HG2	10	0.44
(1,1166)	1:109:A:THR:HG22	1:122:A:MET:HG2	10	0.44
(1,1166)	1:109:A:THR:HG23	1:122:A:MET:HG2	10	0.44
(2,400)	1:120:A:LYS:HD3	1:122:A:MET:HE1	8	0.43
(2,400)	1:120:A:LYS:HD3	1:122:A:MET:HE2	8	0.43
(2,400)	1:120:A:LYS:HD3	1:122:A:MET:HE3	8	0.43
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1762)	1:50:A:ASN:H	1:51:A:LEU:HB2	6	0.43
(1,1177)	1:176:A:LYS:HB2	1:179:A:GLU:HB3	8	0.43
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	6	0.43
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	6	0.43
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	6	0.43
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	3	0.43
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	3	0.43
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	3	0.43
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	5	0.43
(2,313)	1:14:A:VAL:HG21	1:49:A:ARG:HB3	5	0.42
(2,313)	1:14:A:VAL:HG22	1:49:A:ARG:HB3	5	0.42
(2,313)	1:14:A:VAL:HG23	1:49:A:ARG:HB3	5	0.42
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	10	0.42
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	10	0.42
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	10	0.42
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	10	0.42
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	4	0.42
(1,252)	1:17:A:LYS:HB3	1:24:A:TYR:HB3	9	0.42
(1,173)	1:11:A:ILE:HG21	1:46:A:SER:HB3	6	0.42
(1,173)	1:11:A:ILE:HG22	1:46:A:SER:HB3	6	0.42
(1,173)	1:11:A:ILE:HG23	1:46:A:SER:HB3	6	0.42
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	6	0.41
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	6	0.41
(2,365)	1:31:A:GLU:HB3	1:33:A:LEU:HG	4	0.41
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	9	0.41
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	9	0.41
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	9	0.41
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	9	0.41
(1,599)	1:55:A:VAL:HG11	1:83:A:PHE:HB2	3	0.41
(1,599)	1:55:A:VAL:HG12	1:83:A:PHE:HB2	3	0.41
(1,599)	1:55:A:VAL:HG13	1:83:A:PHE:HB2	3	0.41
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	3	0.4
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	3	0.4
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	3	0.4
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	3	0.4
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	3	0.4
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	3	0.4
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	2	0.4
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	2	0.4
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	2	0.4
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	2	0.4
(1,245)	1:17:A:LYS:HB2	1:24:A:TYR:HB3	10	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2528)	1:91:A:SER:HB2	1:96:A:MET:HA	7	0.39
(1,2528)	1:91:A:SER:HB3	1:96:A:MET:HA	7	0.39
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	3	0.39
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	3	0.39
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	3	0.39
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG21	10	0.39
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG22	10	0.39
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG23	10	0.39
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	3	0.39
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	3	0.39
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	3	0.39
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	3	0.39
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	3	0.39
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	3	0.39
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	3	0.39
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	3	0.39
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	3	0.39
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG21	10	0.39
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG22	10	0.39
(1,408)	1:148:A:LYS:HG2	1:188:A:THR:HG23	10	0.39
(2,467)	1:63:A:ARG:HB2	1:66:A:PHE:HZ	8	0.38
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	4	0.38
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	4	0.38
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	4	0.38
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	4	0.38
(1,2188)	1:51:A:LEU:H	1:54:A:GLN:HG3	5	0.38
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	10	0.38
(1,1756)	1:49:A:ARG:HD3	1:50:A:ASN:H	6	0.37
(1,1154)	1:114:A:ASN:HB2	1:116:A:ILE:HG12	6	0.37
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG21	10	0.37
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG22	10	0.37
(1,1033)	1:88:A:TYR:HD1	1:99:A:THR:HG23	10	0.37
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG21	10	0.37
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG22	10	0.37
(1,1033)	1:88:A:TYR:HD2	1:99:A:THR:HG23	10	0.37
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	5	0.37
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	5	0.37
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	5	0.37
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD11	9	0.37
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD12	9	0.37
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD13	9	0.37
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	2	0.37
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	2	0.37
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	2	0.37
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	2	0.37
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	2	0.37
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	2	0.37
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	2	0.37
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	2	0.37
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG2	1	0.36
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG3	1	0.36
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	9	0.36
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	9	0.36
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	9	0.36
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	9	0.36
(1,2141)	1:49:A:ARG:HD3	1:190:A:GLN:HE21	6	0.36
(1,1935)	1:108:A:SER:HB2	1:120:A:LYS:H	7	0.36
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	4	0.36
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	4	0.36
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	4	0.36
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	2	0.36
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	9	0.36
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	9	0.36
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	9	0.36
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	9	0.36
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	9	0.36
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	9	0.36
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	9	0.36
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	9	0.36
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	9	0.36
(1,448)	1:45:A:LEU:HD21	1:46:A:SER:HB2	7	0.36
(1,448)	1:45:A:LEU:HD22	1:46:A:SER:HB2	7	0.36
(1,448)	1:45:A:LEU:HD23	1:46:A:SER:HB2	7	0.36
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	7	0.36
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE1	2	0.36
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE2	2	0.36
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	7	0.35
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	7	0.35
(2,365)	1:31:A:GLU:HB3	1:33:A:LEU:HG	1	0.35
(2,365)	1:31:A:GLU:HB3	1:33:A:LEU:HG	7	0.35
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD11	10	0.35
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD12	10	0.35
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD13	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,817)	1:128:A:ILE:HD11	1:136:A:ILE:HG12	1	0.35
(1,817)	1:128:A:ILE:HD12	1:136:A:ILE:HG12	1	0.35
(1,817)	1:128:A:ILE:HD13	1:136:A:ILE:HG12	1	0.35
(1,599)	1:55:A:VAL:HG11	1:83:A:PHE:HB2	6	0.35
(1,599)	1:55:A:VAL:HG12	1:83:A:PHE:HB2	6	0.35
(1,599)	1:55:A:VAL:HG13	1:83:A:PHE:HB2	6	0.35
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	5	0.35
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	5	0.35
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	5	0.35
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	5	0.35
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	5	0.35
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	5	0.35
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	5	0.35
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	5	0.35
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	5	0.35
(1,252)	1:17:A:LYS:HB3	1:24:A:TYR:HB3	8	0.35
(1,137)	1:92:A:GLN:HB2	1:93:A:PRO:HG3	7	0.35
(1,127)	1:88:A:TYR:HE1	1:97:A:ALA:HB1	10	0.35
(1,127)	1:88:A:TYR:HE1	1:97:A:ALA:HB2	10	0.35
(1,127)	1:88:A:TYR:HE1	1:97:A:ALA:HB3	10	0.35
(1,127)	1:88:A:TYR:HE2	1:97:A:ALA:HB1	10	0.35
(1,127)	1:88:A:TYR:HE2	1:97:A:ALA:HB2	10	0.35
(1,127)	1:88:A:TYR:HE2	1:97:A:ALA:HB3	10	0.35
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG21	9	0.34
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG22	9	0.34
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG23	9	0.34
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG21	6	0.34
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG22	6	0.34
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG23	6	0.34
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	6	0.34
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	6	0.34
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	6	0.34
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE1	9	0.34
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE2	9	0.34
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE3	9	0.34
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	10	0.34
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	8	0.34
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	8	0.34
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	8	0.34
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	2	0.34
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	3	0.34
(2,71)	1:9:A:ASN:HA	1:44:A:LYS:HD2	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG21	10	0.33
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG22	10	0.33
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG23	10	0.33
(1,2271)	1:45:A:LEU:H	1:185:A:ILE:HD11	3	0.33
(1,2271)	1:45:A:LEU:H	1:185:A:ILE:HD12	3	0.33
(1,2271)	1:45:A:LEU:H	1:185:A:ILE:HD13	3	0.33
(1,1373)	1:142:A:VAL:HG21	1:145:A:HIS:HD2	4	0.33
(1,1373)	1:142:A:VAL:HG22	1:145:A:HIS:HD2	4	0.33
(1,1373)	1:142:A:VAL:HG23	1:145:A:HIS:HD2	4	0.33
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD11	4	0.33
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD12	4	0.33
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD13	4	0.33
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	1	0.33
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	1	0.33
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	1	0.33
(1,599)	1:55:A:VAL:HG11	1:83:A:PHE:HB2	4	0.33
(1,599)	1:55:A:VAL:HG12	1:83:A:PHE:HB2	4	0.33
(1,599)	1:55:A:VAL:HG13	1:83:A:PHE:HB2	4	0.33
(1,468)	1:47:A:VAL:HG21	1:148:A:LYS:HD3	1	0.33
(1,468)	1:47:A:VAL:HG22	1:148:A:LYS:HD3	1	0.33
(1,468)	1:47:A:VAL:HG23	1:148:A:LYS:HD3	1	0.33
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD11	7	0.33
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD12	7	0.33
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD13	7	0.33
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE1	4	0.33
(1,123)	1:34:A:GLU:HA	1:37:A:TYR:HE2	4	0.33
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	7	0.32
(2,967)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	7	0.32
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG2	2	0.32
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG3	2	0.32
(2,643)	1:41:A:LEU:HB3	1:183:A:ARG:H	10	0.32
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG21	6	0.32
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG22	6	0.32
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG23	6	0.32
(1,1154)	1:114:A:ASN:HB2	1:116:A:ILE:HG12	5	0.32
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	2	0.32
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	3	0.32
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	6	0.32
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	8	0.32
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	9	0.32
(2,125)	1:31:A:GLU:HB3	1:33:A:LEU:HD21	7	0.31
(2,125)	1:31:A:GLU:HB3	1:33:A:LEU:HD22	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:31:A:GLU:HB3	1:33:A:LEU:HD23	7	0.31
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	5	0.31
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	5	0.31
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	5	0.31
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG2	10	0.31
(1,2411)	1:47:A:VAL:HG11	1:190:A:GLN:HG3	10	0.31
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG2	10	0.31
(1,2411)	1:47:A:VAL:HG12	1:190:A:GLN:HG3	10	0.31
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG2	10	0.31
(1,2411)	1:47:A:VAL:HG13	1:190:A:GLN:HG3	10	0.31
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	1	0.31
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	1	0.31
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	1	0.31
(1,533)	1:14:A:VAL:HA	1:49:A:ARG:HG2	10	0.31
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	1	0.31
(1,529)	1:49:A:ARG:HB2	1:49:A:ARG:HD3	4	0.31
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	5	0.31
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG2	10	0.3
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG3	10	0.3
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG21	8	0.3
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG22	8	0.3
(2,69)	1:17:A:LYS:HB3	1:19:A:ILE:HG23	8	0.3
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	10	0.3
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	10	0.3
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	10	0.3
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	10	0.3
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	10	0.3
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	10	0.3
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	10	0.3
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	10	0.3
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	10	0.3
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	5	0.3
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	5	0.3
