



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 04:56 PM EST

PDB ID : 6ZV3  
BMRB ID : 34540  
Title : TFIIS N-terminal domain (TND) from human MED26  
Authors : Veverka, V.  
Deposited on : 2020-07-23

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

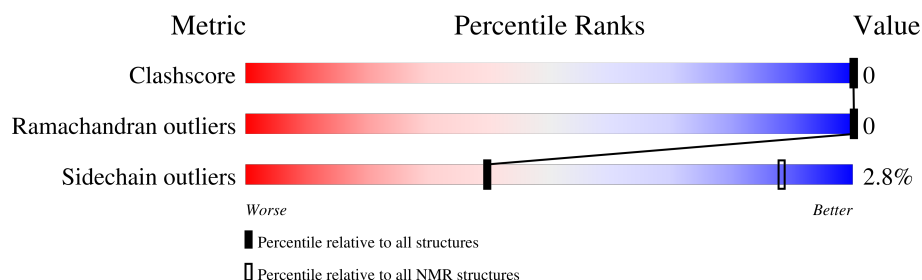
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 89%.

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	90	<div> <div>83%</div> <div>•</div> <div>16%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 50 models. Model 18 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:7-A:82 (76)	0.32	18

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 9 clusters and 6 single-model clusters were found.

Cluster number	Models
1	3, 8, 10, 11, 18, 19, 22, 24, 28, 30, 32, 34, 41, 44, 47, 48, 49, 50
2	2, 4, 17, 21, 27, 31, 39
3	9, 12, 15, 26, 42, 46
4	13, 16, 36
5	5, 20
6	29, 45
7	14, 37
8	7, 38
9	1, 6
Single-model clusters	23; 25; 33; 35; 40; 43

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

There is only 1 type of molecule in this entry. The entry contains 1480 atoms, of which 767 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mediator of RNA polymerase II transcription subunit 26.

Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1480	446	767	131	134	2	

There are 3 discrepancies between the modelled and reference sequences:

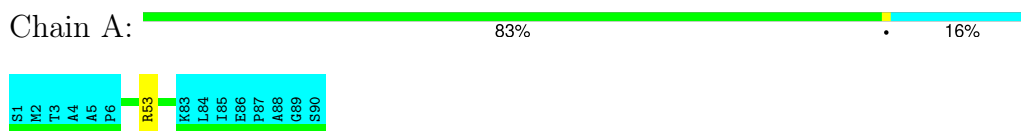
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O95402
A	89	GLY	-	expression tag	UNP O95402
A	90	SER	-	expression tag	UNP O95402

## 4 Residue-property plots

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

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

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26

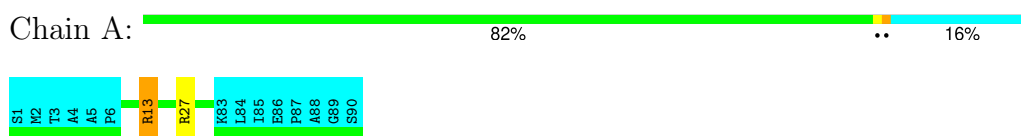


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

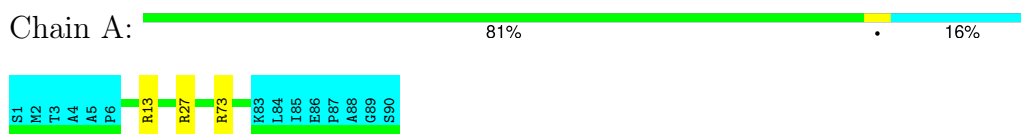
#### 4.2.1 Score per residue for model 1

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



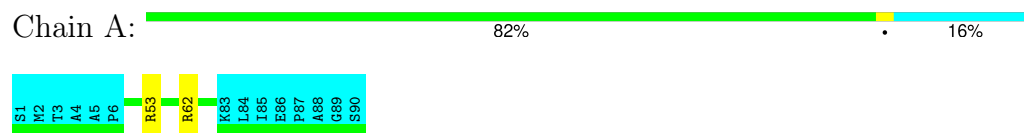
#### 4.2.2 Score per residue for model 2

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



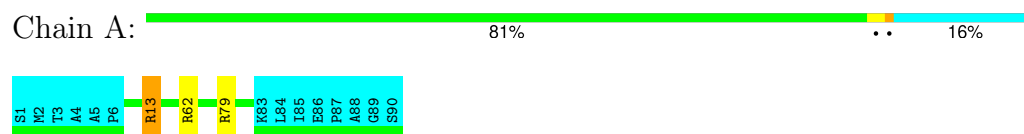
### 4.2.3 Score per residue for model 3

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



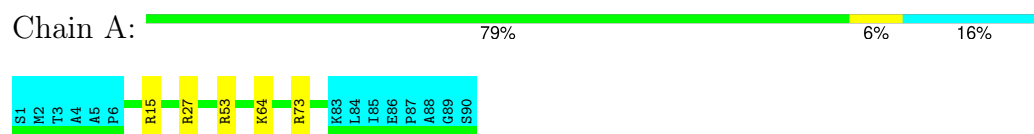
### 4.2.4 Score per residue for model 4

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



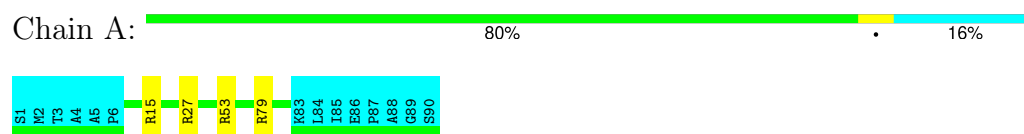
### 4.2.5 Score per residue for model 5

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



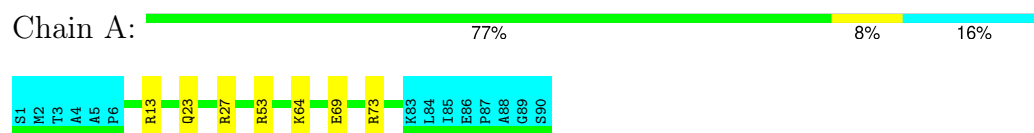
### 4.2.6 Score per residue for model 6

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



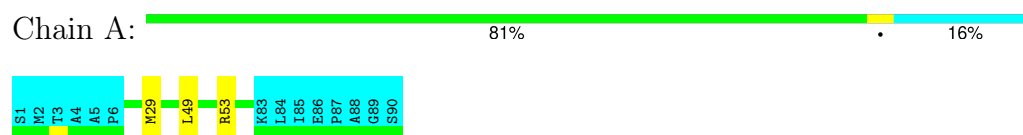
### 4.2.7 Score per residue for model 7

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



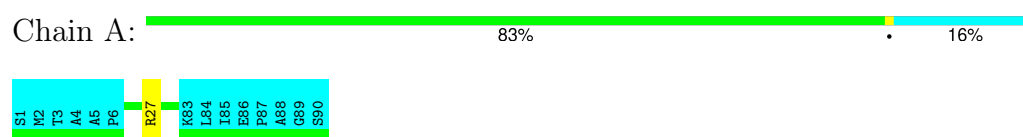
### 4.2.8 Score per residue for model 8

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



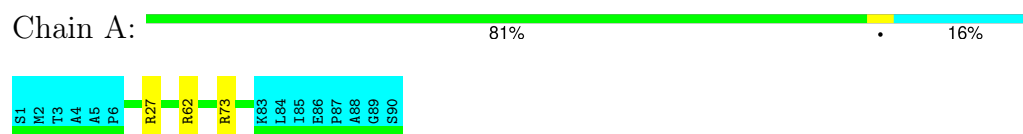
### 4.2.9 Score per residue for model 9

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



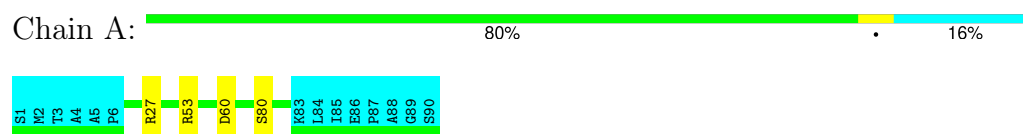
### 4.2.10 Score per residue for model 10

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



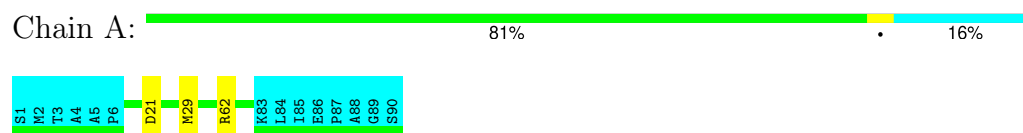
### 4.2.11 Score per residue for model 11

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



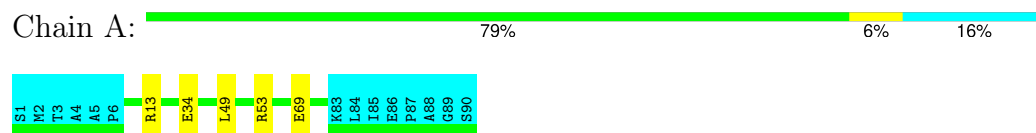
### 4.2.12 Score per residue for model 12

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



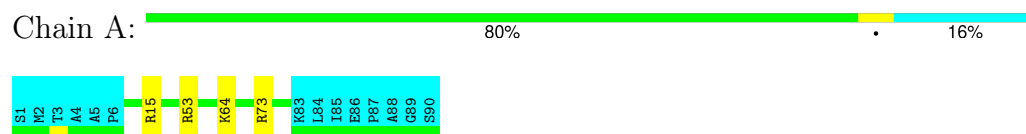
### 4.2.13 Score per residue for model 13

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



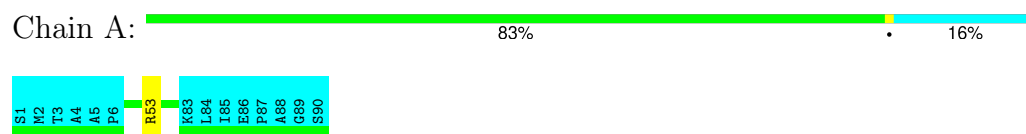
### 4.2.14 Score per residue for model 14

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



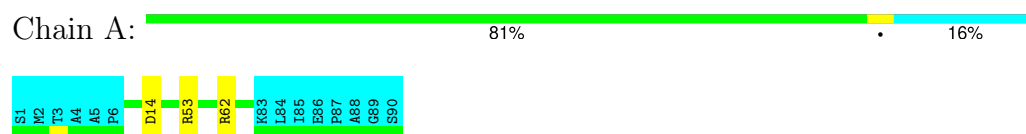
### 4.2.15 Score per residue for model 15

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



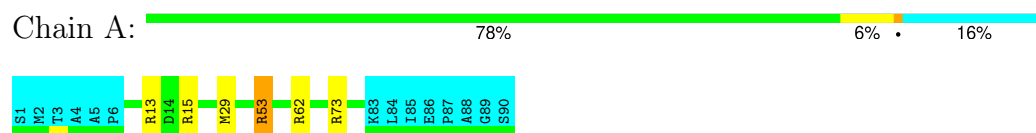
### 4.2.16 Score per residue for model 16

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



### 4.2.17 Score per residue for model 17

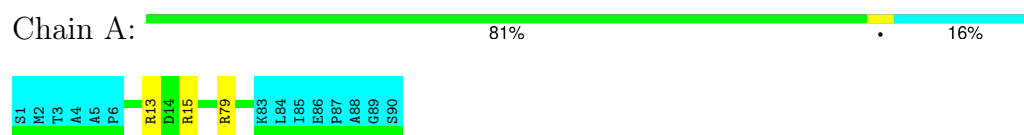
- Molecule 1: Mediator of RNA polymerase II transcription subunit 26





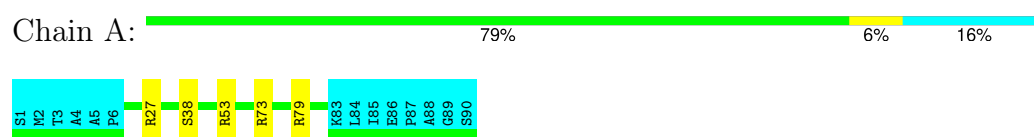
#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



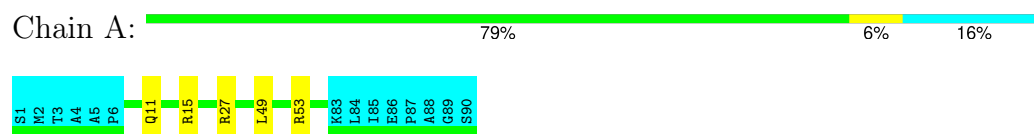
#### 4.2.19 Score per residue for model 19

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



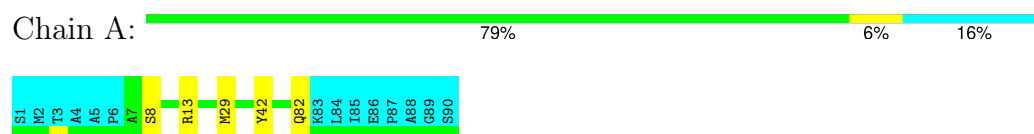
#### 4.2.20 Score per residue for model 20

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



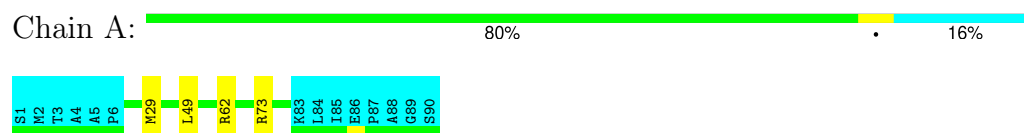
#### 4.2.21 Score per residue for model 21

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



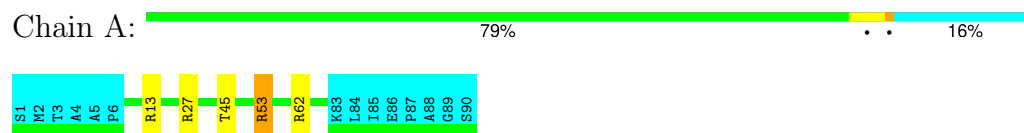
#### 4.2.22 Score per residue for model 22

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



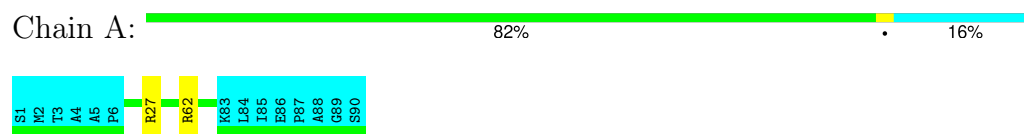
#### 4.2.23 Score per residue for model 23

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



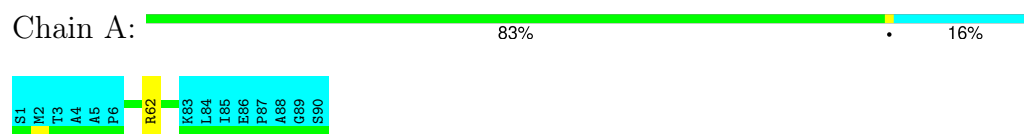
#### 4.2.24 Score per residue for model 24

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



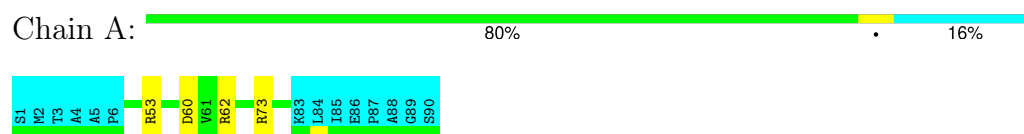
#### 4.2.25 Score per residue for model 25

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



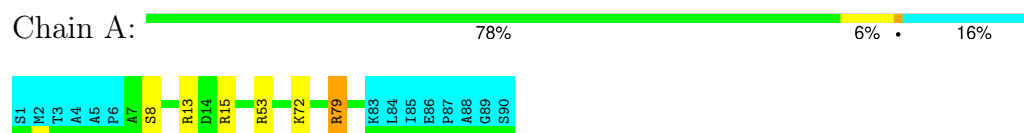
#### 4.2.26 Score per residue for model 26

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



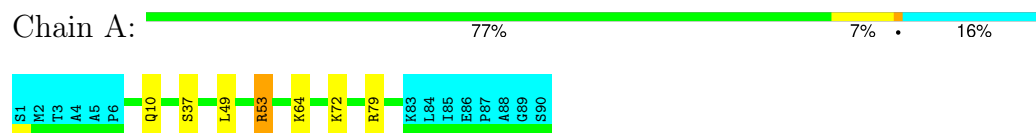
#### 4.2.27 Score per residue for model 27

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



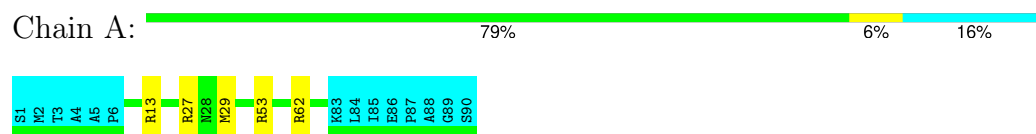
#### 4.2.28 Score per residue for model 28

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



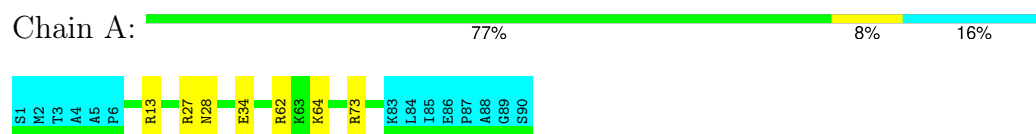
#### 4.2.29 Score per residue for model 29

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



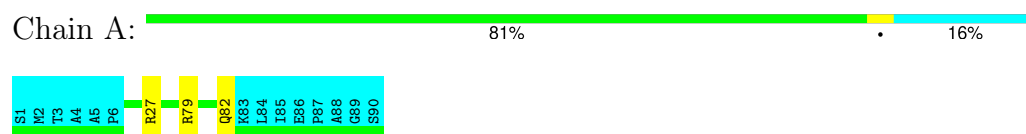
#### 4.2.30 Score per residue for model 30

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



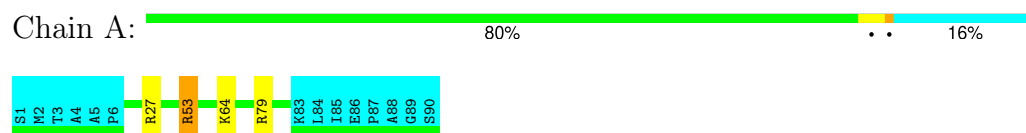
#### 4.2.31 Score per residue for model 31

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



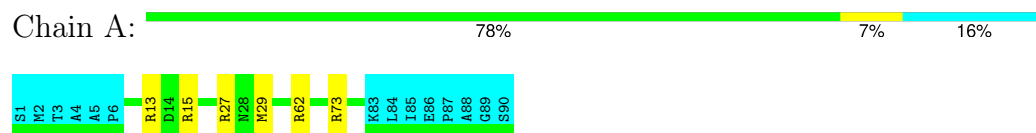
#### 4.2.32 Score per residue for model 32

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



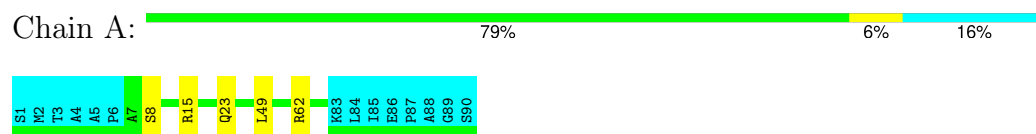
### 4.2.33 Score per residue for model 33