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	5	0.3
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	5	0.3
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	5	0.3
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	5	0.3
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	1	0.3
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	1	0.3
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	1	0.3
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	1	0.3
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	1	0.3
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	1	0.3
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	1	0.3
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	1	0.3
(1,1935)	1:108:A:SER:HB2	1:120:A:LYS:H	3	0.29
(1,1935)	1:108:A:SER:HB2	1:120:A:LYS:H	6	0.29
(1,1262)	1:114:A:ASN:HB3	1:116:A:ILE:HG12	1	0.29
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	1	0.29
(1,625)	1:56:A:LEU:HD21	1:57:A:PHE:HB3	10	0.29
(1,625)	1:56:A:LEU:HD22	1:57:A:PHE:HB3	10	0.29
(1,625)	1:56:A:LEU:HD23	1:57:A:PHE:HB3	10	0.29
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	4	0.29
(1,252)	1:17:A:LYS:HB3	1:24:A:TYR:HB3	6	0.29
(1,245)	1:17:A:LYS:HB2	1:24:A:TYR:HB3	8	0.29
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	6	0.29
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	6	0.29
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	6	0.29
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	1	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	1	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	6	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	6	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	7	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	7	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	10	0.28
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	10	0.28
(1,2789)	1:165:A:LYS:HA	1:165:A:LYS:HE2	3	0.28
(1,2789)	1:165:A:LYS:HA	1:165:A:LYS:HE3	3	0.28
(1,2789)	1:165:A:LYS:HA	1:165:A:LYS:HE2	6	0.28
(1,2789)	1:165:A:LYS:HA	1:165:A:LYS:HE3	6	0.28
(1,2141)	1:49:A:ARG:HD3	1:190:A:GLN:HE21	9	0.28
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	9	0.28
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	9	0.28
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	9	0.28
(1,719)	1:100:A:ILE:HD11	1:110:A:LEU:HB2	1	0.28
(1,719)	1:100:A:ILE:HD12	1:110:A:LEU:HB2	1	0.28
(1,719)	1:100:A:ILE:HD13	1:110:A:LEU:HB2	1	0.28
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	4	0.28
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	4	0.28
(1,266)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	4	0.28
(2,404)	1:58:A:ILE:HD11	1:64:A:PRO:HD3	2	0.27
(2,404)	1:58:A:ILE:HD12	1:64:A:PRO:HD3	2	0.27
(2,404)	1:58:A:ILE:HD13	1:64:A:PRO:HD3	2	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:34:A:GLU:HA	1:38:A:PHE:HB3	6	0.27
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	8	0.27
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	8	0.27
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	8	0.27
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	2	0.27
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	2	0.27
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	9	0.27
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	9	0.27
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	5	0.27
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	5	0.27
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	5	0.27
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	5	0.27
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	10	0.27
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	10	0.27
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	10	0.27
(1,1165)	1:109:A:THR:HB	1:122:A:MET:HG2	10	0.27
(1,1154)	1:114:A:ASN:HB2	1:116:A:ILE:HG12	10	0.27
(1,599)	1:55:A:VAL:HG11	1:83:A:PHE:HB2	2	0.27
(1,599)	1:55:A:VAL:HG12	1:83:A:PHE:HB2	2	0.27
(1,599)	1:55:A:VAL:HG13	1:83:A:PHE:HB2	2	0.27
(1,524)	1:49:A:ARG:HB2	1:51:A:LEU:HB2	7	0.27
(1,245)	1:17:A:LYS:HB2	1:24:A:TYR:HB3	6	0.27
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	1	0.27
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	1	0.27
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	1	0.27
(2,1040)	1:113:A:GLU:HG2	1:116:A:ILE:HD11	4	0.26
(2,1040)	1:113:A:GLU:HG2	1:116:A:ILE:HD12	4	0.26
(2,1040)	1:113:A:GLU:HG2	1:116:A:ILE:HD13	4	0.26
(2,1040)	1:113:A:GLU:HG3	1:116:A:ILE:HD11	4	0.26
(2,1040)	1:113:A:GLU:HG3	1:116:A:ILE:HD12	4	0.26
(2,1040)	1:113:A:GLU:HG3	1:116:A:ILE:HD13	4	0.26
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	7	0.26
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	7	0.26
(2,12)	1:37:A:TYR:HE1	1:38:A:PHE:HZ	1	0.26
(2,12)	1:37:A:TYR:HE2	1:38:A:PHE:HZ	1	0.26
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE2	5	0.26
(1,2824)	1:175:A:LYS:HB2	1:175:A:LYS:HE3	5	0.26
(1,2671)	1:131:A:THR:HA	1:132:A:LYS:HG2	1	0.26
(1,2671)	1:131:A:THR:HA	1:132:A:LYS:HG3	1	0.26
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	7	0.26
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	6	0.26
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	6	0.26
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	7	0.26
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	7	0.26
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	7	0.26
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	4	0.26
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	4	0.26
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	4	0.26
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	4	0.26
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	4	0.26
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	4	0.26
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	4	0.26
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	4	0.26
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	4	0.26
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	4	0.26
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	4	0.26
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	4	0.26
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	2	0.26
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	2	0.26
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	2	0.26
(2,1066)	1:149:A:MET:HB2	1:150:A:GLN:HE21	6	0.25
(2,1066)	1:149:A:MET:HB2	1:150:A:GLN:HE22	6	0.25
(2,1066)	1:149:A:MET:HB3	1:150:A:GLN:HE21	6	0.25
(2,1066)	1:149:A:MET:HB3	1:150:A:GLN:HE22	6	0.25
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	9	0.25
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	9	0.25
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	9	0.25
(1,2499)	1:82:A:ILE:HG12	1:103:A:LYS:HE2	4	0.25
(1,2499)	1:82:A:ILE:HG12	1:103:A:LYS:HE3	4	0.25
(1,2499)	1:82:A:ILE:HG13	1:103:A:LYS:HE2	4	0.25
(1,2499)	1:82:A:ILE:HG13	1:103:A:LYS:HE3	4	0.25
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD11	2	0.25
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD12	2	0.25
(1,628)	1:56:A:LEU:HD21	1:58:A:ILE:HD13	2	0.25
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD11	2	0.25
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD12	2	0.25
(1,628)	1:56:A:LEU:HD22	1:58:A:ILE:HD13	2	0.25
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD11	2	0.25
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD12	2	0.25
(1,628)	1:56:A:LEU:HD23	1:58:A:ILE:HD13	2	0.25
(1,468)	1:47:A:VAL:HG21	1:148:A:LYS:HD3	9	0.25
(1,468)	1:47:A:VAL:HG22	1:148:A:LYS:HD3	9	0.25
(1,468)	1:47:A:VAL:HG23	1:148:A:LYS:HD3	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:17:A:LYS:HD3	1:169:A:LEU:HD21	9	0.25
(1,258)	1:17:A:LYS:HD3	1:169:A:LEU:HD22	9	0.25
(1,258)	1:17:A:LYS:HD3	1:169:A:LEU:HD23	9	0.25
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD11	7	0.24
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD12	7	0.24
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD13	7	0.24
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD11	7	0.24
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD12	7	0.24
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD13	7	0.24
(2,12)	1:37:A:TYR:HE1	1:38:A:PHE:HZ	9	0.24
(2,12)	1:37:A:TYR:HE2	1:38:A:PHE:HZ	9	0.24
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE1	10	0.24
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE2	10	0.24
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE3	10	0.24
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE1	10	0.24
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE2	10	0.24
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE3	10	0.24
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE1	10	0.24
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE2	10	0.24
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE3	10	0.24
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	9	0.24
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	9	0.24
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	9	0.24
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD11	1	0.24
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD12	1	0.24
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD13	1	0.24
(1,654)	1:59:A:ASP:HA	1:87:A:MET:HE1	8	0.24
(1,654)	1:59:A:ASP:HA	1:87:A:MET:HE2	8	0.24
(1,654)	1:59:A:ASP:HA	1:87:A:MET:HE3	8	0.24
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG21	8	0.24
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG22	8	0.24
(1,454)	1:45:A:LEU:HD21	1:47:A:VAL:HG23	8	0.24
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG21	8	0.24
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG22	8	0.24
(1,454)	1:45:A:LEU:HD22	1:47:A:VAL:HG23	8	0.24
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG21	8	0.24
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG22	8	0.24
(1,454)	1:45:A:LEU:HD23	1:47:A:VAL:HG23	8	0.24
(1,93)	1:47:A:VAL:HG21	1:148:A:LYS:HE2	3	0.24
(1,93)	1:47:A:VAL:HG22	1:148:A:LYS:HE2	3	0.24
(1,93)	1:47:A:VAL:HG23	1:148:A:LYS:HE2	3	0.24
(1,93)	1:47:A:VAL:HG21	1:148:A:LYS:HE2	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:47:A:VAL:HG22	1:148:A:LYS:HE2	7	0.24
(1,93)	1:47:A:VAL:HG23	1:148:A:LYS:HE2	7	0.24
(2,891)	1:9:A:ASN:HB2	1:185:A:ILE:HG21	6	0.23
(2,891)	1:9:A:ASN:HB2	1:185:A:ILE:HG22	6	0.23
(2,891)	1:9:A:ASN:HB2	1:185:A:ILE:HG23	6	0.23
(2,891)	1:9:A:ASN:HB3	1:185:A:ILE:HG21	6	0.23
(2,891)	1:9:A:ASN:HB3	1:185:A:ILE:HG22	6	0.23
(2,891)	1:9:A:ASN:HB3	1:185:A:ILE:HG23	6	0.23
(2,106)	1:26:A:ILE:HG12	1:169:A:LEU:HB2	2	0.23
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG21	1	0.23
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG22	1	0.23
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG23	1	0.23
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	2	0.23
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	2	0.23
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	2	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	8	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	8	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	8	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	10	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	10	0.23
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	10	0.23
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	3	0.23
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	3	0.23
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	3	0.23
(1,531)	1:47:A:VAL:HG11	1:49:A:ARG:HD2	5	0.23
(1,531)	1:47:A:VAL:HG12	1:49:A:ARG:HD2	5	0.23
(1,531)	1:47:A:VAL:HG13	1:49:A:ARG:HD2	5	0.23
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	10	0.23
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	10	0.23
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	10	0.23
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	8	0.22
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	8	0.22
(1,2830)	1:175:A:LYS:HD2	1:179:A:GLU:HG2	8	0.22
(1,2830)	1:175:A:LYS:HD2	1:179:A:GLU:HG3	8	0.22
(1,2830)	1:175:A:LYS:HD3	1:179:A:GLU:HG2	8	0.22
(1,2830)	1:175:A:LYS:HD3	1:179:A:GLU:HG3	8	0.22
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	2	0.22
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	2	0.22
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	2	0.22
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	8	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD11	3	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD12	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD13	3	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD11	10	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD12	10	0.22
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD13	10	0.22
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD11	10	0.22
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD12	10	0.22
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD13	10	0.22
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	2	0.22
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	2	0.22
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	2	0.22
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD11	1	0.22
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD12	1	0.22
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD13	1	0.22
(1,269)	1:17:A:LYS:HG2	1:24:A:TYR:HB3	1	0.22
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB1	7	0.22
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB2	7	0.22
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB3	7	0.22
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB1	7	0.22
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB2	7	0.22
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB3	7	0.22
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB1	7	0.22
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB2	7	0.22
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB3	7	0.22
(1,43)	1:100:A:ILE:HD11	1:110:A:LEU:HD21	2	0.22
(1,43)	1:100:A:ILE:HD11	1:110:A:LEU:HD22	2	0.22
(1,43)	1:100:A:ILE:HD11	1:110:A:LEU:HD23	2	0.22
(1,43)	1:100:A:ILE:HD12	1:110:A:LEU:HD21	2	0.22
(1,43)	1:100:A:ILE:HD12	1:110:A:LEU:HD22	2	0.22
(1,43)	1:100:A:ILE:HD12	1:110:A:LEU:HD23	2	0.22
(1,43)	1:100:A:ILE:HD13	1:110:A:LEU:HD21	2	0.22
(1,43)	1:100:A:ILE:HD13	1:110:A:LEU:HD22	2	0.22
(1,43)	1:100:A:ILE:HD13	1:110:A:LEU:HD23	2	0.22
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG2	4	0.21
(2,966)	1:61:A:GLY:HA3	1:63:A:ARG:HG3	4	0.21
(2,962)	1:59:A:ASP:HB2	1:87:A:MET:HB3	4	0.21
(2,962)	1:59:A:ASP:HB3	1:87:A:MET:HB3	4	0.21
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD11	2	0.21
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD12	2	0.21
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD13	2	0.21
(1,179)	1:12:A:ASN:HA	1:49:A:ARG:HG3	8	0.21
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	2	0.2
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD21	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD22	6	0.2
(2,87)	1:18:A:PHE:HB3	1:23:A:LEU:HD23	6	0.2
(2,13)	1:30:A:ASP:HA	1:37:A:TYR:HE1	4	0.2
(2,13)	1:30:A:ASP:HA	1:37:A:TYR:HE2	4	0.2
(1,2499)	1:82:A:ILE:HG12	1:103:A:LYS:HE2	6	0.2
(1,2499)	1:82:A:ILE:HG12	1:103:A:LYS:HE3	6	0.2
(1,2499)	1:82:A:ILE:HG13	1:103:A:LYS:HE2	6	0.2
(1,2499)	1:82:A:ILE:HG13	1:103:A:LYS:HE3	6	0.2
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	10	0.2
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	10	0.2
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	10	0.2
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	10	0.2
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	10	0.2
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	10	0.2
(1,2142)	1:147:A:ASN:HB2	1:190:A:GLN:HE21	5	0.2
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	4	0.2
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	6	0.2
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	6	0.2
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	6	0.2
(1,1154)	1:114:A:ASN:HB2	1:116:A:ILE:HG12	2	0.2
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	3	0.2
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	3	0.2
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	3	0.2
(1,531)	1:47:A:VAL:HG11	1:49:A:ARG:HD2	7	0.2
(1,531)	1:47:A:VAL:HG12	1:49:A:ARG:HD2	7	0.2
(1,531)	1:47:A:VAL:HG13	1:49:A:ARG:HD2	7	0.2
(1,524)	1:49:A:ARG:HB2	1:51:A:LEU:HB2	10	0.2
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	3	0.2
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	3	0.2
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	3	0.2
(1,300)	1:21:A:ASN:HB2	1:119:A:PHE:HD1	1	0.2
(1,300)	1:21:A:ASN:HB2	1:119:A:PHE:HD2	1	0.2
(1,178)	1:12:A:ASN:HA	1:49:A:ARG:HD2	2	0.2
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	4	0.19
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	9	0.19
(1,2272)	1:45:A:LEU:H	1:185:A:ILE:HG21	6	0.19
(1,2272)	1:45:A:LEU:H	1:185:A:ILE:HG22	6	0.19
(1,2272)	1:45:A:LEU:H	1:185:A:ILE:HG23	6	0.19
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE1	3	0.19
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE2	3	0.19
(1,1323)	1:57:A:PHE:HB2	1:87:A:MET:HE3	3	0.19
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:175:A:LYS:HB2	1:179:A:GLU:HG2	6	0.19
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	4	0.19
(1,1006)	1:161:A:LEU:HD21	1:174:A:LEU:HB3	4	0.19
(1,1006)	1:161:A:LEU:HD22	1:174:A:LEU:HB3	4	0.19
(1,1006)	1:161:A:LEU:HD23	1:174:A:LEU:HB3	4	0.19
(1,855)	1:13:A:PHE:HE1	1:185:A:ILE:HD11	6	0.19
(1,855)	1:13:A:PHE:HE1	1:185:A:ILE:HD12	6	0.19
(1,855)	1:13:A:PHE:HE1	1:185:A:ILE:HD13	6	0.19
(1,855)	1:13:A:PHE:HE2	1:185:A:ILE:HD11	6	0.19
(1,855)	1:13:A:PHE:HE2	1:185:A:ILE:HD12	6	0.19
(1,855)	1:13:A:PHE:HE2	1:185:A:ILE:HD13	6	0.19
(1,640)	1:56:A:LEU:HG	1:58:A:ILE:HD11	9	0.19
(1,640)	1:56:A:LEU:HG	1:58:A:ILE:HD12	9	0.19
(1,640)	1:56:A:LEU:HG	1:58:A:ILE:HD13	9	0.19
(1,623)	1:56:A:LEU:HD21	1:66:A:PHE:HE1	8	0.19
(1,623)	1:56:A:LEU:HD21	1:66:A:PHE:HE2	8	0.19
(1,623)	1:56:A:LEU:HD22	1:66:A:PHE:HE1	8	0.19
(1,623)	1:56:A:LEU:HD22	1:66:A:PHE:HE2	8	0.19
(1,623)	1:56:A:LEU:HD23	1:66:A:PHE:HE1	8	0.19
(1,623)	1:56:A:LEU:HD23	1:66:A:PHE:HE2	8	0.19
(1,502)	1:48:A:ILE:HG21	1:57:A:PHE:HZ	6	0.19
(1,502)	1:48:A:ILE:HG22	1:57:A:PHE:HZ	6	0.19
(1,502)	1:48:A:ILE:HG23	1:57:A:PHE:HZ	6	0.19
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD11	7	0.19
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD12	7	0.19
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD13	7	0.19
(2,922)	1:32:A:ASN:HA	1:34:A:GLU:HG2	7	0.18
(2,922)	1:32:A:ASN:HA	1:34:A:GLU:HG3	7	0.18
(2,921)	1:30:A:ASP:HB2	1:37:A:TYR:HE1	1	0.18
(2,921)	1:30:A:ASP:HB2	1:37:A:TYR:HE2	1	0.18
(2,921)	1:30:A:ASP:HB3	1:37:A:TYR:HE1	1	0.18
(2,921)	1:30:A:ASP:HB3	1:37:A:TYR:HE2	1	0.18
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE1	2	0.18
(2,450)	1:65:A:LEU:HB3	1:66:A:PHE:HE2	2	0.18
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	1	0.18
(2,152)	1:43:A:SER:HB3	1:180:A:LEU:HD11	5	0.18
(2,152)	1:43:A:SER:HB3	1:180:A:LEU:HD12	5	0.18
(2,152)	1:43:A:SER:HB3	1:180:A:LEU:HD13	5	0.18
(2,106)	1:26:A:ILE:HG12	1:169:A:LEU:HB2	8	0.18
(1,2435)	1:58:A:ILE:HG21	1:63:A:ARG:HD2	2	0.18
(1,2435)	1:58:A:ILE:HG21	1:63:A:ARG:HD3	2	0.18
(1,2435)	1:58:A:ILE:HG22	1:63:A:ARG:HD2	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2435)	1:58:A:ILE:HG22	1:63:A:ARG:HD3	2	0.18
(1,2435)	1:58:A:ILE:HG23	1:63:A:ARG:HD2	2	0.18
(1,2435)	1:58:A:ILE:HG23	1:63:A:ARG:HD3	2	0.18
(1,1935)	1:108:A:SER:HB2	1:120:A:LYS:H	1	0.18
(1,1864)	1:56:A:LEU:HB2	1:85:A:ILE:H	4	0.18
(1,1263)	1:142:A:VAL:HB	1:145:A:HIS:HD2	3	0.18
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG21	9	0.18
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG22	9	0.18
(1,1257)	1:11:A:ILE:HG12	1:185:A:ILE:HG23	9	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	7	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	7	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	7	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	8	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	8	0.18
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	8	0.18
(1,1154)	1:114:A:ASN:HB2	1:116:A:ILE:HG12	8	0.18
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD21	2	0.18
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD22	2	0.18
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD23	2	0.18
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD11	9	0.18
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD12	9	0.18
(1,831)	1:80:A:ARG:HA	1:82:A:ILE:HD13	9	0.18
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	5	0.18
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	5	0.18
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	5	0.18
(1,257)	1:120:A:LYS:HD2	1:135:A:ILE:HG21	6	0.18
(1,257)	1:120:A:LYS:HD2	1:135:A:ILE:HG22	6	0.18
(1,257)	1:120:A:LYS:HD2	1:135:A:ILE:HG23	6	0.18
(1,93)	1:47:A:VAL:HG21	1:148:A:LYS:HE2	5	0.18
(1,93)	1:47:A:VAL:HG22	1:148:A:LYS:HE2	5	0.18
(1,93)	1:47:A:VAL:HG23	1:148:A:LYS:HE2	5	0.18
(2,1006)	1:89:A:LYS:HA	1:96:A:MET:HG2	1	0.17
(2,1006)	1:89:A:LYS:HA	1:96:A:MET:HG3	1	0.17
(2,467)	1:63:A:ARG:HB2	1:66:A:PHE:HZ	6	0.17
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	6	0.17
(2,106)	1:26:A:ILE:HG12	1:169:A:LEU:HB2	1	0.17
(2,61)	1:44:A:LYS:HA	1:185:A:ILE:HG21	6	0.17
(2,61)	1:44:A:LYS:HA	1:185:A:ILE:HG22	6	0.17
(2,61)	1:44:A:LYS:HA	1:185:A:ILE:HG23	6	0.17
(1,2475)	1:75:A:ARG:HG2	1:76:A:ASP:HB2	10	0.17
(1,2475)	1:75:A:ARG:HG2	1:76:A:ASP:HB3	10	0.17
(1,2475)	1:75:A:ARG:HG3	1:76:A:ASP:HB2	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2475)	1:75:A:ARG:HG3	1:76:A:ASP:HB3	10	0.17
(1,2413)	1:47:A:VAL:HG21	1:190:A:GLN:HG2	9	0.17
(1,2413)	1:47:A:VAL:HG21	1:190:A:GLN:HG3	9	0.17
(1,2413)	1:47:A:VAL:HG22	1:190:A:GLN:HG2	9	0.17
(1,2413)	1:47:A:VAL:HG22	1:190:A:GLN:HG3	9	0.17
(1,2413)	1:47:A:VAL:HG23	1:190:A:GLN:HG2	9	0.17
(1,2413)	1:47:A:VAL:HG23	1:190:A:GLN:HG3	9	0.17
(1,2363)	1:32:A:ASN:H	1:34:A:GLU:HG2	7	0.17
(1,2363)	1:32:A:ASN:H	1:34:A:GLU:HG3	7	0.17
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	9	0.17
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	9	0.17
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	10	0.17
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	3	0.17
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	3	0.17
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	3	0.17
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	6	0.17
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD11	7	0.17
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD12	7	0.17
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD13	7	0.17
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	1	0.17
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	1	0.17
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	1	0.17
(1,300)	1:21:A:ASN:HB2	1:119:A:PHE:HD1	4	0.17
(1,300)	1:21:A:ASN:HB2	1:119:A:PHE:HD2	4	0.17
(1,186)	1:14:A:VAL:HA	1:49:A:ARG:HB3	8	0.17
(1,93)	1:47:A:VAL:HG21	1:148:A:LYS:HE2	9	0.17
(1,93)	1:47:A:VAL:HG22	1:148:A:LYS:HE2	9	0.17
(1,93)	1:47:A:VAL:HG23	1:148:A:LYS:HE2	9	0.17
(2,658)	1:9:A:ASN:HD22	1:44:A:LYS:HA	10	0.16
(2,343)	1:131:A:THR:HA	1:135:A:ILE:HD11	7	0.16
(2,343)	1:131:A:THR:HA	1:135:A:ILE:HD12	7	0.16
(2,343)	1:131:A:THR:HA	1:135:A:ILE:HD13	7	0.16
(2,328)	1:65:A:LEU:HD21	1:69:A:MET:HE1	10	0.16
(2,328)	1:65:A:LEU:HD21	1:69:A:MET:HE2	10	0.16
(2,328)	1:65:A:LEU:HD21	1:69:A:MET:HE3	10	0.16
(2,328)	1:65:A:LEU:HD22	1:69:A:MET:HE1	10	0.16
(2,328)	1:65:A:LEU:HD22	1:69:A:MET:HE2	10	0.16
(2,328)	1:65:A:LEU:HD22	1:69:A:MET:HE3	10	0.16
(2,328)	1:65:A:LEU:HD23	1:69:A:MET:HE1	10	0.16
(2,328)	1:65:A:LEU:HD23	1:69:A:MET:HE2	10	0.16
(2,328)	1:65:A:LEU:HD23	1:69:A:MET:HE3	10	0.16
(1,1935)	1:108:A:SER:HB2	1:120:A:LYS:H	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	1	0.16
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	5	0.16
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	3	0.16
(1,1114)	1:162:A:ALA:HB1	1:175:A:LYS:HB3	8	0.16
(1,1114)	1:162:A:ALA:HB2	1:175:A:LYS:HB3	8	0.16
(1,1114)	1:162:A:ALA:HB3	1:175:A:LYS:HB3	8	0.16
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD21	7	0.16
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD22	7	0.16
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD23	7	0.16
(1,537)	1:49:A:ARG:HG2	1:51:A:LEU:HD11	10	0.16
(1,537)	1:49:A:ARG:HG2	1:51:A:LEU:HD12	10	0.16
(1,537)	1:49:A:ARG:HG2	1:51:A:LEU:HD13	10	0.16
(1,524)	1:49:A:ARG:HB2	1:51:A:LEU:HB2	6	0.16
(1,186)	1:14:A:VAL:HA	1:49:A:ARG:HB3	3	0.16
(1,58)	1:82:A:ILE:HD11	1:84:A:ILE:HD11	8	0.16
(1,58)	1:82:A:ILE:HD11	1:84:A:ILE:HD12	8	0.16
(1,58)	1:82:A:ILE:HD11	1:84:A:ILE:HD13	8	0.16
(1,58)	1:82:A:ILE:HD12	1:84:A:ILE:HD11	8	0.16
(1,58)	1:82:A:ILE:HD12	1:84:A:ILE:HD12	8	0.16
(1,58)	1:82:A:ILE:HD12	1:84:A:ILE:HD13	8	0.16
(1,58)	1:82:A:ILE:HD13	1:84:A:ILE:HD11	8	0.16
(1,58)	1:82:A:ILE:HD13	1:84:A:ILE:HD12	8	0.16
(1,58)	1:82:A:ILE:HD13	1:84:A:ILE:HD13	8	0.16
(2,663)	1:47:A:VAL:HG11	1:190:A:GLN:HE21	8	0.15
(2,663)	1:47:A:VAL:HG12	1:190:A:GLN:HE21	8	0.15
(2,663)	1:47:A:VAL:HG13	1:190:A:GLN:HE21	8	0.15
(2,436)	1:58:A:ILE:HD11	1:66:A:PHE:HD1	8	0.15
(2,436)	1:58:A:ILE:HD11	1:66:A:PHE:HD2	8	0.15
(2,436)	1:58:A:ILE:HD12	1:66:A:PHE:HD1	8	0.15
(2,436)	1:58:A:ILE:HD12	1:66:A:PHE:HD2	8	0.15
(2,436)	1:58:A:ILE:HD13	1:66:A:PHE:HD1	8	0.15
(2,436)	1:58:A:ILE:HD13	1:66:A:PHE:HD2	8	0.15
(2,222)	1:56:A:LEU:HD21	1:66:A:PHE:HZ	2	0.15
(2,222)	1:56:A:LEU:HD22	1:66:A:PHE:HZ	2	0.15
(2,222)	1:56:A:LEU:HD23	1:66:A:PHE:HZ	2	0.15
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	3	0.15
(2,146)	1:41:A:LEU:HD21	1:44:A:LYS:HE3	2	0.15
(2,146)	1:41:A:LEU:HD22	1:44:A:LYS:HE3	2	0.15
(2,146)	1:41:A:LEU:HD23	1:44:A:LYS:HE3	2	0.15
(2,103)	1:26:A:ILE:HD11	1:170:A:PHE:HE1	5	0.15
(2,103)	1:26:A:ILE:HD11	1:170:A:PHE:HE2	5	0.15
(2,103)	1:26:A:ILE:HD12	1:170:A:PHE:HE1	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,103)	1:26:A:ILE:HD12	1:170:A:PHE:HE2	5	0.15
(2,103)	1:26:A:ILE:HD13	1:170:A:PHE:HE1	5	0.15
(2,103)	1:26:A:ILE:HD13	1:170:A:PHE:HE2	5	0.15
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	10	0.15
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	10	0.15
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	10	0.15
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	10	0.15
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	2	0.15
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	9	0.15
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	9	0.15
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	9	0.15
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	9	0.15
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	9	0.15
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	9	0.15
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	9	0.15
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	9	0.15
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	9	0.15
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	9	0.15
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD21	5	0.15
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD22	5	0.15
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD23	5	0.15
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD21	6	0.15
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD22	6	0.15
(1,1003)	1:179:A:GLU:HB2	1:180:A:LEU:HD23	6	0.15
(1,817)	1:128:A:ILE:HD11	1:136:A:ILE:HG12	6	0.15
(1,817)	1:128:A:ILE:HD12	1:136:A:ILE:HG12	6	0.15
(1,817)	1:128:A:ILE:HD13	1:136:A:ILE:HG12	6	0.15
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD11	5	0.15
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD12	5	0.15
(1,800)	1:56:A:LEU:HB2	1:85:A:ILE:HD13	5	0.15
(1,786)	1:58:A:ILE:HG12	1:84:A:ILE:HG21	9	0.15
(1,786)	1:58:A:ILE:HG12	1:84:A:ILE:HG22	9	0.15
(1,786)	1:58:A:ILE:HG12	1:84:A:ILE:HG23	9	0.15
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	6	0.15
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	6	0.15
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	6	0.15
(1,546)	1:159:A:TYR:HD1	1:176:A:LYS:HG2	1	0.15
(1,546)	1:159:A:TYR:HD2	1:176:A:LYS:HG2	1	0.15
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	7	0.15
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	7	0.15
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	7	0.15
(1,468)	1:47:A:VAL:HG21	1:148:A:LYS:HD3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,468)	1:47:A:VAL:HG22	1:148:A:LYS:HD3	7	0.15
(1,468)	1:47:A:VAL:HG23	1:148:A:LYS:HD3	7	0.15
(1,453)	1:45:A:LEU:HD21	1:185:A:ILE:HD11	1	0.15
(1,453)	1:45:A:LEU:HD21	1:185:A:ILE:HD12	1	0.15
(1,453)	1:45:A:LEU:HD21	1:185:A:ILE:HD13	1	0.15
(1,453)	1:45:A:LEU:HD22	1:185:A:ILE:HD11	1	0.15
(1,453)	1:45:A:LEU:HD22	1:185:A:ILE:HD12	1	0.15
(1,453)	1:45:A:LEU:HD22	1:185:A:ILE:HD13	1	0.15
(1,453)	1:45:A:LEU:HD23	1:185:A:ILE:HD11	1	0.15
(1,453)	1:45:A:LEU:HD23	1:185:A:ILE:HD12	1	0.15
(1,453)	1:45:A:LEU:HD23	1:185:A:ILE:HD13	1	0.15
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD11	4	0.15
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD12	4	0.15
(1,335)	1:18:A:PHE:HB3	1:23:A:LEU:HD13	4	0.15