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



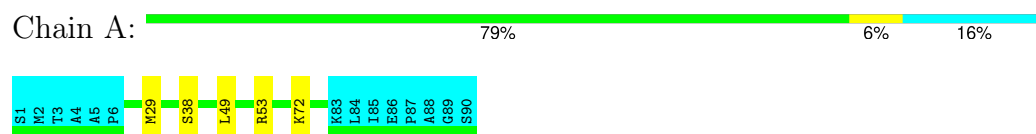
### 4.2.34 Score per residue for model 34

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



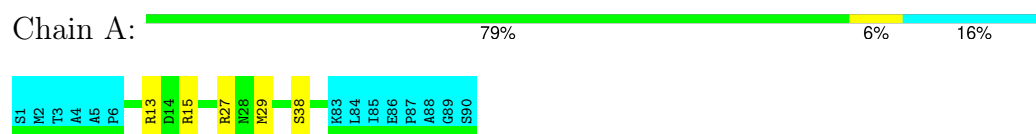
### 4.2.35 Score per residue for model 35

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



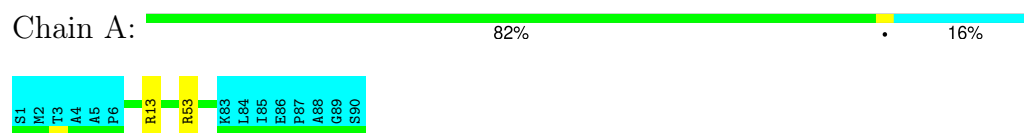
### 4.2.36 Score per residue for model 36

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



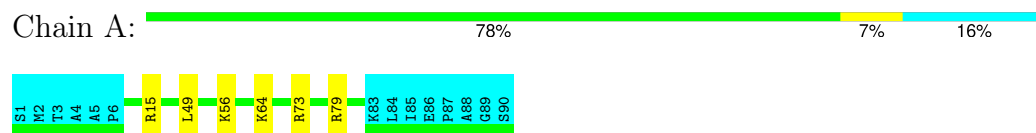
### 4.2.37 Score per residue for model 37

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



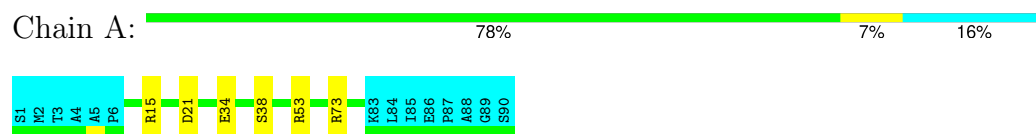
#### 4.2.38 Score per residue for model 38

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



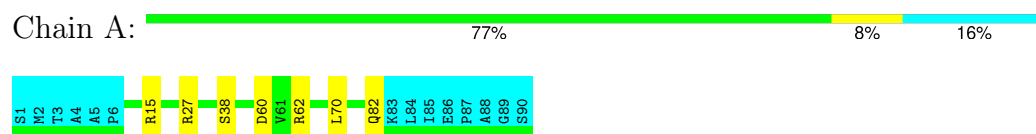
#### 4.2.39 Score per residue for model 39

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



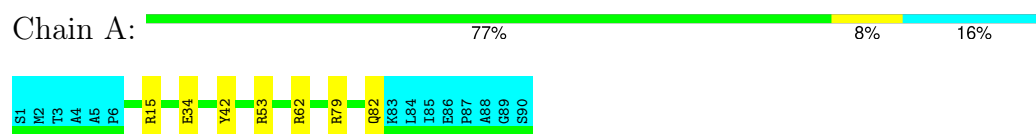
#### 4.2.40 Score per residue for model 40

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



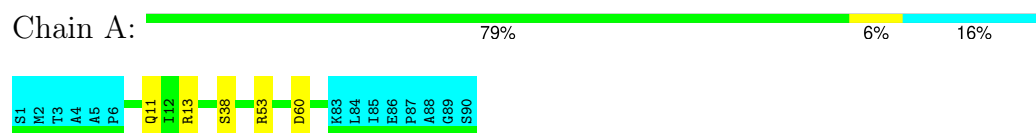
#### 4.2.41 Score per residue for model 41

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



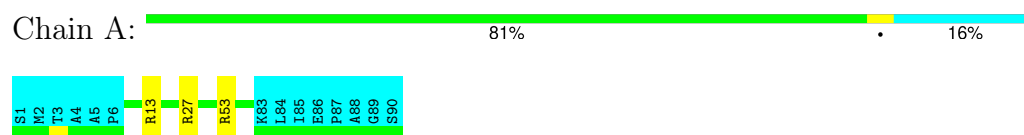
#### 4.2.42 Score per residue for model 42

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



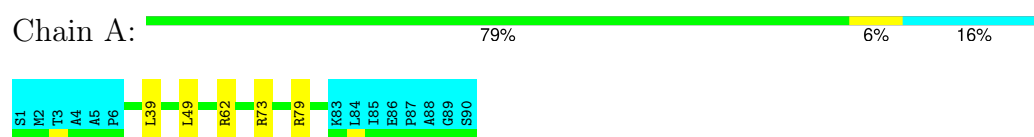
#### 4.2.43 Score per residue for model 43

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



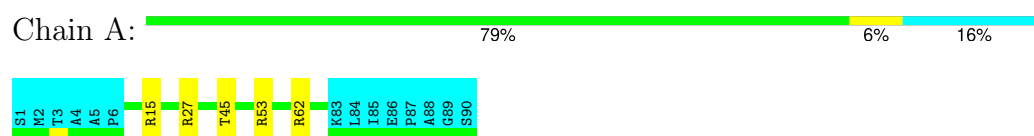
#### 4.2.44 Score per residue for model 44

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



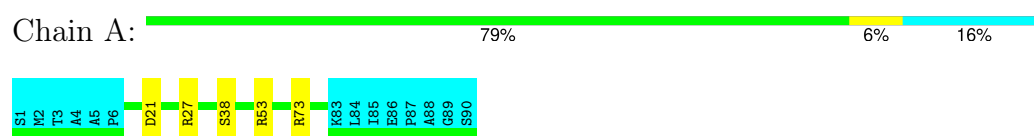
#### 4.2.45 Score per residue for model 45

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



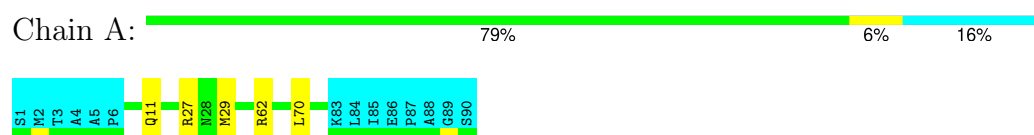
#### 4.2.46 Score per residue for model 46

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



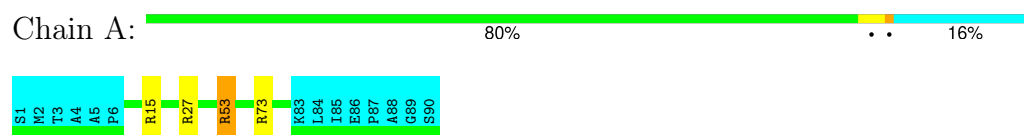
#### 4.2.47 Score per residue for model 47

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



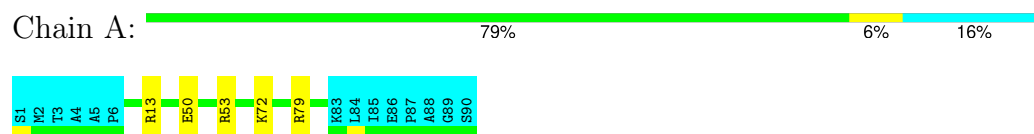
#### 4.2.48 Score per residue for model 48

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



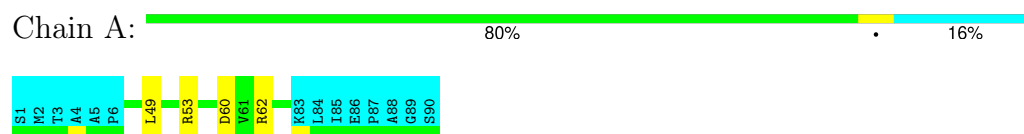
#### 4.2.49 Score per residue for model 49

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



#### 4.2.50 Score per residue for model 50

- Molecule 1: Mediator of RNA polymerase II transcription subunit 26



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
YASARA	refinement	

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	1138
Number of shifts mapped to atoms	1138
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%



## 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	0.78±0.14	0±0/624 ( 0.0± 0.0%)	0.83±0.08	3±1/838 ( 0.3± 0.2%)
All	All	0.79	2/31200 ( 0.0%)	0.83	138/41900 ( 0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	42	TYR	CD1-CE1	5.16	1.47	1.39	41	1
1	A	42	TYR	CD2-CE2	5.11	1.47	1.39	21	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	ARG	NE-CZ-NH1	9.54	125.07	120.30	33	16
1	A	79	ARG	NE-CZ-NH1	9.44	125.02	120.30	27	11
1	A	62	ARG	NE-CZ-NH1	8.45	124.53	120.30	40	17
1	A	13	ARG	NE-CZ-NH1	8.14	124.37	120.30	43	18
1	A	73	ARG	NE-CZ-NH1	8.13	124.36	120.30	48	16
1	A	27	ARG	NE-CZ-NH1	7.79	124.20	120.30	45	21
1	A	53	ARG	NE-CZ-NH1	7.66	124.13	120.30	14	18
1	A	73	ARG	NE-CZ-NH2	-6.82	116.89	120.30	22	1
1	A	53	ARG	NE-CZ-NH2	-6.76	116.92	120.30	49	2
1	A	62	ARG	NE-CZ-NH2	-6.13	117.24	120.30	29	8
1	A	27	ARG	NE-CZ-NH2	-5.68	117.46	120.30	31	6
1	A	79	ARG	NE-CZ-NH2	-5.29	117.65	120.30	18	3
1	A	13	ARG	NE-CZ-NH2	-5.16	117.72	120.30	18	1

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	30900	33300	33300	-

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 -.