(1,299)	1:21:A:ASN:HB3	1:119:A:PHE:HB3	10	0.15
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	10	0.15
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	10	0.15
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	10	0.15
(2,905)	1:17:A:LYS:HE2	1:24:A:TYR:HD1	5	0.14
(2,905)	1:17:A:LYS:HE2	1:24:A:TYR:HD2	5	0.14
(2,905)	1:17:A:LYS:HE3	1:24:A:TYR:HD1	5	0.14
(2,905)	1:17:A:LYS:HE3	1:24:A:TYR:HD2	5	0.14
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD11	2	0.14
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD12	2	0.14
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD13	2	0.14
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD11	2	0.14
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD12	2	0.14
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD13	2	0.14
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD11	7	0.14
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD12	7	0.14
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD13	7	0.14
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	8	0.14
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	10	0.14
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG21	2	0.14
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG22	2	0.14
(1,2795)	1:165:A:LYS:HE2	1:185:A:ILE:HG23	2	0.14
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	2	0.14
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	2	0.14
(1,2795)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	2	0.14
(1,2771)	1:163:A:CYS:HB2	1:185:A:ILE:HD11	6	0.14
(1,2771)	1:163:A:CYS:HB2	1:185:A:ILE:HD12	6	0.14
(1,2771)	1:163:A:CYS:HB2	1:185:A:ILE:HD13	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2771)	1:163:A:CYS:HB3	1:185:A:ILE:HD11	6	0.14
(1,2771)	1:163:A:CYS:HB3	1:185:A:ILE:HD12	6	0.14
(1,2771)	1:163:A:CYS:HB3	1:185:A:ILE:HD13	6	0.14
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG21	8	0.14
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG22	8	0.14
(1,2651)	1:120:A:LYS:HD2	1:135:A:ILE:HG23	8	0.14
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	8	0.14
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	8	0.14
(1,2651)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	8	0.14
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	2	0.14
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	2	0.14
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	2	0.14
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	2	0.14
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	2	0.14
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	2	0.14
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	3	0.14
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	3	0.14
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	3	0.14
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	3	0.14
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	3	0.14
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	3	0.14
(1,2435)	1:58:A:ILE:HG21	1:63:A:ARG:HD2	9	0.14
(1,2435)	1:58:A:ILE:HG21	1:63:A:ARG:HD3	9	0.14
(1,2435)	1:58:A:ILE:HG22	1:63:A:ARG:HD2	9	0.14
(1,2435)	1:58:A:ILE:HG22	1:63:A:ARG:HD3	9	0.14
(1,2435)	1:58:A:ILE:HG23	1:63:A:ARG:HD2	9	0.14
(1,2435)	1:58:A:ILE:HG23	1:63:A:ARG:HD3	9	0.14
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	3	0.14
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	4	0.14
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	4	0.14
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	4	0.14
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	4	0.14
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	4	0.14
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	4	0.14
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	4	0.14
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	4	0.14
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	4	0.14
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	8	0.14
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	8	0.14
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	8	0.14
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	8	0.14
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	8	0.14
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	8	0.14
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	8	0.14
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	8	0.14
(1,1158)	1:57:A:PHE:HZ	1:189:A:VAL:HB	8	0.14
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	2	0.14
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	2	0.14
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	2	0.14
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	4	0.14
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	4	0.14
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	4	0.14
(1,475)	1:47:A:VAL:HG11	1:190:A:GLN:HB3	3	0.14
(1,475)	1:47:A:VAL:HG12	1:190:A:GLN:HB3	3	0.14
(1,475)	1:47:A:VAL:HG13	1:190:A:GLN:HB3	3	0.14
(1,379)	1:14:A:VAL:HG11	1:28:A:GLU:HB2	2	0.14
(1,379)	1:14:A:VAL:HG12	1:28:A:GLU:HB2	2	0.14
(1,379)	1:14:A:VAL:HG13	1:28:A:GLU:HB2	2	0.14
(1,186)	1:14:A:VAL:HA	1:49:A:ARG:HB3	4	0.14
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB1	5	0.14
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB2	5	0.14
(1,77)	1:11:A:ILE:HD11	1:27:A:ALA:HB3	5	0.14
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB1	5	0.14
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB2	5	0.14
(1,77)	1:11:A:ILE:HD12	1:27:A:ALA:HB3	5	0.14
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB1	5	0.14
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB2	5	0.14
(1,77)	1:11:A:ILE:HD13	1:27:A:ALA:HB3	5	0.14
(2,1039)	1:113:A:GLU:HG2	1:116:A:ILE:HG21	9	0.13
(2,1039)	1:113:A:GLU:HG2	1:116:A:ILE:HG22	9	0.13
(2,1039)	1:113:A:GLU:HG2	1:116:A:ILE:HG23	9	0.13
(2,1039)	1:113:A:GLU:HG3	1:116:A:ILE:HG21	9	0.13
(2,1039)	1:113:A:GLU:HG3	1:116:A:ILE:HG22	9	0.13
(2,1039)	1:113:A:GLU:HG3	1:116:A:ILE:HG23	9	0.13
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE2	9	0.13
(1,2781)	1:164:A:GLU:HG2	1:165:A:LYS:HE3	9	0.13
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE2	9	0.13
(1,2781)	1:164:A:GLU:HG3	1:165:A:LYS:HE3	9	0.13
(1,2594)	1:110:A:LEU:HD21	1:112:A:CYS:HB2	1	0.13
(1,2594)	1:110:A:LEU:HD21	1:112:A:CYS:HB3	1	0.13
(1,2594)	1:110:A:LEU:HD22	1:112:A:CYS:HB2	1	0.13
(1,2594)	1:110:A:LEU:HD22	1:112:A:CYS:HB3	1	0.13
(1,2594)	1:110:A:LEU:HD23	1:112:A:CYS:HB2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2594)	1:110:A:LEU:HD23	1:112:A:CYS:HB3	1	0.13
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	6	0.13
(1,1250)	1:11:A:ILE:HG13	1:185:A:ILE:HG21	5	0.13
(1,1250)	1:11:A:ILE:HG13	1:185:A:ILE:HG22	5	0.13
(1,1250)	1:11:A:ILE:HG13	1:185:A:ILE:HG23	5	0.13
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG21	1	0.13
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG22	1	0.13
(1,1162)	1:165:A:LYS:HE3	1:185:A:ILE:HG23	1	0.13
(1,1043)	1:99:A:THR:HB	1:109:A:THR:HG21	10	0.13
(1,1043)	1:99:A:THR:HB	1:109:A:THR:HG22	10	0.13
(1,1043)	1:99:A:THR:HB	1:109:A:THR:HG23	10	0.13
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD11	2	0.13
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD12	2	0.13
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD13	2	0.13
(1,761)	1:102:A:VAL:HG21	1:108:A:SER:HB3	10	0.13
(1,761)	1:102:A:VAL:HG22	1:108:A:SER:HB3	10	0.13
(1,761)	1:102:A:VAL:HG23	1:108:A:SER:HB3	10	0.13
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD11	8	0.13
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD12	8	0.13
(1,720)	1:85:A:ILE:HG12	1:100:A:ILE:HD13	8	0.13
(1,357)	1:17:A:LYS:HG3	1:26:A:ILE:HD11	8	0.13
(1,357)	1:17:A:LYS:HG3	1:26:A:ILE:HD12	8	0.13
(1,357)	1:17:A:LYS:HG3	1:26:A:ILE:HD13	8	0.13
(1,299)	1:21:A:ASN:HB3	1:119:A:PHE:HB3	5	0.13
(1,229)	1:15:A:ALA:HA	1:54:A:GLN:HB2	5	0.13
(1,212)	1:14:A:VAL:HG11	1:49:A:ARG:HB3	7	0.13
(1,212)	1:14:A:VAL:HG12	1:49:A:ARG:HB3	7	0.13
(1,212)	1:14:A:VAL:HG13	1:49:A:ARG:HB3	7	0.13
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD11	8	0.12
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD12	8	0.12
(2,889)	1:9:A:ASN:HB2	1:41:A:LEU:HD13	8	0.12
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD11	8	0.12
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD12	8	0.12
(2,889)	1:9:A:ASN:HB3	1:41:A:LEU:HD13	8	0.12
(1,2783)	1:164:A:GLU:HG2	1:173:A:ILE:HG21	3	0.12
(1,2783)	1:164:A:GLU:HG2	1:173:A:ILE:HG22	3	0.12
(1,2783)	1:164:A:GLU:HG2	1:173:A:ILE:HG23	3	0.12
(1,2783)	1:164:A:GLU:HG3	1:173:A:ILE:HG21	3	0.12
(1,2783)	1:164:A:GLU:HG3	1:173:A:ILE:HG22	3	0.12
(1,2783)	1:164:A:GLU:HG3	1:173:A:ILE:HG23	3	0.12
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG21	1	0.12
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG22	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:120:A:LYS:HD3	1:135:A:ILE:HG23	1	0.12
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD11	1	0.12
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD12	1	0.12
(1,820)	1:83:A:PHE:HA	1:84:A:ILE:HD13	1	0.12
(1,317)	1:22:A:THR:HG21	1:171:A:LYS:HB3	10	0.12
(1,317)	1:22:A:THR:HG22	1:171:A:LYS:HB3	10	0.12
(1,317)	1:22:A:THR:HG23	1:171:A:LYS:HB3	10	0.12
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD11	1	0.12
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD12	1	0.12
(1,149)	1:45:A:LEU:HA	1:185:A:ILE:HD13	1	0.12
(2,387)	1:148:A:LYS:HD3	1:188:A:THR:HB	3	0.11
(2,344)	1:99:A:THR:HB	1:135:A:ILE:HG21	10	0.11
(2,344)	1:99:A:THR:HB	1:135:A:ILE:HG22	10	0.11
(2,344)	1:99:A:THR:HB	1:135:A:ILE:HG23	10	0.11
(2,202)	1:51:A:LEU:HB3	1:52:A:ASN:HB3	7	0.11
(2,171)	1:37:A:TYR:HD1	1:41:A:LEU:HD11	7	0.11
(2,171)	1:37:A:TYR:HD1	1:41:A:LEU:HD12	7	0.11
(2,171)	1:37:A:TYR:HD1	1:41:A:LEU:HD13	7	0.11
(2,171)	1:37:A:TYR:HD2	1:41:A:LEU:HD11	7	0.11
(2,171)	1:37:A:TYR:HD2	1:41:A:LEU:HD12	7	0.11
(2,171)	1:37:A:TYR:HD2	1:41:A:LEU:HD13	7	0.11
(2,106)	1:26:A:ILE:HG12	1:169:A:LEU:HB2	3	0.11
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE21	3	0.11
(1,2736)	1:149:A:MET:HG2	1:150:A:GLN:HE22	3	0.11
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE21	3	0.11
(1,2736)	1:149:A:MET:HG3	1:150:A:GLN:HE22	3	0.11
(1,2587)	1:107:A:ILE:HG21	1:123:A:ASN:HB2	10	0.11
(1,2587)	1:107:A:ILE:HG21	1:123:A:ASN:HB3	10	0.11
(1,2587)	1:107:A:ILE:HG22	1:123:A:ASN:HB2	10	0.11
(1,2587)	1:107:A:ILE:HG22	1:123:A:ASN:HB3	10	0.11
(1,2587)	1:107:A:ILE:HG23	1:123:A:ASN:HB2	10	0.11
(1,2587)	1:107:A:ILE:HG23	1:123:A:ASN:HB3	10	0.11
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE2	9	0.11
(1,2497)	1:82:A:ILE:HG21	1:103:A:LYS:HE3	9	0.11
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE2	9	0.11
(1,2497)	1:82:A:ILE:HG22	1:103:A:LYS:HE3	9	0.11
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE2	9	0.11
(1,2497)	1:82:A:ILE:HG23	1:103:A:LYS:HE3	9	0.11
(1,2383)	1:41:A:LEU:HD11	1:44:A:LYS:HD2	3	0.11
(1,2383)	1:41:A:LEU:HD11	1:44:A:LYS:HD3	3	0.11
(1,2383)	1:41:A:LEU:HD12	1:44:A:LYS:HD2	3	0.11
(1,2383)	1:41:A:LEU:HD12	1:44:A:LYS:HD3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2383)	1:41:A:LEU:HD13	1:44:A:LYS:HD2	3	0.11
(1,2383)	1:41:A:LEU:HD13	1:44:A:LYS:HD3	3	0.11
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE1	2	0.11
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE2	2	0.11
(1,1384)	1:45:A:LEU:HD11	1:186:A:MET:HE3	2	0.11
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE1	2	0.11
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE2	2	0.11
(1,1384)	1:45:A:LEU:HD12	1:186:A:MET:HE3	2	0.11
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE1	2	0.11
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE2	2	0.11
(1,1384)	1:45:A:LEU:HD13	1:186:A:MET:HE3	2	0.11
(1,1343)	1:16:A:MET:HE1	1:54:A:GLN:HG2	1	0.11
(1,1343)	1:16:A:MET:HE2	1:54:A:GLN:HG2	1	0.11
(1,1343)	1:16:A:MET:HE3	1:54:A:GLN:HG2	1	0.11
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE1	9	0.11
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE2	9	0.11
(1,1339)	1:58:A:ILE:HD11	1:69:A:MET:HE3	9	0.11
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE1	9	0.11
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE2	9	0.11
(1,1339)	1:58:A:ILE:HD12	1:69:A:MET:HE3	9	0.11
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE1	9	0.11
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE2	9	0.11
(1,1339)	1:58:A:ILE:HD13	1:69:A:MET:HE3	9	0.11
(1,1213)	1:176:A:LYS:HG3	1:179:A:GLU:HB3	6	0.11
(1,1146)	1:108:A:SER:HB2	1:119:A:PHE:HB2	7	0.11
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD11	9	0.11
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD12	9	0.11
(1,865)	1:11:A:ILE:HG12	1:185:A:ILE:HD13	9	0.11
(1,526)	1:49:A:ARG:HA	1:49:A:ARG:HD3	1	0.11
(1,524)	1:49:A:ARG:HB2	1:51:A:LEU:HB2	3	0.11
(1,178)	1:12:A:ASN:HA	1:49:A:ARG:HD2	8	0.11
(1,119)	1:159:A:TYR:HE1	1:176:A:LYS:HG2	1	0.11
(1,119)	1:159:A:TYR:HE2	1:176:A:LYS:HG2	1	0.11
(2,407)	1:61:A:GLY:HA3	1:63:A:ARG:HD3	2	0.1
(2,407)	1:61:A:GLY:HA3	1:63:A:ARG:HD2	2	0.1
(2,351)	1:162:A:ALA:HB1	1:179:A:GLU:HB2	10	0.1
(2,351)	1:162:A:ALA:HB2	1:179:A:GLU:HB2	10	0.1
(2,351)	1:162:A:ALA:HB3	1:179:A:GLU:HB2	10	0.1
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD11	8	0.1
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD12	8	0.1
(2,218)	1:64:A:PRO:HB3	1:65:A:LEU:HD13	8	0.1
(1,2475)	1:75:A:ARG:HG2	1:76:A:ASP:HB2	1	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2475)	1:75:A:ARG:HG2	1:76:A:ASP:HB3	1	0.1
(1,2475)	1:75:A:ARG:HG3	1:76:A:ASP:HB2	1	0.1
(1,2475)	1:75:A:ARG:HG3	1:76:A:ASP:HB3	1	0.1
(1,2325)	1:17:A:LYS:HE2	1:19:A:ILE:HD11	5	0.1
(1,2325)	1:17:A:LYS:HE2	1:19:A:ILE:HD12	5	0.1
(1,2325)	1:17:A:LYS:HE2	1:19:A:ILE:HD13	5	0.1
(1,2325)	1:17:A:LYS:HE3	1:19:A:ILE:HD11	5	0.1
(1,2325)	1:17:A:LYS:HE3	1:19:A:ILE:HD12	5	0.1
(1,2325)	1:17:A:LYS:HE3	1:19:A:ILE:HD13	5	0.1
(1,1517)	1:50:A:ASN:HD22	1:54:A:GLN:H	8	0.1
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG11	2	0.1
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG12	2	0.1
(1,776)	1:23:A:LEU:HB3	1:102:A:VAL:HG13	2	0.1
(1,641)	1:66:A:PHE:HE1	1:107:A:ILE:HG21	9	0.1
(1,641)	1:66:A:PHE:HE1	1:107:A:ILE:HG22	9	0.1
(1,641)	1:66:A:PHE:HE1	1:107:A:ILE:HG23	9	0.1
(1,641)	1:66:A:PHE:HE2	1:107:A:ILE:HG21	9	0.1
(1,641)	1:66:A:PHE:HE2	1:107:A:ILE:HG22	9	0.1
(1,641)	1:66:A:PHE:HE2	1:107:A:ILE:HG23	9	0.1
(1,540)	1:12:A:ASN:HB2	1:49:A:ARG:HG3	2	0.1
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD11	6	0.1
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD12	6	0.1
(1,490)	1:13:A:PHE:HA	1:48:A:ILE:HD13	6	0.1
(1,93)	1:47:A:VAL:HG21	1:148:A:LYS:HE2	2	0.1
(1,93)	1:47:A:VAL:HG22	1:148:A:LYS:HE2	2	0.1
(1,93)	1:47:A:VAL:HG23	1:148:A:LYS:HE2	2	0.1

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

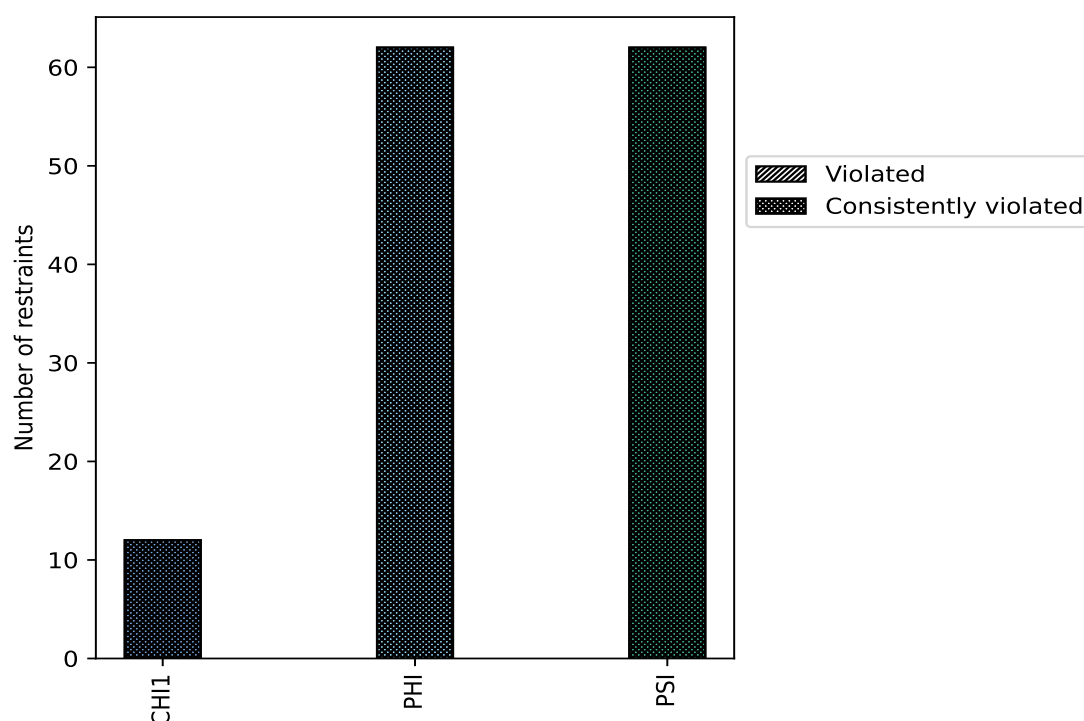
### 10.1 Summary of dihedral-angle violations [i](#)

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>
CHI1	12	8.8	12	100.0	8.8	12	100.0	8.8
PHI	62	45.6	62	100.0	45.6	62	100.0	45.6
PSI	62	45.6	62	100.0	45.6	62	100.0	45.6
Total	136	100.0	136	100.0	100.0	136	100.0	100.0

<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](#)



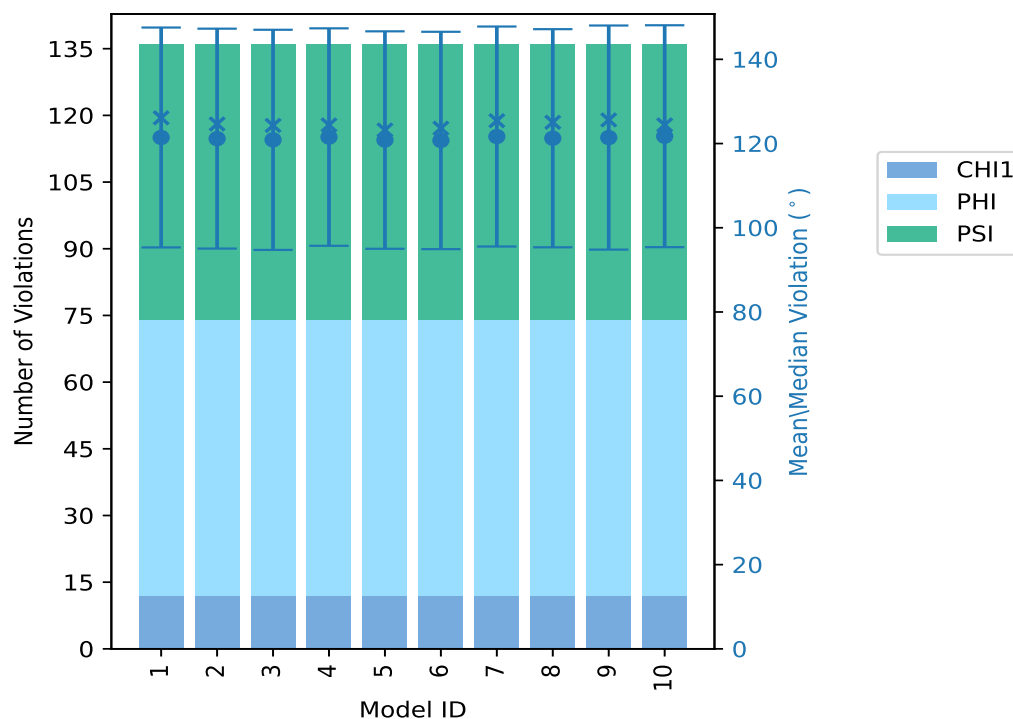
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 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 (°)
	CHI1	PHI	PSI	Total				
1	12	62	62	136	121.44	174.7	26.11	126.11
2	12	62	62	136	121.17	173.96	26.11	124.65
3	12	62	62	136	120.88	171.72	26.14	124.3
4	12	62	62	136	121.54	172.75	25.82	124.41
5	12	62	62	136	120.83	173.3	25.82	123.22
6	12	62	62	136	120.73	178.52	25.81	123.64
7	12	62	62	136	121.67	174.88	26.12	125.42
8	12	62	62	136	121.26	177.48	25.9	125.05
9	12	62	62	136	121.42	176.78	26.61	125.61
10	12	62	62	136	121.74	173.74	26.35	124.42

### 10.2.1 Bar graph : Dihedral 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



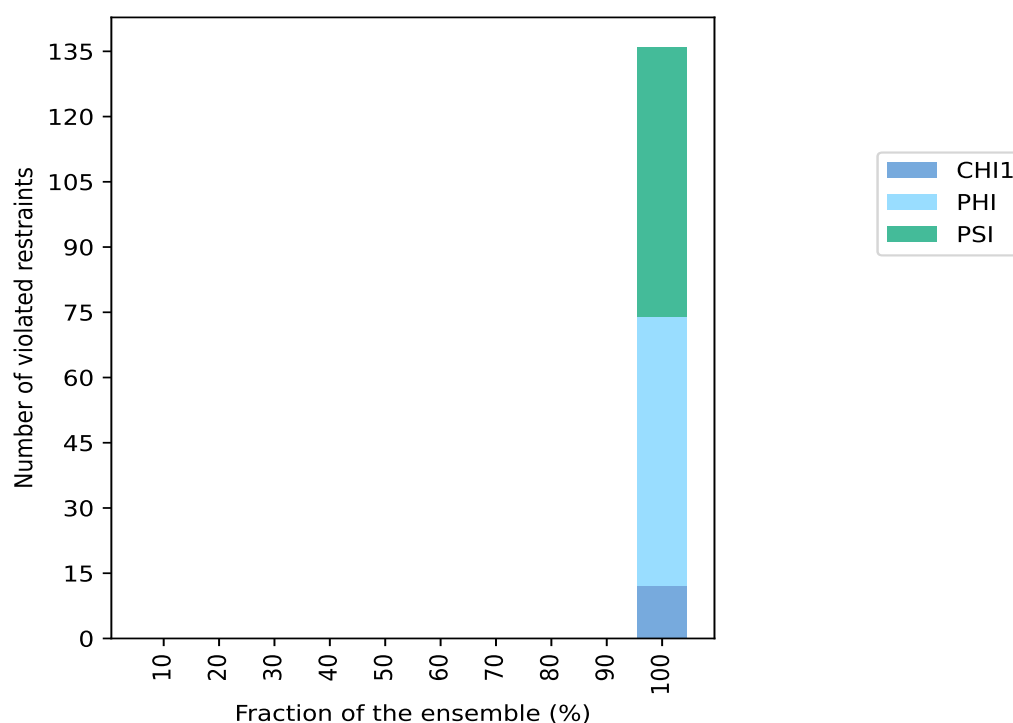
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints				Fraction of the ensemble	
CHI1	PHI	PSI	Total	Count <sup>1</sup>	%
0	0	0	0	1	10.0
0	0	0	0	2	20.0
0	0	0	0	3	30.0
0	0	0	0	4	40.0
0	0	0	0	5	50.0
0	0	0	0	6	60.0
0	0	0	0	7	70.0
0	0	0	0	8	80.0
0	0	0	0	9	90.0
12	62	62	136	10	100.0

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

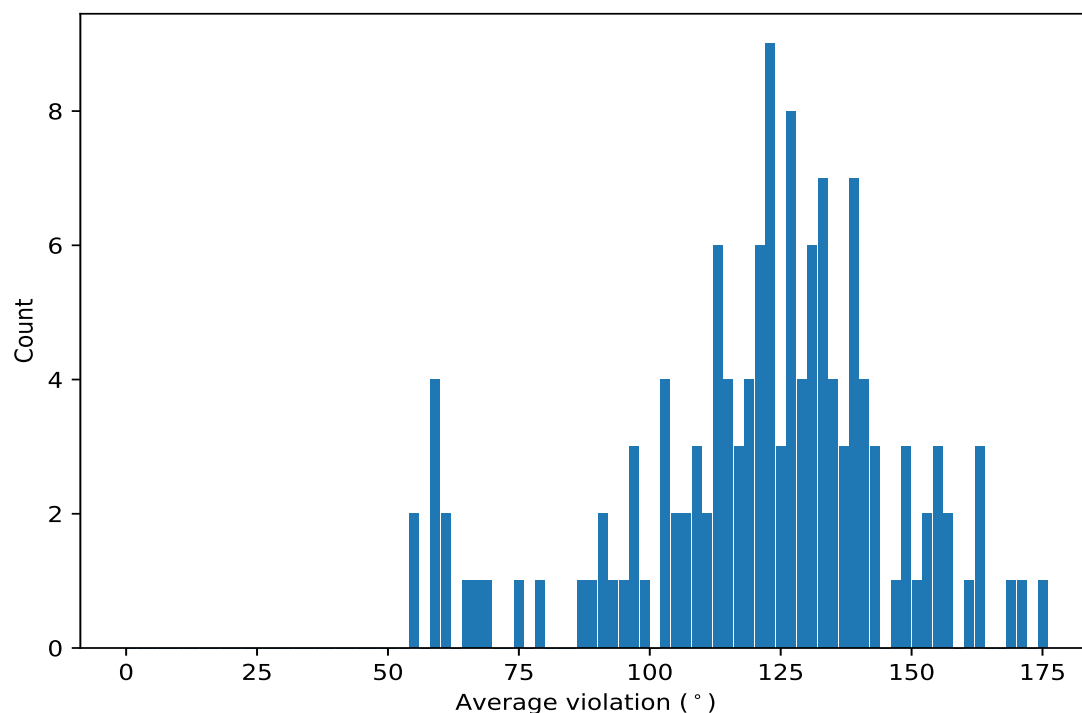
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

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



### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Media
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	10	174.14	2.83	174.33
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	10	171.62	1.1	171.32
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	10	168.94	3.44	169.36
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	10	163.28	1.57	163.49
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	10	162.42	2.24	162.14
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	10	162.41	2.82	162.14
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	10	160.25	1.66	159.66
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	10	156.46	2.14	156.7
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	10	156.06	2.84	155.58
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	10	155.45	1.96	155.39
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	10	155.14	0.83	155.4
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	10	154.6	1.54	154.29
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	10	153.91	2.09	153.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Media
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	10	153.39	5.95	153.92
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	10	150.51	2.93	150.12
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	10	149.93	3.15	150.04
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	10	149.86	1.95	149.6
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	10	148.37	2.0	148.52
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	10	146.84	1.81	146.28
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	10	143.95	3.83	144.49
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	10	143.5	4.76	144.9
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	10	142.94	1.85	142.72
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	10	141.61	1.14	141.62
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	10	141.61	1.78	141.34
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	10	141.12	6.58	143.12
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	10	140.63	9.87	135.78
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	10	139.7	3.05	139.68
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	10	139.44	8.42	137.85
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	10	139.44	1.17	139.15
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	10	139.38	2.93	139.1
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	10	138.86	5.05	139.83
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	10	138.68	1.74	138.56
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	10	138.57	1.95	138.32
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	10	136.91	1.38	136.9
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	10	136.68	5.54	134.65
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	10	136.11	6.69	132.29
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	10	135.56	1.17	135.15
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	10	135.4	4.21	137.5
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	10	135.03	4.94	136.88
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	10	134.1	1.97	134.18
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	10	133.94	5.29	132.66
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	10	133.79	0.84	133.82
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	10	133.65	0.82	133.7
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	10	133.36	7.36	135.36
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	10	133.33	4.59	134.23
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	10	132.36	7.01	136.24
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	10	132.28	2.17	132.66
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	10	131.86	13.3	126.54
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	10	131.86	3.27	132.78
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	10	131.56	1.84	131.83
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	10	131.44	0.99	131.18
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	10	131.42	2.52	130.75
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	10	131.35	2.33	131.24
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	10	129.67	1.6	130.32
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	10	129.54	1.33	130.02
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	10	129.07	3.24	130.26
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	10	128.01	1.77	128.18
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	10	127.96	2.84	127.22
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	10	127.68	1.96	128.21
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	10	126.88	1.93	126.97
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	10	126.84	2.84	125.76
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	10	126.67	1.69	126.74
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	10	126.49	1.62	126.8
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	10	126.4	3.47	126.56