There are no clashes.

## 6.3 Torsion angles [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	76/90 (84%)	76±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	3800/4500 (84%)	3795 (100%)	5 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/79 (87%)	67±1 (97±2%)	2±1 (3±2%)	40	88
All	All	3450/3950 (87%)	3355 (97%)	95 (3%)	40	88

All 27 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	53	ARG	15
1	A	29	MET	10
1	A	49	LEU	10
1	A	64	LYS	7
1	A	38	SER	7
1	A	60	ASP	5
1	A	34	GLU	4
1	A	82	GLN	4
1	A	72	LYS	4
1	A	21	ASP	3
1	A	11	GLN	3
1	A	8	SER	3
1	A	13	ARG	2
1	A	23	GLN	2
1	A	69	GLU	2
1	A	45	THR	2
1	A	70	LEU	2
1	A	80	SER	1
1	A	14	ASP	1
1	A	62	ARG	1
1	A	79	ARG	1
1	A	10	GLN	1
1	A	37	SER	1
1	A	28	ASN	1
1	A	56	LYS	1
1	A	39	LEU	1
1	A	50	GLU	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1138
Number of shifts mapped to atoms	1138
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	$-0.40 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	86	$0.20 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	84	$-0.24 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	81	$0.50 \pm 0.48$	None needed (imprecise)

#### 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 89%, i.e. 1007 atoms were assigned a chemical shift out of a possible 1126. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	371/375 (99%)	149/150 (99%)	150/152 (99%)	72/73 (99%)
Sidechain	618/730 (85%)	424/470 (90%)	187/221 (85%)	7/39 (18%)

*Continued on next page...*

Continued from previous page...

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	18/21 (86%)	10/10 (100%)	7/10 (70%)	1/1 (100%)
Overall	1007/1126 (89%)	583/630 (93%)	344/383 (90%)	80/113 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1137 atoms were assigned a chemical shift out of a possible 1291. 0 out of 15 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	424/442 (96%)	171/177 (97%)	172/180 (96%)	81/85 (95%)
Sidechain	695/828 (84%)	477/536 (89%)	211/252 (84%)	7/40 (18%)
Aromatic	18/21 (86%)	10/10 (100%)	7/10 (70%)	1/1 (100%)
Overall	1137/1291 (88%)	658/723 (91%)	390/442 (88%)	89/126 (71%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

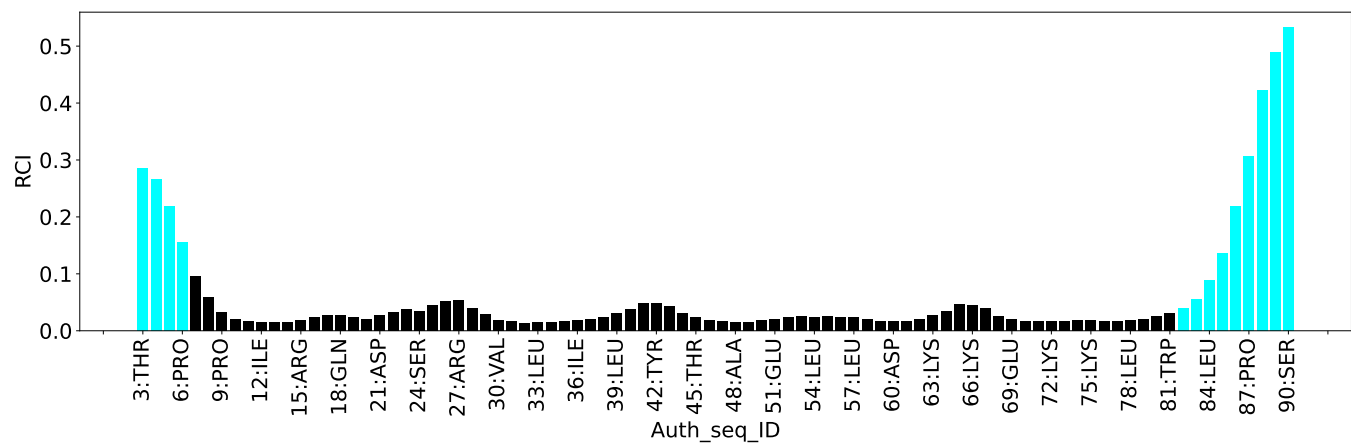
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	52	THR	HG1	4.63	0.08 – 2.19	16.6

#### 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	1827
Intra-residue ( $ i-j =0$ )	506
Sequential ( $ i-j =1$ )	393
Medium range ( $ i-j >1$ and $ i-j <5$ )	445
Long range ( $ i-j \geq 5$ )	483
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	144
Number of unmapped restraints	0
Number of restraints per residue	21.9
Number of long range restraints per residue <sup>1</sup>	5.4

<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)	11.0	0.2
0.2-0.5 (Medium)	6.6	0.5
>0.5 (Large)	None	None



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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.3	4.92
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

## 9 Distance violation analysis [i](#)

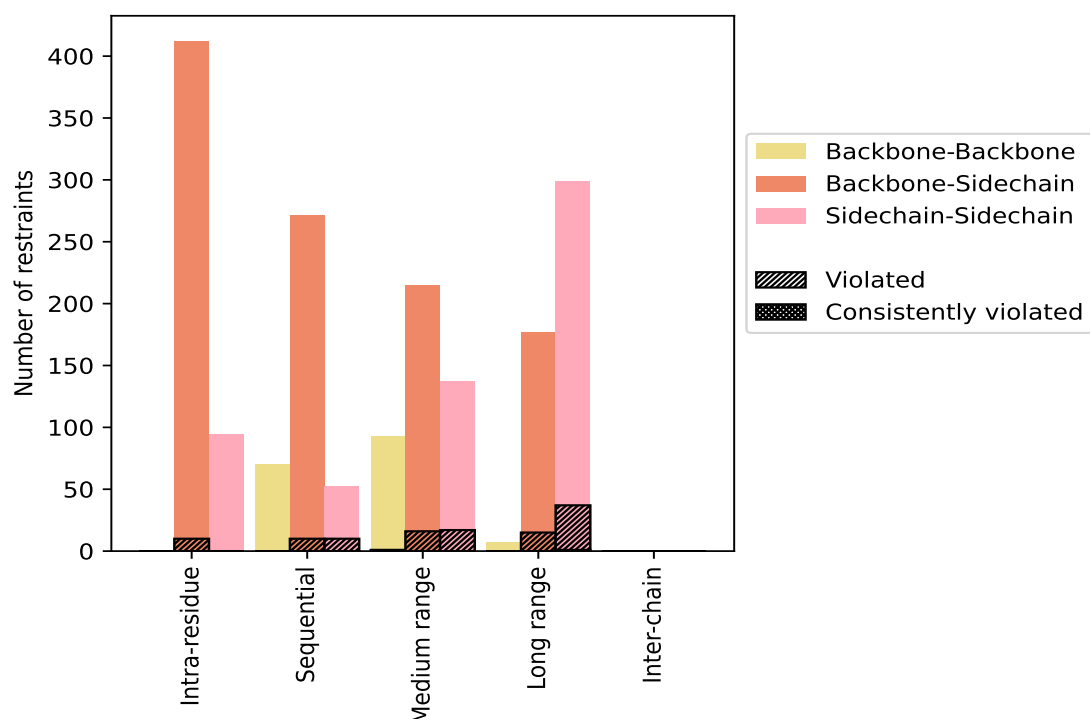
### 9.1 Summary of distance violations [i](#)

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>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">506</a>	<a href="#">27.7</a>	<a href="#">10</a>	<a href="#">2.0</a>	<a href="#">0.5</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	412	22.6	10	2.4	0.5	0	0.0	0.0
Sidechain-Sidechain	94	5.1	0	0.0	0.0	0	0.0	0.0
<a href="#">Sequential ( i-j =1)</a>	<a href="#">393</a>	<a href="#">21.5</a>	<a href="#">20</a>	<a href="#">5.1</a>	<a href="#">1.1</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	70	3.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	271	14.8	10	3.7	0.5	0	0.0	0.0
Sidechain-Sidechain	52	2.8	10	19.2	0.5	0	0.0	0.0
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">445</a>	<a href="#">24.4</a>	<a href="#">34</a>	<a href="#">7.6</a>	<a href="#">1.9</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	93	5.1	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	215	11.8	16	7.4	0.9	0	0.0	0.0
Sidechain-Sidechain	137	7.5	17	12.4	0.9	0	0.0	0.0
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">483</a>	<a href="#">26.4</a>	<a href="#">52</a>	<a href="#">10.8</a>	<a href="#">2.8</a>	<a href="#">1</a>	<a href="#">0.2</a>	<a href="#">0.1</a>
Backbone-Backbone	7	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	177	9.7	15	8.5	0.8	0	0.0	0.0
Sidechain-Sidechain	299	16.4	37	12.4	2.0	1	0.3	0.1
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
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
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">1827</a>	<a href="#">100.0</a>	<a href="#">116</a>	<a href="#">6.3</a>	<a href="#">6.3</a>	<a href="#">1</a>	<a href="#">0.1</a>	<a href="#">0.1</a>
Backbone-Backbone	170	9.3	1	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	1075	58.8	51	4.7	2.8	0	0.0	0.0
Sidechain-Sidechain	582	31.9	64	11.0	3.5	1	0.2	0.1

<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	2	4	0	4	0	10	0.15	0.25	0.05	0.13
2	1	4	3	7	0	15	0.18	0.27	0.05	0.19
3	0	4	2	7	0	13	0.18	0.5	0.11	0.14
4	1	3	2	6	0	12	0.21	0.32	0.07	0.22
5	0	3	0	8	0	11	0.16	0.32	0.06	0.13
6	0	1	0	2	0	3	0.14	0.2	0.04	0.11
7	0	3	0	5	0	8	0.14	0.19	0.03	0.13
8	1	4	3	9	0	17	0.17	0.26	0.05	0.17
9	0	3	0	5	0	8	0.2	0.47	0.1	0.16
10	0	3	0	3	0	6	0.16	0.28	0.06	0.14

*Continued on next page...*

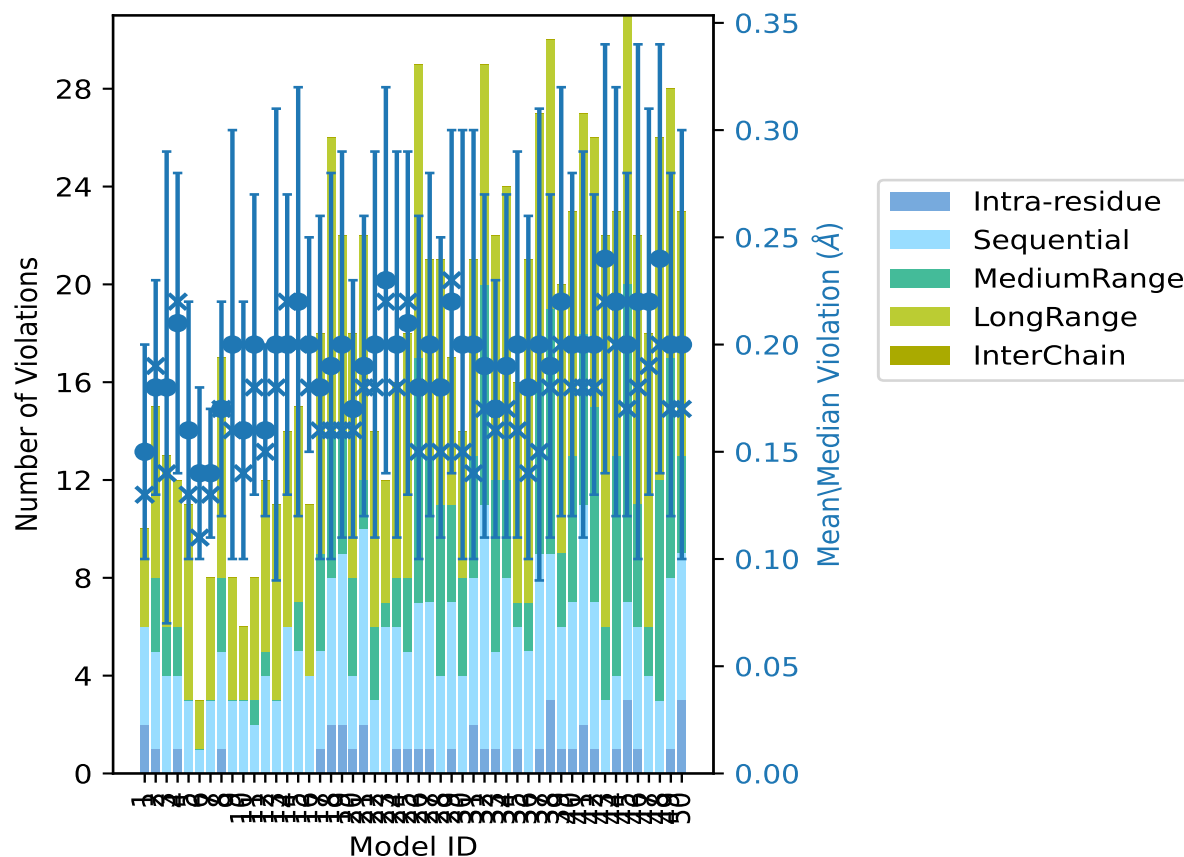
*Continued from previous page...*

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	0	2	1	5	0	8	0.2	0.36	0.07	0.18
12	0	4	1	7	0	12	0.16	0.25	0.04	0.15
13	0	3	0	8	0	11	0.2	0.5	0.11	0.18
14	0	6	0	8	0	14	0.2	0.31	0.07	0.22
15	0	5	2	8	0	15	0.22	0.47	0.1	0.2
16	0	4	0	7	0	11	0.2	0.28	0.05	0.18
17	1	4	4	9	0	18	0.18	0.44	0.08	0.16
18	2	6	6	12	0	26	0.19	0.46	0.09	0.16
19	2	7	5	8	0	22	0.2	0.46	0.09	0.16
20	1	3	4	10	0	18	0.17	0.31	0.06	0.16
21	2	8	2	10	0	22	0.19	0.35	0.07	0.18
22	0	3	3	8	0	14	0.2	0.49	0.09	0.18
23	0	6	1	5	0	12	0.23	0.39	0.09	0.22
24	1	5	2	8	0	16	0.2	0.45	0.09	0.18
25	1	4	3	10	0	18	0.21	0.42	0.08	0.22
26	1	6	10	12	0	29	0.18	0.4	0.08	0.15
27	1	6	6	8	0	21	0.2	0.37	0.08	0.18
28	0	4	7	10	0	21	0.18	0.36	0.07	0.15
29	1	6	4	6	0	17	0.22	0.42	0.08	0.23
30	0	4	4	6	0	14	0.2	0.38	0.1	0.15
31	2	6	5	8	0	21	0.2	0.49	0.1	0.14
32	1	10	9	9	0	29	0.19	0.48	0.08	0.17
33	1	4	7	10	0	22	0.17	0.29	0.06	0.16
34	0	8	4	12	0	24	0.19	0.41	0.08	0.17
35	1	5	1	9	0	16	0.2	0.44	0.09	0.16
36	0	5	2	14	0	21	0.18	0.41	0.08	0.14
37	1	8	7	11	0	27	0.2	0.44	0.11	0.15
38	3	6	10	11	0	30	0.19	0.43	0.08	0.18
39	1	5	3	11	0	20	0.22	0.48	0.1	0.2
40	1	6	6	10	0	23	0.2	0.35	0.08	0.18
41	2	9	7	9	0	27	0.2	0.43	0.09	0.18
42	1	6	8	11	0	26	0.2	0.42	0.07	0.18
43	0	3	3	16	0	22	0.24	0.48	0.1	0.22
44	1	3	9	10	0	23	0.22	0.43	0.1	0.2
45	3	4	13	11	0	31	0.2	0.4	0.08	0.17
46	1	5	5	11	0	22	0.22	0.46	0.12	0.18
47	0	4	2	12	0	18	0.22	0.45	0.09	0.19
48	0	3	9	14	0	26	0.24	0.46	0.1	0.2
49	1	7	9	11	0	28	0.2	0.38	0.08	0.17
50	3	6	4	10	0	23	0.2	0.46	0.1	0.17

<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 ⓘ



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

### 9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1711(IR:496, SQ:373, MR:411, LR:431, 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>	%
5	5	12	13	0	35	1	2.0
0	3	4	6	0	13	2	4.0
1	0	3	8	0	12	3	6.0
1	0	2	2	0	5	4	8.0

*Continued on next page...*

*Continued from previous page...*

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>	%
1	2	0	2	0	5	5	10.0
0	0	2	3	0	5	6	12.0
1	0	1	4	0	6	7	14.0
0	0	1	1	0	2	8	16.0
0	1	1	1	0	3	9	18.0
0	1	0	1	0	2	10	20.0
0	1	1	3	0	5	11	22.0
0	1	1	0	0	2	12	24.0
0	0	1	0	0	1	13	26.0
0	0	1	0	0	1	14	28.0
0	0	1	0	0	1	15	30.0
0	0	0	0	0	0	16	32.0
1	0	1	0	0	2	17	34.0
0	0	0	0	0	0	18	36.0
0	0	0	1	0	1	19	38.0
0	1	0	0	0	1	20	40.0
0	0	1	0	0	1	21	42.0
0	0	1	0	0	1	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
0	0	0	0	0	0	25	50.0
0	0	0	0	0	0	26	52.0
0	0	0	1	0	1	27	54.0
0	1	0	1	0	2	28	56.0
0	0	0	0	0	0	29	58.0
0	1	0	1	0	2	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	1	0	1	32	64.0
0	2	0	0	0	2	33	66.0
0	1	0	0	0	1	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	1	0	1	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	0	0	0	40	80.0
0	0	0	0	0	0	41	82.0
0	0	0	0	0	0	42	84.0
0	0	0	0	0	0	43	86.0
0	0	0	0	0	0	44	88.0
0	0	0	0	0	0	45	90.0