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Media
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	10	126.04	1.93	126.68
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	10	125.58	5.11	126.36
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	10	124.71	1.49	125.04
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	10	124.42	2.55	124.2
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	10	123.85	2.1	123.86
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	10	123.63	1.68	123.6
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	10	123.51	2.13	122.96
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	10	123.24	1.58	123.33
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	10	122.95	9.97	129.28
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	10	122.83	1.25	122.59
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	10	122.71	3.22	123.21
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	10	122.68	5.9	122.71
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	10	122.35	1.65	122.26
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	10	121.96	2.26	122.5
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	10	121.57	1.71	121.69
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	10	121.35	5.09	123.56
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	10	121.22	2.19	121.22
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	10	120.91	5.39	120.1
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	10	120.11	2.09	119.72
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	10	119.8	8.65	116.49
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	10	119.23	2.6	118.58
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	10	118.64	2.15	118.36
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	10	118.07	3.61	118.28
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	10	117.74	4.16	117.3
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	10	116.95	5.88	117.46
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	10	116.86	3.03	117.34
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	10	115.54	2.24	116.25
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	10	115.15	2.66	114.94
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	10	114.38	2.84	115.1
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	10	114.09	3.32	114.38
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	10	113.83	2.71	114.48
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	10	113.74	2.7	113.55
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	10	113.73	2.77	112.71
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	10	113.52	4.93	113.28
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	10	113.39	4.21	111.66
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	10	112.78	2.83	113.02
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	10	111.57	0.97	111.37
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	10	111.42	1.9	110.98
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	10	109.97	1.82	110.12
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	10	109.78	1.64	109.79
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	10	108.8	3.1	108.7
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	10	106.76	3.45	106.31
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	10	106.67	4.6	104.9
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	10	105.31	4.85	105.46
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	10	104.81	1.45	105.2
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	10	103.85	2.81	102.34
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	10	103.68	6.06	103.02
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	10	103.07	3.44	101.52
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	10	102.61	4.33	101.2
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	10	98.38	5.42	97.93
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	10	97.77	3.65	97.38

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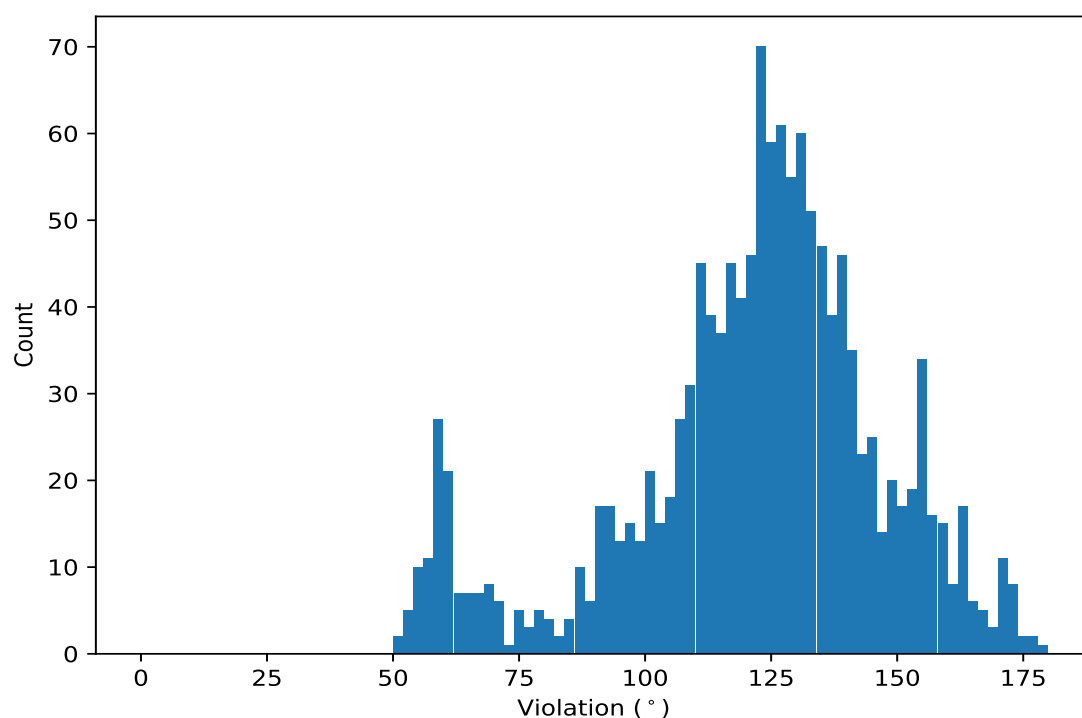
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Media
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	10	97.18	6.32	99.13
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	10	96.94	2.07	96.5
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	10	95.27	4.21	94.9
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	10	92.46	1.28	92.51
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	10	91.88	3.14	90.46
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	10	91.47	2.7	91.62
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	10	89.08	4.13	90.54
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	10	86.52	3.6	86.93
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	10	78.49	5.36	78.08
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	10	75.54	3.82	74.8
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	10	69.39	5.57	67.85
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	10	67.2	4.2	67.46
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	10	65.27	2.87	65.77
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	10	61.48	4.22	59.79
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	10	60.12	2.34	59.08
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	10	59.97	1.21	59.96
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	10	59.59	2.03	59.45
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	10	58.92	1.67	58.59
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	10	58.73	1.48	58.98
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	10	54.88	3.5	53.34
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	10	54.47	0.85	54.4

<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 ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	6	178.52
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	8	177.48
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	9	176.78
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	7	174.88
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	1	174.7
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	2	173.96
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	10	173.74
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	10	173.47
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	5	173.3
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	5	172.87
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	4	172.75
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	6	172.52
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	5	172.18
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	3	171.72
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	4	171.66
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	7	171.47
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	3	171.17
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	9	171.15
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	9	171.04
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	2	170.86
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	3	170.58

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	8	170.35
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	2	170.25
(1,132)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:CB	1:102:A:VAL:CG1	1	170.03
(1,134)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:CB	1:83:A:PHE:CG	10	168.83
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	4	168.48
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	7	168.17
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	1	167.31
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	9	166.87
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	6	166.4
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	6	166.37
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	8	166.07
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	10	165.46
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	9	165.27
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	8	165.05
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	2	164.71
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	2	164.32
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	10	164.12
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	9	163.68
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	7	163.67
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	7	163.63
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	10	163.63
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	8	163.35
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	5	163.07
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	10	162.76
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	7	162.71
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	4	162.39
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	5	162.36
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	3	162.34
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	5	162.21
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	3	162.14
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	10	162.13
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	1	162.13
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	1	162.07
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	8	162.02
(1,108)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1:174:A:LEU:N	6	161.79
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	3	161.67
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	3	161.34
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	4	161.25
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	7	161.16
(1,120)	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1:189:A:VAL:N	1	160.5
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	5	160.31
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	2	160.29
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	6	159.86
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	2	159.79
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	6	159.73
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	1	159.53
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	3	159.45
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	4	159.21
(1,48)	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1:99:A:THR:N	10	159.13
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	6	159.11
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	4	158.91

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	10	158.5
(1,96)	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1:163:A:CYS:N	8	158.4
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	9	158.3
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	4	158.26
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	7	158.16
(1,54)	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1:102:A:VAL:N	9	158.16
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	3	157.97
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	9	157.91
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	5	157.78
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	8	157.77
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	8	157.6
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	7	157.48
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	2	156.89
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	10	156.75
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	1	156.61
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	1	156.4
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	6	156.36
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	9	156.3
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	3	156.29
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	8	156.28
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	2	156.13
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	10	156.07
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	4	155.9
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	9	155.89
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	8	155.8
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	1	155.79
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	9	155.79
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	2	155.7
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	7	155.66
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	7	155.59
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	2	155.52
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	5	155.46
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	1	155.45
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	2	155.37
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	9	155.35
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	10	155.27
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	5	155.19
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	9	154.96
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	2	154.95
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	3	154.95
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	4	154.81
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	6	154.7
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	5	154.61
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	1	154.58
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	4	154.54
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	9	154.5
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	1	154.46
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	8	154.44
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	10	154.43
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	10	154.34
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	1	154.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	4	154.22
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	5	154.18
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	7	154.17
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	6	154.14
(1,8)	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1:17:A:LYS:N	3	154.07
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	9	153.95
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	1	153.94
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	8	153.53
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	3	153.51
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	7	153.34
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	4	153.23
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	3	153.2
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	5	153.18
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	6	153.15
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	6	153.14
(1,86)	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1:151:A:PHE:N	5	152.73
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	7	152.69
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	4	152.58
(1,92)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1:161:A:LEU:N	2	152.54
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	9	152.37
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	6	152.3
(1,70)	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1:119:A:PHE:N	9	152.21
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	8	152.15
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	4	152.01
(1,76)	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1:138:A:PHE:N	4	151.88
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	8	151.49
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	7	151.23
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	8	151.06
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	7	151.01
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	1	150.87
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	1	150.83
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	7	150.65
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	2	150.56
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	2	150.5
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	3	150.44
(1,6)	1:15:A:ALA:N	1:15:A:ALA:CA	1:15:A:ALA:C	1:16:A:MET:N	10	150.41
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	2	150.17
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	2	150.16
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	6	150.14
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	3	150.14
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	5	150.07
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	10	149.94
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	10	149.9
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	4	149.84
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	1	149.84
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	3	149.83
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	7	149.7
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	4	149.62
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	8	149.49
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	5	149.43
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	4	149.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	4	149.32
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	7	149.23
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	5	149.07
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	10	149.02
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	9	148.72
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	1	148.64
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	9	148.64
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	6	148.54
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	1	148.4
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	4	148.23
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	5	147.64
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	4	147.61
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	7	147.43
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	5	147.38
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	1	147.17
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	10	146.98
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	6	146.94
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	9	146.92
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	8	146.91
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	5	146.77
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	8	146.39
(1,82)	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1:141:A:SER:N	3	146.26
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	9	146.17
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	7	146.09
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	10	145.89
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	9	145.89
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	8	145.79
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	8	145.78
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	2	145.68
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	2	145.66
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	3	145.64
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	7	145.58
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	3	145.38
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	1	145.37
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	5	145.21
(1,16)	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1:25:A:PHE:N	10	145.2
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	1	144.89
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	6	144.85
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	8	144.8
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	8	144.75
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	8	144.51
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	10	144.45
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	3	144.44
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	9	144.41
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	4	144.32
(1,24)	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1:48:A:ILE:N	9	144.22
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	7	144.13
(1,68)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:CYS:N	6	144.13
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	2	144.09
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	5	143.82
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	8	143.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	1	143.64
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	6	143.5
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	10	143.46
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	2	143.38
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	10	143.34
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	1	143.31
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	1	143.27
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	3	143.27
(1,104)	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1:172:A:LEU:N	10	143.2
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	4	143.11
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	10	142.76
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	10	142.72
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	4	142.62
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	9	142.62
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	9	142.55
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	7	142.48
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	6	142.48
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	6	142.41
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	7	142.14
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	5	142.1
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	5	142.06
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	6	141.96
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	3	141.93
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	6	141.92
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	9	141.91
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	4	141.91
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	1	141.78
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	4	141.58
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	7	141.4
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	2	141.39
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	2	141.34
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	8	141.14
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	7	141.13
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	8	141.12
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	3	141.01
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	5	140.96
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	7	140.91
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	3	140.88
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	10	140.86
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	5	140.85
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	7	140.79
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	6	140.64
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	3	140.63
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	2	140.57
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	9	140.57
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	5	140.55
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	4	140.41
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	5	140.31
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	2	140.3
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	8	140.23
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	2	140.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	1	140.18
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	2	140.14
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	8	140.13
(1,10)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:PHE:N	5	140.1
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	1	140.02
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	7	139.99
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	9	139.9
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	7	139.83
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	10	139.82
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	10	139.75
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	2	139.66
(1,18)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1:26:A:ILE:N	9	139.5
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	1	139.48
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	10	139.47
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	9	139.39
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	3	139.37
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	6	139.33
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	4	139.22
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	7	139.21
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	8	139.11
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	10	139.05
(1,98)	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1:164:A:GLU:N	7	139.03
(1,114)	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1:186:A:MET:N	6	138.94
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	1	138.91
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	5	138.91
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	6	138.87
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	8	138.86
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	9	138.83
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	2	138.81
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	8	138.68
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	1	138.66
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	9	138.65
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	2	138.6
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	3	138.49
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	1	138.41
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	3	138.36
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	10	138.33
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	9	138.33
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	3	138.31
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	6	138.29
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	6	138.26
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	4	138.2
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	8	138.15
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	10	138.15
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	3	138.12
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	7	138.11
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	6	138.08
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	2	138.03
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	1	138.02
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	7	138.0
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	1	138.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	6	137.97
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	2	137.96
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	3	137.9
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	4	137.82
(1,22)	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1:47:A:VAL:N	9	137.78
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	4	137.74
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	6	137.72
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	2	137.7
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	6	137.64
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	10	137.63
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	7	137.47
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	7	137.46
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	2	137.4
(1,112)	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1:176:A:LYS:N	5	137.38
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	5	137.36
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	1	137.32
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	9	137.28
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	3	137.24
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	4	137.19
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	4	137.1
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	6	136.98
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	8	136.81
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	3	136.77
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	8	136.74
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	7	136.7
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	8	136.65
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	1	136.62
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	6	136.6
(1,84)	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1:150:A:GLN:N	2	136.54
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	1	136.46
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	1	136.4
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	5	136.38
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	7	136.28
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	3	136.19
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	8	136.19
(1,62)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:THR:N	6	136.15
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	8	136.15
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	7	136.09
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	3	136.02
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	4	135.96
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	7	135.91
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	4	135.86
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	4	135.85
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	10	135.76
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	1	135.73
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	6	135.72
(1,53)	1:100:A:ILE:C	1:101:A:SER:N	1:101:A:SER:CA	1:101:A:SER:C	5	135.59
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	5	135.52
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	2	135.48
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	9	135.42
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	6	135.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	3	135.37
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	6	135.28
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	7	135.26
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	5	135.25
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	4	135.23
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	3	135.08
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	5	135.02
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	8	135.01
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	6	135.01
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	4	134.99
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	5	134.98
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	8	134.94
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	8	134.94
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	8	134.83
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	5	134.82
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	1	134.79
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	6	134.77
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	7	134.77
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	4	134.75
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	4	134.72
(1,4)	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1:14:A:VAL:N	4	134.65
(1,100)	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1:165:A:LYS:N	1	134.63
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	2	134.55
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	1	134.42
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	2	134.38
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	4	134.37
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	2	134.37
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	2	134.32
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	9	134.3
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	9	134.29
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	6	134.26
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	2	134.19
(1,102)	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1:171:A:LYS:N	3	134.04
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	10	134.04
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	7	134.0
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	3	133.9
(1,90)	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1:153:A:SER:N	10	133.87
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	9	133.85
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	2	133.85
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	1	133.83
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	2	133.81
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	10	133.8
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	2	133.78
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	3	133.77
(1,122)	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1:190:A:GLN:N	10	133.75
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	2	133.73
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	8	133.67
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	8	133.67
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	4	133.66
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	5	133.56
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	4	133.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	5	133.42
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	1	133.41
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	8	133.41
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	7	133.39
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	7	133.31
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	10	133.24
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	9	133.21
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	8	133.19
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	10	133.11
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	3	133.09
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	7	133.04
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	3	133.02
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	1	133.01
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	3	133.01
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	7	132.99
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	5	132.98
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	8	132.94
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	4	132.92
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	3	132.88
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	10	132.88
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	3	132.72
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	4	132.72
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	1	132.67
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	6	132.65
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	5	132.62
(1,7)	1:15:A:ALA:C	1:16:A:MET:N	1:16:A:MET:CA	1:16:A:MET:C	5	132.6
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	1	132.59
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	3	132.49
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	10	132.49
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	5	132.35
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	2	132.32
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	1	132.27
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	5	132.26
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	7	132.13
(1,95)	1:161:A:LEU:C	1:162:A:ALA:N	1:162:A:ALA:CA	1:162:A:ALA:C	10	132.03
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	6	131.99
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	5	131.97
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	9	131.93
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	6	131.92
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	7	131.84
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	3	131.77
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	9	131.74
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	1	131.73
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	9	131.7
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	3	131.7
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	3	131.7
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	4	131.61
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	6	131.6
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	2	131.53
(1,50)	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1:100:A:ILE:N	5	131.36
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	3	131.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	1	131.11
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	9	131.0
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	2	130.99
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	8	130.98
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	10	130.96
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	3	130.95
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	4	130.89
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	4	130.84
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	9	130.83
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	2	130.8
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	6	130.8
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	9	130.76
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	6	130.75
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	8	130.72
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	9	130.69
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	6	130.68
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	2	130.67
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	10	130.67
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	8	130.66
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	7	130.64
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	7	130.61
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	7	130.56
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	7	130.52
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	10	130.49
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	6	130.47
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	6	130.47
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	4	130.47
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	4	130.46
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	1	130.42
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	6	130.39
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	4	130.38
(1,64)	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1:110:A:LEU:N	8	130.35
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	8	130.35
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	2	130.31
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	2	130.3
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	10	130.25
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	5	130.24
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	8	130.24
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	1	130.17
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	10	130.16
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	2	130.1
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	9	130.07
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	6	130.05
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	8	130.05
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	5	129.98
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	10	129.96
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	5	129.94
(1,23)	1:46:A:SER:C	1:47:A:VAL:N	1:47:A:VAL:CA	1:47:A:VAL:C	9	129.86
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	10	129.85
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	3	129.83
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	6	129.78