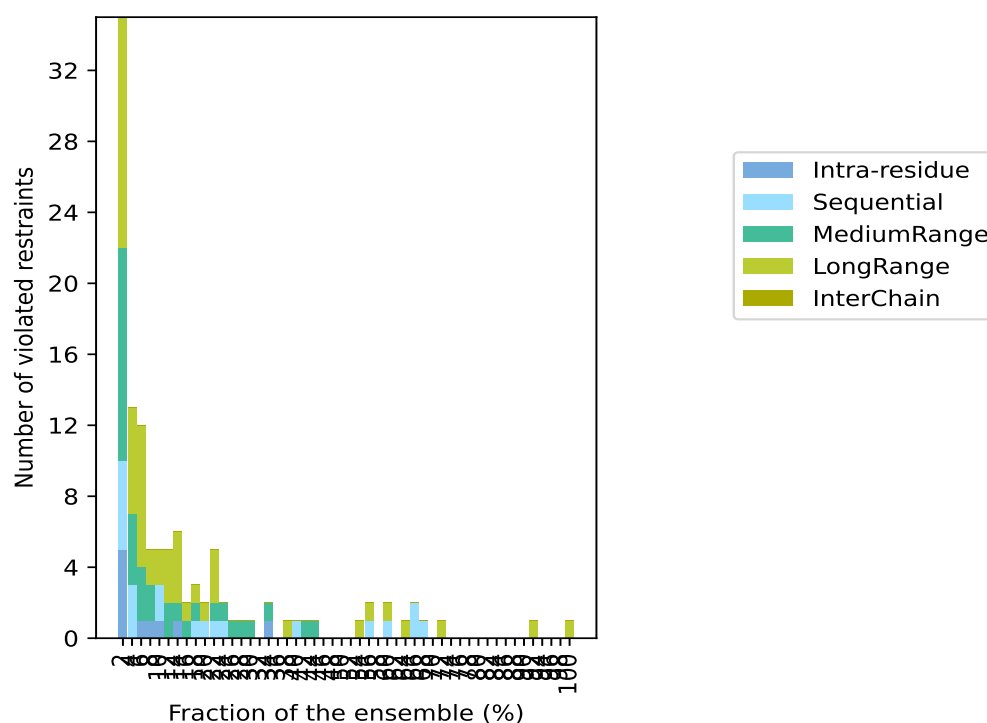
*Continued on next page...*

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	0	1	0	1	46	92.0
0	0	0	0	0	0	47	94.0
0	0	0	0	0	0	48	96.0
0	0	0	0	0	0	49	98.0
0	0	0	1	0	1	50	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

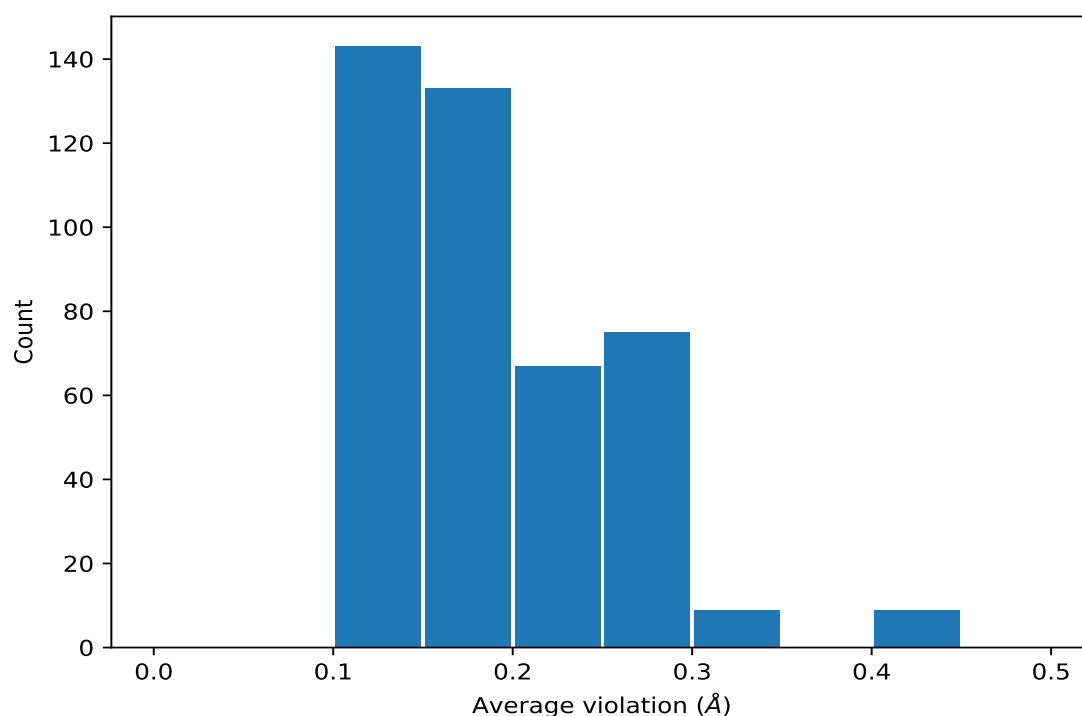
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	50	0.27	0.09	0.26
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	50	0.27	0.09	0.26
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	50	0.27	0.09	0.26
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	46	0.32	0.11	0.3
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	46	0.32	0.11	0.3
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	46	0.32	0.11	0.3
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	36	0.28	0.08	0.27
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	36	0.28	0.08	0.27
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	36	0.28	0.08	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	34	0.27	0.07	0.26

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	34	0.27	0.07	0.26
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	34	0.27	0.07	0.26
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	33	0.19	0.06	0.17
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	33	0.19	0.06	0.17
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	33	0.19	0.06	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	33	0.17	0.05	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	33	0.17	0.05	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	32	0.21	0.07	0.2
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	32	0.21	0.07	0.2
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	32	0.21	0.07	0.2
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	30	0.19	0.06	0.18
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	30	0.19	0.06	0.18
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	30	0.19	0.06	0.18
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	30	0.19	0.06	0.18
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	30	0.19	0.06	0.18
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	30	0.19	0.06	0.18
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	30	0.17	0.05	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	30	0.17	0.05	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	28	0.2	0.06	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	28	0.2	0.06	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	28	0.2	0.06	0.19
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	28	0.19	0.08	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	28	0.19	0.08	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	28	0.19	0.08	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	28	0.19	0.08	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	28	0.19	0.08	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	28	0.19	0.08	0.17
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	27	0.23	0.08	0.22
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	27	0.23	0.08	0.22
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	22	0.21	0.08	0.2
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	22	0.21	0.08	0.2
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	22	0.21	0.08	0.2
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	21	0.18	0.07	0.15
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	21	0.18	0.07	0.15
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	21	0.18	0.07	0.15
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	20	0.12	0.02	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	20	0.12	0.02	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	20	0.12	0.02	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	20	0.12	0.02	0.11
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	19	0.2	0.09	0.17
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	19	0.2	0.09	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	17	0.16	0.05	0.16
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	17	0.15	0.03	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	17	0.15	0.03	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	17	0.15	0.03	0.14
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	15	0.18	0.07	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	15	0.18	0.07	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	15	0.18	0.07	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	15	0.18	0.07	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	15	0.18	0.07	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	15	0.18	0.07	0.16
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	14	0.14	0.03	0.12
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	13	0.17	0.05	0.15
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	13	0.17	0.05	0.15
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	13	0.17	0.05	0.15
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	13	0.17	0.05	0.15
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	13	0.17	0.05	0.15
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	13	0.17	0.05	0.15
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	12	0.16	0.04	0.16
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	12	0.16	0.04	0.16
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	12	0.12	0.01	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	12	0.12	0.01	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	12	0.12	0.01	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	12	0.12	0.01	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	12	0.12	0.01	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	12	0.12	0.01	0.12
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	11	0.3	0.09	0.29
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	11	0.3	0.09	0.29
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	11	0.2	0.07	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	11	0.15	0.03	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	11	0.15	0.03	0.14
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	11	0.14	0.02	0.14
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	11	0.14	0.02	0.14
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	11	0.14	0.02	0.14
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	11	0.12	0.01	0.12
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	11	0.12	0.01	0.12
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	11	0.12	0.01	0.12
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	10	0.19	0.05	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	10	0.19	0.05	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	10	0.19	0.05	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	10	0.19	0.05	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	10	0.19	0.05	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	10	0.19	0.05	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	10	0.15	0.05	0.14
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	10	0.15	0.05	0.14
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	10	0.15	0.05	0.14
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	10	0.15	0.05	0.14
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	10	0.15	0.05	0.14
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	10	0.15	0.05	0.14
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	9	0.17	0.05	0.18
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	9	0.17	0.05	0.18
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	9	0.15	0.04	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	9	0.15	0.04	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	9	0.15	0.04	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	9	0.15	0.04	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	9	0.15	0.04	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	9	0.15	0.04	0.14
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	9	0.14	0.03	0.13
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	9	0.14	0.03	0.13
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	9	0.14	0.03	0.13
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	9	0.14	0.03	0.13
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	9	0.14	0.03	0.13
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	9	0.14	0.03	0.13
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	8	0.31	0.06	0.3
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	8	0.31	0.06	0.3
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	8	0.31	0.06	0.3
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	8	0.31	0.06	0.3
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	8	0.31	0.06	0.3
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	8	0.31	0.06	0.3
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	8	0.14	0.03	0.14
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	8	0.14	0.03	0.14
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	8	0.14	0.03	0.14
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	7	0.18	0.04	0.18
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	7	0.18	0.04	0.18
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	7	0.18	0.04	0.18
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	7	0.18	0.06	0.14
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	7	0.18	0.06	0.14
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	7	0.18	0.06	0.14
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	7	0.16	0.02	0.16
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	7	0.16	0.02	0.16
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	7	0.15	0.03	0.14
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	7	0.15	0.03	0.14
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	7	0.15	0.03	0.14
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	7	0.15	0.05	0.13
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	7	0.15	0.05	0.13
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	7	0.15	0.05	0.13
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	7	0.13	0.02	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	7	0.13	0.02	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	7	0.13	0.02	0.12
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	6	0.43	0.08	0.48
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	6	0.43	0.08	0.48
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	6	0.19	0.05	0.2
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	6	0.19	0.05	0.2
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	6	0.17	0.05	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	6	0.17	0.05	0.15
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	6	0.17	0.04	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	6	0.17	0.04	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	6	0.17	0.04	0.17
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	6	0.15	0.02	0.16
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD11	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD12	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD13	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD11	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD12	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD13	5	0.27	0.16	0.17

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD11	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD12	5	0.27	0.16	0.17
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD13	5	0.27	0.16	0.17
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE1	5	0.24	0.1	0.29
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE2	5	0.24	0.1	0.29
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE1	5	0.24	0.1	0.29
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE2	5	0.24	0.1	0.29
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE1	5	0.24	0.1	0.29
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE2	5	0.24	0.1	0.29
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD2	5	0.16	0.05	0.15
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD3	5	0.16	0.05	0.15
(1,1737)	1:68:A:GLU:HG2	1:69:A:GLU:H	5	0.14	0.03	0.13
(1,1737)	1:68:A:GLU:HG3	1:69:A:GLU:H	5	0.14	0.03	0.13
(1,567)	1:58:A:ILE:HD11	1:59:A:ASN:H	5	0.12	0.01	0.12
(1,567)	1:58:A:ILE:HD12	1:59:A:ASN:H	5	0.12	0.01	0.12
(1,567)	1:58:A:ILE:HD13	1:59:A:ASN:H	5	0.12	0.01	0.12
(1,40)	1:12:A:ILE:HD11	1:39:A:LEU:HG	4	0.16	0.07	0.12
(1,40)	1:12:A:ILE:HD12	1:39:A:LEU:HG	4	0.16	0.07	0.12
(1,40)	1:12:A:ILE:HD13	1:39:A:LEU:HG	4	0.16	0.07	0.12
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD11	4	0.15	0.02	0.15
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD12	4	0.15	0.02	0.15
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD13	4	0.15	0.02	0.15
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD11	4	0.15	0.02	0.15
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD12	4	0.15	0.02	0.15
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD13	4	0.15	0.02	0.15
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE2	4	0.14	0.03	0.15
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE3	4	0.14	0.03	0.15
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD11	4	0.12	0.02	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD12	4	0.12	0.02	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD13	4	0.12	0.02	0.11
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD1	4	0.11	0.01	0.11
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD2	4	0.11	0.01	0.11
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD11	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD12	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD13	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD21	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD22	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD23	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD11	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD12	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD13	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD21	3	0.28	0.02	0.29

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD22	3	0.28	0.02	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD23	3	0.28	0.02	0.29
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD11	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD12	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD13	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD11	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD12	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD13	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD11	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD12	3	0.28	0.1	0.22
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD13	3	0.28	0.1	0.22
(1,1527)	1:39:A:LEU:HD11	1:44:A:ILE:H	3	0.26	0.08	0.27
(1,1527)	1:39:A:LEU:HD12	1:44:A:ILE:H	3	0.26	0.08	0.27
(1,1527)	1:39:A:LEU:HD13	1:44:A:ILE:H	3	0.26	0.08	0.27
(1,1527)	1:39:A:LEU:HD21	1:44:A:ILE:H	3	0.26	0.08	0.27
(1,1527)	1:39:A:LEU:HD22	1:44:A:ILE:H	3	0.26	0.08	0.27
(1,1527)	1:39:A:LEU:HD23	1:44:A:ILE:H	3	0.26	0.08	0.27
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD11	3	0.25	0.1	0.3
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD12	3	0.25	0.1	0.3
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD13	3	0.25	0.1	0.3
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG11	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG12	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG13	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG21	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG22	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG23	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG11	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG12	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG13	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG21	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG22	3	0.25	0.04	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG23	3	0.25	0.04	0.26
(1,192)	1:26:A:ILE:HD11	1:32:A:VAL:H	3	0.17	0.06	0.16
(1,192)	1:26:A:ILE:HD12	1:32:A:VAL:H	3	0.17	0.06	0.16
(1,192)	1:26:A:ILE:HD13	1:32:A:VAL:H	3	0.17	0.06	0.16
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD21	3	0.16	0.03	0.18
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD22	3	0.16	0.03	0.18
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD23	3	0.16	0.03	0.18
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB2	3	0.16	0.03	0.15
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB3	3	0.16	0.03	0.15
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG21	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG22	3	0.14	0.01	0.14

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG23	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG21	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG22	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG23	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG21	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG22	3	0.14	0.01	0.14
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG23	3	0.14	0.01	0.14
(1,335)	1:36:A:ILE:HG21	1:77:A:LEU:H	3	0.14	0.02	0.16
(1,335)	1:36:A:ILE:HG22	1:77:A:LEU:H	3	0.14	0.02	0.16
(1,335)	1:36:A:ILE:HG23	1:77:A:LEU:H	3	0.14	0.02	0.16
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG21	3	0.13	0.01	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG22	3	0.13	0.01	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG23	3	0.13	0.01	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG21	3	0.13	0.01	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG22	3	0.13	0.01	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG23	3	0.13	0.01	0.14
(1,454)	1:49:A:LEU:HG	1:55:A:GLY:HA3	3	0.1	0.0	0.1
(1,370)	1:7:A:ALA:HB1	1:42:A:TYR:HE1	2	0.22	0.08	0.22
(1,370)	1:7:A:ALA:HB1	1:42:A:TYR:HE2	2	0.22	0.08	0.22
(1,370)	1:7:A:ALA:HB2	1:42:A:TYR:HE1	2	0.22	0.08	0.22
(1,370)	1:7:A:ALA:HB2	1:42:A:TYR:HE2	2	0.22	0.08	0.22
(1,370)	1:7:A:ALA:HB3	1:42:A:TYR:HE1	2	0.22	0.08	0.22
(1,370)	1:7:A:ALA:HB3	1:42:A:TYR:HE2	2	0.22	0.08	0.22
(1,1605)	1:49:A:LEU:HD11	1:84:A:LEU:HB2	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD11	1:84:A:LEU:HB3	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD12	1:84:A:LEU:HB2	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD12	1:84:A:LEU:HB3	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD13	1:84:A:LEU:HB2	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD13	1:84:A:LEU:HB3	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD21	1:84:A:LEU:HB2	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD21	1:84:A:LEU:HB3	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD22	1:84:A:LEU:HB2	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD22	1:84:A:LEU:HB3	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD23	1:84:A:LEU:HB2	2	0.22	0.04	0.22
(1,1605)	1:49:A:LEU:HD23	1:84:A:LEU:HB3	2	0.22	0.04	0.22
(1,474)	1:49:A:LEU:HD21	1:81:A:TRP:HD1	2	0.18	0.04	0.18
(1,474)	1:49:A:LEU:HD22	1:81:A:TRP:HD1	2	0.18	0.04	0.18
(1,474)	1:49:A:LEU:HD23	1:81:A:TRP:HD1	2	0.18	0.04	0.18
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG21	2	0.18	0.08	0.18
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG22	2	0.18	0.08	0.18
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG23	2	0.18	0.08	0.18
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG21	2	0.18	0.08	0.18

*Continued on next page...*

*Continued from previous page...*

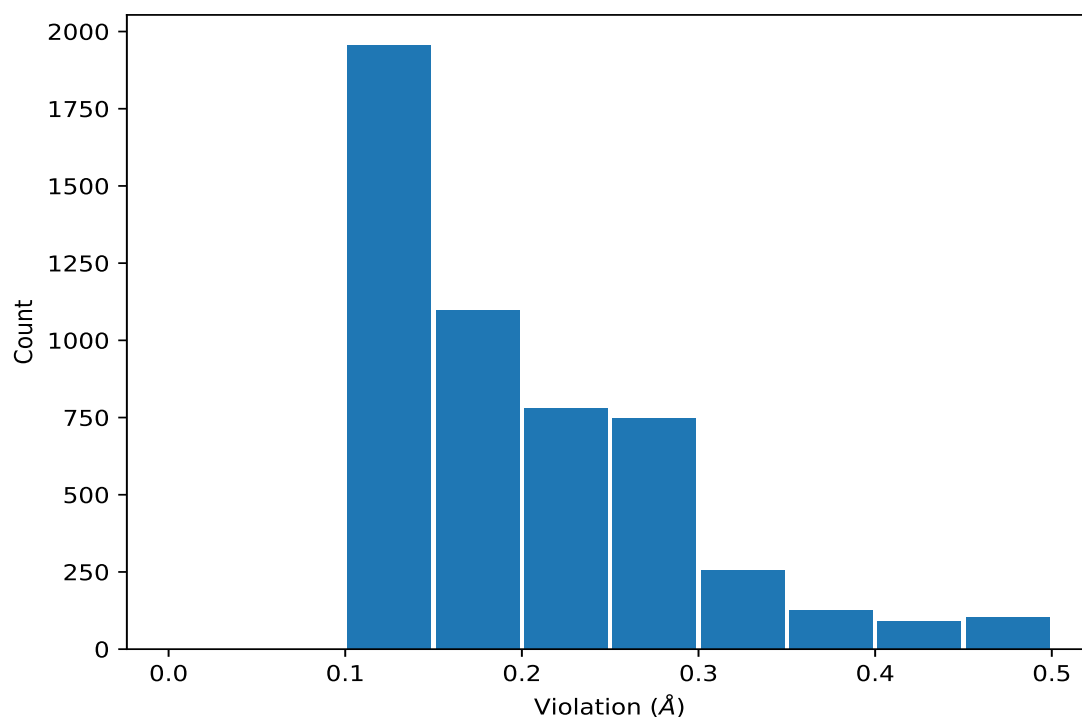
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG22	2	0.18	0.08	0.18
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG23	2	0.18	0.08	0.18
(1,427)	1:45:A:THR:HG21	1:46:A:LYS:H	2	0.16	0.01	0.16
(1,427)	1:45:A:THR:HG22	1:46:A:LYS:H	2	0.16	0.01	0.16
(1,427)	1:45:A:THR:HG23	1:46:A:LYS:H	2	0.16	0.01	0.16
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG11	2	0.15	0.04	0.15
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG12	2	0.15	0.04	0.15
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG13	2	0.15	0.04	0.15
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG21	2	0.15	0.04	0.15
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG22	2	0.15	0.04	0.15
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG23	2	0.15	0.04	0.15
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD21	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD22	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD23	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD21	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD22	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD23	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD21	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD22	2	0.14	0.03	0.14
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD23	2	0.14	0.03	0.14
(1,701)	1:74:A:ALA:HA	1:77:A:LEU:HB3	2	0.14	0.04	0.14
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG21	2	0.14	0.01	0.14
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG22	2	0.14	0.01	0.14
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG23	2	0.14	0.01	0.14
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD21	2	0.14	0.02	0.14
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD22	2	0.14	0.02	0.14
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD23	2	0.14	0.02	0.14
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD11	2	0.14	0.02	0.14
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD12	2	0.14	0.02	0.14
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD13	2	0.14	0.02	0.14
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD21	2	0.14	0.02	0.14
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD22	2	0.14	0.02	0.14
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD23	2	0.14	0.02	0.14
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE1	2	0.11	0.01	0.11
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE2	2	0.11	0.01	0.11
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE3	2	0.11	0.01	0.11
(1,1562)	1:44:A:ILE:HG21	1:84:A:LEU:HB2	2	0.11	0.0	0.11
(1,1562)	1:44:A:ILE:HG21	1:84:A:LEU:HB3	2	0.11	0.0	0.11
(1,1562)	1:44:A:ILE:HG22	1:84:A:LEU:HB2	2	0.11	0.0	0.11
(1,1562)	1:44:A:ILE:HG22	1:84:A:LEU:HB3	2	0.11	0.0	0.11
(1,1562)	1:44:A:ILE:HG23	1:84:A:LEU:HB2	2	0.11	0.0	0.11
(1,1562)	1:44:A:ILE:HG23	1:84:A:LEU:HB3	2	0.11	0.0	0.11