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	1	129.76
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	1	129.75
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	7	129.71
(1,74)	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1:121:A:GLU:N	10	129.66
(1,56)	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1:103:A:LYS:N	5	129.6
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	3	129.59
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	2	129.54
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	8	129.47
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	4	129.44
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	10	129.42
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	7	129.35
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1	129.34
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	1	129.26
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	8	129.19
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	3	129.18
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	9	129.14
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	9	129.11
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	5	129.1
(1,9)	1:16:A:MET:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	4	129.06
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	10	129.05
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	7	129.02
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	8	129.0
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	6	128.86
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	6	128.85
(1,111)	1:174:A:LEU:C	1:175:A:LYS:N	1:175:A:LYS:CA	1:175:A:LYS:C	4	128.8
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	1	128.75
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	1	128.72
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	10	128.7
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	9	128.68
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	9	128.65
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	3	128.64
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	2	128.54
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	1	128.53
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	8	128.52
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	1	128.43
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	9	128.42
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	3	128.41
(1,94)	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1:162:A:ALA:N	4	128.33
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	2	128.33
(1,32)	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1:58:A:ILE:N	9	128.33
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	10	128.26
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	2	128.24
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	8	128.19
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	5	128.18
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	4	128.18
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	9	128.17
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	4	128.12
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	8	128.0
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	8	127.95
(1,46)	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1:98:A:VAL:N	7	127.92
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	8	127.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	3	127.87
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	3	127.86
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	8	127.84
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	7	127.79
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	3	127.77
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	8	127.77
(1,78)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1:139:A:GLN:N	2	127.75
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	6	127.69
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	1	127.68
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	2	127.61
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	4	127.58
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	2	127.48
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	4	127.43
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	7	127.39
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	3	127.37
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	5	127.23
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	1	127.23
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	7	127.21
(1,26)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:ARG:N	5	127.14
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	6	127.0
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	2	126.99
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	7	126.97
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	9	126.95
(1,69)	1:117:A:ILE:C	1:118:A:SER:N	1:118:A:SER:CA	1:118:A:SER:C	6	126.92
(1,107)	1:172:A:LEU:C	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:C	6	126.84
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	4	126.82
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	7	126.82
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	5	126.8
(1,83)	1:148:A:LYS:C	1:149:A:MET:N	1:149:A:MET:CA	1:149:A:MET:C	9	126.8
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	1	126.8
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	7	126.8
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	9	126.78
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	9	126.77
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	8	126.76
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	7	126.71
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	1	126.69
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	8	126.69
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	5	126.61
(1,72)	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1:120:A:LYS:N	10	126.56
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	1	126.56
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	9	126.56
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	6	126.55
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	9	126.53
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	4	126.49
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	6	126.46
(1,81)	1:139:A:GLN:C	1:140:A:ARG:N	1:140:A:ARG:CA	1:140:A:ARG:C	1	126.35
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	9	126.35
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	5	126.27
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	10	126.26
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	1	126.26
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	9	126.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	9	126.2
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	2	126.19
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	2	126.16
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	5	126.11
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	4	126.09
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	3	126.05
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	2	126.02
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	1	125.96
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	3	125.94
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1	125.92
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	5	125.89
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	6	125.87
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	6	125.83
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	7	125.78
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	7	125.68
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	9	125.68
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	3	125.61
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	10	125.6
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	7	125.59
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	9	125.54
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	8	125.54
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	4	125.52
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	8	125.47
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	10	125.45
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	5	125.3
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	10	125.3
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	10	125.27
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	3	125.27
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	2	125.26
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	7	125.24
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	5	125.23
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	5	125.21
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	10	125.11
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	4	125.07
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	10	125.04
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	7	124.99
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	5	124.92
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	7	124.89
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	10	124.89
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	3	124.89
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	6	124.86
(1,36)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1:83:A:PHE:N	2	124.85
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	3	124.85
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	1	124.85
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	4	124.77
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	2	124.67
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	5	124.65
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	8	124.63
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	2	124.63
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	4	124.49
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	10	124.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	2	124.39
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	3	124.38
(1,85)	1:149:A:MET:C	1:150:A:GLN:N	1:150:A:GLN:CA	1:150:A:GLN:C	10	124.38
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	2	124.38
(1,40)	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1:85:A:ILE:N	10	124.38
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	4	124.33
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	8	124.31
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	1	124.28
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	3	124.23
(1,116)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:PHE:N	6	124.17
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	7	124.12
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	10	124.04
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	10	124.04
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	9	124.02
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	7	124.01
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	1	123.99
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	5	123.96
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	8	123.95
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	4	123.89
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	2	123.86
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	9	123.85
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	3	123.79
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	2	123.79
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	8	123.73
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	9	123.68
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	4	123.66
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	6	123.65
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	5	123.63
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	6	123.63
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	10	123.62
(1,52)	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1:101:A:SER:N	2	123.61
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	9	123.61
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	6	123.6
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	6	123.57
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	8	123.55
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	10	123.49
(1,34)	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1:59:A:ASP:N	3	123.45
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	2	123.43
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	9	123.42
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	8	123.41
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	1	123.39
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	9	123.25
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	4	123.2
(1,47)	1:97:A:ALA:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	10	123.16
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	4	123.13
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	3	123.1
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	1	123.09
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	1	123.07
(1,30)	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1:57:A:PHE:N	10	123.04
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	9	122.97
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	6	122.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	10	122.93
(1,66)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:SER:N	10	122.91
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	8	122.9
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	8	122.9
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	10	122.85
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	4	122.81
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	5	122.8
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	3	122.8
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	4	122.8
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	2	122.65
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	6	122.64
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	5	122.61
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	8	122.57
(1,113)	1:184:A:SER:C	1:185:A:ILE:N	1:185:A:ILE:CA	1:185:A:ILE:C	9	122.54
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	3	122.51
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	6	122.46
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	3	122.4
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	1	122.37
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	2	122.35
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	9	122.31
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	3	122.29
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	3	122.27
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	9	122.25
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	7	122.25
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	3	122.22
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	1	122.2
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	2	122.19
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	7	122.15
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	7	122.11
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	5	122.11
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	7	122.09
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	5	122.06
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	9	122.05
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	6	122.0
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	6	121.98
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	10	121.96
(1,28)	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1:56:A:LEU:N	7	121.95
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	5	121.93
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	4	121.92
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	6	121.9
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	3	121.9
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	7	121.87
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	3	121.84
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	9	121.83
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	10	121.79
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	5	121.76
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	7	121.72
(1,5)	1:13:A:PHE:C	1:14:A:VAL:N	1:14:A:VAL:CA	1:14:A:VAL:C	4	121.69
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	10	121.66
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	1	121.64
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	1	121.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	9	121.54
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	10	121.52
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	2	121.51
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	1	121.45
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	1	121.41
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	5	121.32
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	5	121.28
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	5	121.25
(1,58)	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1:104:A:CYS:N	4	121.19
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	8	120.93
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	5	120.91
(1,20)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1:27:A:ALA:N	6	120.89
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	7	120.88
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	6	120.88
(1,110)	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1:175:A:LYS:N	8	120.86
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	6	120.86
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	7	120.83
(1,27)	1:54:A:GLN:C	1:55:A:VAL:N	1:55:A:VAL:CA	1:55:A:VAL:C	1	120.81
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	9	120.8
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	8	120.65
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	5	120.64
(1,55)	1:101:A:SER:C	1:102:A:VAL:N	1:102:A:VAL:CA	1:102:A:VAL:C	4	120.57
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	10	120.47
(1,119)	1:187:A:PHE:C	1:188:A:THR:N	1:188:A:THR:CA	1:188:A:THR:C	5	120.39
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	6	120.39
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	9	120.32
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	8	120.19
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	1	120.18
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	4	120.15
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	5	119.99
(1,44)	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1:87:A:MET:N	3	119.98
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	9	119.96
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	7	119.91
(1,14)	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1:24:A:TYR:N	8	119.9
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	4	119.89
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	9	119.86
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	5	119.85
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	4	119.54
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	9	119.52
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	6	119.46
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	2	119.43
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	4	119.36
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	2	119.34
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	2	119.28
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	2	119.25
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	10	119.17
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	5	119.15
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	1	119.13
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	1	119.05
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	6	119.04
(1,118)	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1:188:A:THR:N	4	118.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	10	118.86
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	6	118.8
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	10	118.75
(1,2)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:PHE:N	4	118.68
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	10	118.61
(1,99)	1:163:A:CYS:C	1:164:A:GLU:N	1:164:A:GLU:CA	1:164:A:GLU:C	8	118.6
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	4	118.47
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	7	118.42
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	7	118.37
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	4	118.36
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	3	118.35
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	5	118.18
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	5	118.17
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	5	118.13
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	6	118.12
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	5	118.1
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	2	118.1
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	8	118.06
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	6	118.02
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	3	117.97
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	10	117.95
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	10	117.89
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	7	117.87
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	3	117.68
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	10	117.68
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	6	117.57
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	2	117.42
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	1	117.41
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	3	117.35
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	1	117.32
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	4	117.31
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	2	117.28
(1,88)	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1:152:A:GLU:N	4	117.24
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	2	117.24
(1,121)	1:188:A:THR:C	1:189:A:VAL:N	1:189:A:VAL:CA	1:189:A:VAL:C	6	117.13
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	6	117.11
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	2	117.1
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	6	117.05
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	4	117.03
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	10	117.01
(1,124)	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1:191:A:ASN:N	3	117.0
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	4	116.96
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	8	116.95
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	8	116.75
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	10	116.67
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	3	116.66
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	10	116.59
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	8	116.59
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	5	116.57
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	4	116.49
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	5	116.47

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	6	116.34
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	10	116.34
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	7	116.28
(1,106)	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1:173:A:ILE:N	9	116.24
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	9	116.2
(1,35)	1:81:A:THR:C	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:C	3	116.18
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	7	116.17
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	2	116.16
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	2	116.11
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	6	116.1
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	8	116.08
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	5	116.01
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	4	116.01
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	2	115.95
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	3	115.93
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	3	115.87
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	7	115.82
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	2	115.76
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	7	115.72
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	5	115.69
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	3	115.65
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	8	115.6
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	8	115.57
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	2	115.54
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	5	115.4
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	5	115.36
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	4	115.28
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	7	115.11
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	5	115.07
(1,75)	1:136:A:ILE:C	1:137:A:PHE:N	1:137:A:PHE:CA	1:137:A:PHE:C	1	115.02
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	3	115.0
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	7	114.92
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	7	114.84
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	4	114.77
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	2	114.73
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	3	114.65
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	5	114.61
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1	114.61
(1,80)	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1:140:A:ARG:N	9	114.6
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	7	114.6
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	8	114.58
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	3	114.52
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	1	114.42
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	1	114.39
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	3	114.32
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	3	114.28
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	2	114.23
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	2	114.2
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	8	114.07
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	4	114.02
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	1	113.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	4	113.94
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	7	113.79
(1,60)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1:108:A:SER:N	3	113.79
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	10	113.79
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	2	113.76
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	8	113.76
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	7	113.65
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	9	113.63
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	10	113.62
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	5	113.48
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	2	113.48
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	4	113.31
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	4	113.23
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1	113.15
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1	113.06
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	4	113.06
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	8	113.04
(1,67)	1:110:A:LEU:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	3	113.0
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	8	112.92
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	8	112.9
(1,87)	1:150:A:GLN:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	4	112.84
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	8	112.84
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	2	112.83
(1,21)	1:45:A:LEU:C	1:46:A:SER:N	1:46:A:SER:CA	1:46:A:SER:C	7	112.68
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	6	112.6
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	6	112.52
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	4	112.52
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	6	112.24
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	4	112.23
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	7	112.22
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	9	112.19
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	2	112.19
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	9	112.11
(1,38)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:ILE:N	10	112.11
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	10	112.06
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	8	112.04
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	9	112.02
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	1	112.01
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	3	111.97
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	3	111.92
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	10	111.88
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	7	111.77
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	5	111.77
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	1	111.75
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	7	111.74
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	1	111.63
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	2	111.63
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	6	111.59
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	3	111.53
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	7	111.43
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	7	111.41

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	2	111.4
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	5	111.34
(1,42)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:SER:N	5	111.33
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	5	111.29
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	6	111.21
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	1	111.06
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	6	111.03
(1,89)	1:151:A:PHE:C	1:152:A:GLU:N	1:152:A:GLU:CA	1:152:A:GLU:C	2	111.02
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	5	110.98
(1,49)	1:98:A:VAL:C	1:99:A:THR:N	1:99:A:THR:CA	1:99:A:THR:C	5	110.98
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	3	110.95
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	3	110.93
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	8	110.89
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	6	110.88
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	10	110.87
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	9	110.7
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	3	110.64
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	8	110.6
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	5	110.59
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	9	110.52
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	7	110.44
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	1	110.32
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	1	110.3
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	9	110.29
(1,61)	1:107:A:ILE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1	110.28
(1,41)	1:84:A:ILE:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	8	110.17
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	9	110.14
(1,11)	1:17:A:LYS:C	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	10	110.08
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	9	110.05
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	3	110.03
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	8	110.01
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	9	110.0
(1,71)	1:118:A:SER:C	1:119:A:PHE:N	1:119:A:PHE:CA	1:119:A:PHE:C	1	109.99
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	6	109.98
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	8	109.98
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	6	109.96
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	10	109.95
(1,97)	1:162:A:ALA:C	1:163:A:CYS:N	1:163:A:CYS:CA	1:163:A:CYS:C	4	109.89
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	9	109.86
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	2	109.83
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	10	109.82
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	6	109.77
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	10	109.64
(1,15)	1:23:A:LEU:C	1:24:A:TYR:N	1:24:A:TYR:CA	1:24:A:TYR:C	9	109.61
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	7	109.58
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	1	109.55
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	9	109.43
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	9	109.42
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	3	109.38
(1,17)	1:24:A:TYR:C	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:C	9	109.19
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	4	109.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	2	109.0
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	9	109.0
(1,31)	1:56:A:LEU:C	1:57:A:PHE:N	1:57:A:PHE:CA	1:57:A:PHE:C	6	108.91
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	10	108.75
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	4	108.68
(1,29)	1:55:A:VAL:C	1:56:A:LEU:N	1:56:A:LEU:CA	1:56:A:LEU:C	8	108.62
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	2	108.55
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	4	108.5
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	5	108.45
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	6	108.3
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	8	108.18
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	6	108.05
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	5	107.93
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	6	107.89
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	6	107.85
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	3	107.76
(1,103)	1:170:A:PHE:C	1:171:A:LYS:N	1:171:A:LYS:CA	1:171:A:LYS:C	3	107.69
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	10	107.63
(1,91)	1:159:A:TYR:C	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:C	1	107.62
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	5	107.61
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	5	107.57
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	4	107.52
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	7	107.39
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	9	107.28
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	10	106.86
(1,19)	1:25:A:PHE:C	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:C	9	106.86
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	8	106.82
(1,109)	1:173:A:ILE:C	1:174:A:LEU:N	1:174:A:LEU:CA	1:174:A:LEU:C	4	106.76
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	10	106.64
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	5	106.55
(1,63)	1:108:A:SER:C	1:109:A:THR:N	1:109:A:THR:CA	1:109:A:THR:C	2	106.51
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	1	106.37
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	9	106.34
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	4	106.31
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	6	106.26
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	5	106.25
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	7	106.24
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	2	106.24
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	9	106.17
(1,73)	1:119:A:PHE:C	1:120:A:LYS:N	1:120:A:LYS:CA	1:120:A:LYS:C	8	105.83
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	9	105.73
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	10	105.69
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	8	105.53
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	4	105.47
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	2	105.4
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	7	104.98
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	8	104.92
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	1	104.91
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	7	104.88
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	5	104.8
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	5	104.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	7	104.61
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	4	104.46
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	8	104.17
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	10	104.09
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	10	104.09
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	7	104.08
(1,39)	1:83:A:PHE:C	1:84:A:ILE:N	1:84:A:ILE:CA	1:84:A:ILE:C	1	103.93
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	6	103.8
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	3	103.63
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	3	103.26
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	7	103.16
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1	102.98
(1,25)	1:47:A:VAL:C	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	5	102.81
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	6	102.78
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	6	102.71
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	3	102.68
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	7	102.63
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	2	102.59
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	6	102.4
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	10	102.09
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	8	102.08
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	2	101.99
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	9	101.82
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	7	101.78
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	7	101.71
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	4	101.58
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	1	101.42
(1,101)	1:169:A:LEU:C	1:170:A:PHE:N	1:170:A:PHE:CA	1:170:A:PHE:C	2	101.36
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	5	101.33
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	1	101.09
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	5	101.06
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	10	100.97
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	4	100.7
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	2	100.61
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	6	100.5
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	7	100.48
(1,12)	1:18:A:PHE:N	1:18:A:PHE:CA	1:18:A:PHE:C	1:19:A:ILE:N	1	100.38
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	7	100.28
(1,51)	1:99:A:THR:C	1:100:A:ILE:N	1:100:A:ILE:CA	1:100:A:ILE:C	2	100.28
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	9	100.21
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	3	100.17
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	5	100.02
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	9	99.83
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	1	99.74
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	3	99.65
(1,57)	1:102:A:VAL:C	1:103:A:LYS:N	1:103:A:LYS:CA	1:103:A:LYS:C	1	99.38
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	3	99.28
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	5	99.2
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	3	99.07
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	4	99.06
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1	99.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	6	98.54
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	2	98.4
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	3	98.28
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	8	98.01
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	2	97.8
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	2	97.74
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	7	97.57
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	4	97.39
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	6	97.35
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	9	97.18
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	3	97.17
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	5	97.15
(1,33)	1:57:A:PHE:C	1:58:A:ILE:N	1:58:A:ILE:CA	1:58:A:ILE:C	8	96.68
(1,77)	1:137:A:PHE:C	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:C	8	96.54
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	8	96.54
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	10	96.46
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	2	96.19
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	7	96.03
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	5	96.03
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	6	95.98
(1,1)	1:11:A:ILE:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	8	95.96
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	4	95.32
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	10	95.26
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	7	94.67
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	9	94.55
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	10	94.43
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	9	94.39
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	8	94.31
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	3	94.19
(1,59)	1:106:A:LYS:C	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:C	1	94.15
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	7	94.11
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	8	94.06
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	5	93.64
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	10	93.64
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	9	93.6
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	6	93.6
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	9	93.36
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	5	93.15
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	1	93.06
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	6	92.78
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	4	92.67
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1	92.57
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	3	92.45
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	3	92.3
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	1	92.24
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	6	92.18
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	4	92.16
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	2	92.16
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	2	92.1
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	4	91.97
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	7	91.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:12:A:ASN:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	4	91.91
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	6	91.27
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	4	91.11
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	7	90.99
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	1	90.98
(1,45)	1:96:A:MET:C	1:97:A:ALA:N	1:97:A:ALA:CA	1:97:A:ALA:C	8	90.95
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	2	90.93
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	8	90.9
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	10	90.71
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	4	90.64
(1,13)	1:22:A:THR:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	10	90.49
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	2	90.2
(1,79)	1:138:A:PHE:C	1:139:A:GLN:N	1:139:A:GLN:CA	1:139:A:GLN:C	10	90.16
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	5	90.12
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	8	90.1
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	10	89.94
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1	89.32
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	9	89.26
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	3	89.15
(1,37)	1:82:A:ILE:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	3	88.9
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	8	88.32
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	8	87.99
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	7	87.72
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	6	87.52
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	9	87.49
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	10	87.38
(1,117)	1:186:A:MET:C	1:187:A:PHE:N	1:187:A:PHE:CA	1:187:A:PHE:C	9	86.86
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	4	86.77
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	8	86.67
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	1	86.37
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	5	86.14
(1,43)	1:85:A:ILE:C	1:86:A:SER:N	1:86:A:SER:CA	1:86:A:SER:C	9	85.8
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	2	85.25
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	5	84.67
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	3	84.26
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1	82.37
(1,65)	1:109:A:THR:C	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	6	82.33
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	6	81.55
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	3	80.73
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	9	80.28
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	6	80.07
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	10	79.3
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	10	79.17
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	1	79.07
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	7	78.89
(1,105)	1:171:A:LYS:C	1:172:A:LEU:N	1:172:A:LEU:CA	1:172:A:LEU:C	6	78.5
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	9	77.1
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	7	77.08
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	8	76.43
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	2	75.26
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	5	75.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	5	75.01
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	2	74.59
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	4	74.32
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	5	72.23
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	8	71.58
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	8	71.3
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	7	71.16
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1	70.95
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	4	70.16
(1,123)	1:189:A:VAL:C	1:190:A:GLN:N	1:190:A:GLN:CA	1:190:A:GLN:C	3	70.06
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	3	69.97
(1,115)	1:185:A:ILE:C	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	6	69.84
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	7	69.7
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	1	69.68
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	6	69.06
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	1	69.05
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	9	68.54
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	1	68.01
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	2	67.69
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	5	67.66
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	9	67.57
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	2	67.08
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	6	67.01
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	8	66.81
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	4	66.39
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	5	65.55
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	1	65.5
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	10	64.86
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	1	64.84
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	7	64.73
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	10	64.72
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	3	64.01
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	3	63.66
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	8	63.52
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	6	63.17
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	9	62.35
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	8	62.18
(1,93)	1:160:A:PHE:C	1:161:A:LEU:N	1:161:A:LEU:CA	1:161:A:LEU:C	10	62.1
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	2	62.04
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	6	61.99
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	10	61.67
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	1	61.49
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	9	61.24
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	4	61.09
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	10	61.09
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	6	60.78
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	5	60.65
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	1	60.64
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	5	60.54
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	5	60.49
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	2	60.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	4	60.39
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	2	60.37
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	1	60.35
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	9	60.35
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	10	60.32
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	4	60.3
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	5	60.29
(1,135)	1:138:A:PHE:N	1:138:A:PHE:CA	1:138:A:PHE:CB	1:138:A:PHE:CG	3	60.24
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	2	60.14
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	6	59.91
(1,136)	1:160:A:PHE:N	1:160:A:PHE:CA	1:160:A:PHE:CB	1:160:A:PHE:CG	4	59.8
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	9	59.65
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	8	59.63
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	7	59.62
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	3	59.38
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	6	59.3
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	7	59.29
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	6	59.29
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	2	59.25
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	3	59.11
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	7	59.06
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	10	58.98
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	7	58.92
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	9	58.82
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	1	58.79
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	5	58.78
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	10	58.76
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	8	58.68
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	4	58.65
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	2	58.61
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	7	58.39
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	8	58.39
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	9	58.35
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	3	58.32
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	7	58.19
(1,131)	1:173:A:ILE:N	1:173:A:ILE:CA	1:173:A:ILE:CB	1:173:A:ILE:CG1	10	58.14
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	8	57.92
(1,129)	1:128:A:ILE:N	1:128:A:ILE:CA	1:128:A:ILE:CB	1:128:A:ILE:CG1	4	57.75
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	5	57.33
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	2	57.29
(1,128)	1:117:A:ILE:N	1:117:A:ILE:CA	1:117:A:ILE:CB	1:117:A:ILE:CG1	9	57.27
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	3	57.18
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	10	57.09
(1,126)	1:82:A:ILE:N	1:82:A:ILE:CA	1:82:A:ILE:CB	1:82:A:ILE:CG1	4	56.68
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	8	56.36
(1,125)	1:26:A:ILE:N	1:26:A:ILE:CA	1:26:A:ILE:CB	1:26:A:ILE:CG1	4	56.01
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	1	56.0
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	8	55.46
(1,130)	1:135:A:ILE:N	1:135:A:ILE:CA	1:135:A:ILE:CB	1:135:A:ILE:CG1	3	55.01
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	10	54.82
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	5	54.57

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*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	4	54.49
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	9	54.38
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	3	54.31
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	6	54.22
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	9	54.14
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	2	54.07
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	6	53.58
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	1	53.11
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	3	52.81
(1,127)	1:107:A:ILE:N	1:107:A:ILE:CA	1:107:A:ILE:CB	1:107:A:ILE:CG1	7	52.61
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	7	52.42
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	2	51.82
(1,133)	1:25:A:PHE:N	1:25:A:PHE:CA	1:25:A:PHE:CB	1:25:A:PHE:CG	5	51.55