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	3	0.5
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	3	0.5
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	3	0.5
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	3	0.5
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	3	0.5
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	3	0.5
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	3	0.5

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	3	0.5
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	3	0.5
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	13	0.5
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	13	0.5
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	13	0.5
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	13	0.5
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	13	0.5
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	13	0.5
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	13	0.5
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	13	0.5
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	13	0.5
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	22	0.49
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	22	0.49
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	22	0.49
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	22	0.49
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	22	0.49
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	22	0.49
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	22	0.49
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	22	0.49
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	22	0.49
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	31	0.49
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	31	0.49
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	31	0.49
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	32	0.48
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	32	0.48
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	32	0.48
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	43	0.48
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	43	0.48
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	43	0.48
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	39	0.48
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	39	0.48
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	39	0.48
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD11	15	0.47
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD12	15	0.47
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD13	15	0.47
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD11	15	0.47
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD12	15	0.47
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD13	15	0.47
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD11	15	0.47
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD12	15	0.47
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD13	15	0.47
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	9	0.47

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	9	0.47
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	9	0.47
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	9	0.47
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	9	0.47
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	9	0.47
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	9	0.47
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	9	0.47
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	9	0.47
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	39	0.46
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	39	0.46
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	39	0.46
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	19	0.46
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	19	0.46
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	19	0.46
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	46	0.46
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	46	0.46
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	46	0.46
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	50	0.46
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	50	0.46
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	50	0.46
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	48	0.46
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	48	0.46
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	48	0.46
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	48	0.46
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	48	0.46
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	48	0.46
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	48	0.46
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	48	0.46
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	48	0.46
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	18	0.46
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	18	0.46
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	18	0.46
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	18	0.46
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	18	0.46
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	18	0.46
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	18	0.46
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	18	0.46
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	18	0.46
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD11	46	0.45
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD12	46	0.45
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD13	46	0.45
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD11	46	0.45

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD12	46	0.45
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD13	46	0.45
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD11	46	0.45
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD12	46	0.45
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD13	46	0.45
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	24	0.45
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	24	0.45
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	24	0.45
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	47	0.45
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	47	0.45
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	47	0.45
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	17	0.44
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	17	0.44
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	17	0.44
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	37	0.44
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	37	0.44
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	37	0.44
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	35	0.44
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	35	0.44
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	35	0.44
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	35	0.44
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	35	0.44
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	35	0.44
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	35	0.44
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	35	0.44
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	35	0.44
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	38	0.43
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	38	0.43
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	38	0.43
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	41	0.43
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	41	0.43
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	41	0.43
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	44	0.43
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	44	0.43
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	44	0.43
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	46	0.42
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	46	0.42
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	46	0.42
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	46	0.42
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	46	0.42
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	46	0.42
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD11	44	0.42

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD12	44	0.42
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD13	44	0.42
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD11	44	0.42
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD12	44	0.42
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD13	44	0.42
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD11	44	0.42
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD12	44	0.42
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD13	44	0.42
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	37	0.42
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	37	0.42
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	37	0.42
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	25	0.42
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	25	0.42
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	25	0.42
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	29	0.42
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	29	0.42
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	29	0.42
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	42	0.42
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	42	0.42
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	42	0.42
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	48	0.42
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	48	0.42
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	48	0.42
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	48	0.42
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	48	0.42
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	48	0.42
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	48	0.42
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	48	0.42
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	48	0.42
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	43	0.41
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	43	0.41
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	43	0.41
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	34	0.41
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	34	0.41
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	34	0.41
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	34	0.41
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	34	0.41
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	34	0.41
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	34	0.41
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	34	0.41
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	34	0.41
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	36	0.41

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	36	0.41
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	36	0.41
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	48	0.41
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	48	0.41
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	48	0.41
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	44	0.4
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	44	0.4
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	44	0.4
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	44	0.4
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	44	0.4
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	44	0.4
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	26	0.4
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	26	0.4
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	26	0.4
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	45	0.4
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	45	0.4
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	45	0.4
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	48	0.39
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	48	0.39
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	48	0.39
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	23	0.39
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	23	0.39
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	23	0.39
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	34	0.39
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	34	0.39
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	34	0.39
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	39	0.39
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	39	0.39
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	39	0.39
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	41	0.38
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	41	0.38
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	41	0.38
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	41	0.38
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	41	0.38
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	41	0.38
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	41	0.38
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	41	0.38
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	41	0.38
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	24	0.38
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	24	0.38
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	24	0.38
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	30	0.38

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	30	0.38
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	30	0.38
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	41	0.38
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	41	0.38
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	41	0.38
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	49	0.38
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	49	0.38
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	49	0.38
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	45	0.37
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	45	0.37
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	45	0.37
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	45	0.37
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	45	0.37
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	45	0.37
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE1	37	0.37
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE2	37	0.37
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE1	37	0.37
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE2	37	0.37
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE1	37	0.37
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE2	37	0.37
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	50	0.37
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	50	0.37
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	50	0.37
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	27	0.37
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	27	0.37
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	27	0.37
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	30	0.37
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	30	0.37
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	30	0.37
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	38	0.37
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	38	0.37
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	38	0.37
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	38	0.37
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	38	0.37
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	38	0.37
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	38	0.37
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	38	0.37
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	38	0.37
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	37	0.36
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	37	0.36
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	37	0.36
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	37	0.36

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	37	0.36
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	37	0.36
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	28	0.36
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	28	0.36
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	28	0.36
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	30	0.36
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	30	0.36
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	30	0.36
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	48	0.36
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	48	0.36
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	48	0.36
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	11	0.36
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	11	0.36
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	11	0.36
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	11	0.36
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	11	0.36
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	11	0.36
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	11	0.36
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	11	0.36
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	11	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	15	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	15	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	15	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	15	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	15	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	15	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	15	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	15	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	15	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	49	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	49	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	49	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	49	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	49	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	49	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	49	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	49	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	49	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	50	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	50	0.36
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	50	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	50	0.36

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	50	0.36
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	50	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	50	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	50	0.36
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	50	0.36
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	36	0.36
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	36	0.36
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	36	0.36
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	50	0.36
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	50	0.36
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	50	0.36
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	50	0.36
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	50	0.36
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	50	0.36
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	50	0.36
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	50	0.36
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	50	0.36
(1,1527)	1:39:A:LEU:HD11	1:44:A:ILE:H	43	0.35
(1,1527)	1:39:A:LEU:HD12	1:44:A:ILE:H	43	0.35
(1,1527)	1:39:A:LEU:HD13	1:44:A:ILE:H	43	0.35
(1,1527)	1:39:A:LEU:HD21	1:44:A:ILE:H	43	0.35
(1,1527)	1:39:A:LEU:HD22	1:44:A:ILE:H	43	0.35
(1,1527)	1:39:A:LEU:HD23	1:44:A:ILE:H	43	0.35
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	46	0.35
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	46	0.35
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	46	0.35
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	46	0.35
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	46	0.35
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	46	0.35
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	40	0.35
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	40	0.35
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	40	0.35
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	27	0.35
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	27	0.35
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	27	0.35
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	27	0.35
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	27	0.35
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	27	0.35
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	27	0.35
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	27	0.35
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	27	0.35
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	23	0.35

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	23	0.35
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	23	0.35
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	21	0.35
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	21	0.35
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	21	0.35
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	25	0.35
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	25	0.35
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	25	0.35
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	44	0.35
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	44	0.35
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	44	0.35
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	44	0.35
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	44	0.35
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	44	0.35
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	44	0.35
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	44	0.35
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	44	0.35
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	46	0.35
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	46	0.35
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	46	0.35
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	46	0.35
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	46	0.35
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	46	0.35
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	46	0.35
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	46	0.35
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	46	0.35
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	26	0.34
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	26	0.34
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	26	0.34
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	26	0.34
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	26	0.34
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	26	0.34
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD11	49	0.34
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD12	49	0.34
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD13	49	0.34
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	21	0.34
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	21	0.34
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	21	0.34
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	42	0.34
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	42	0.34
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	42	0.34
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	42	0.34

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	42	0.34
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	42	0.34
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	42	0.34
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	42	0.34
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	42	0.34
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	35	0.34
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	35	0.34
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	35	0.34
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	19	0.34
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	19	0.34
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	19	0.34
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	31	0.34
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	31	0.34
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	31	0.34
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	31	0.34
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	31	0.34
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	31	0.34
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	31	0.34
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	31	0.34
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	31	0.34
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	31	0.34
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	31	0.34
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	31	0.34
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	31	0.34
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	31	0.34
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	31	0.34
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	23	0.33
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	23	0.33
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	23	0.33
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	23	0.33
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	23	0.33
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	23	0.33
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	23	0.33
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	23	0.33
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	23	0.33
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	23	0.33
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	23	0.33
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	23	0.33
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	23	0.33
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	23	0.33
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	23	0.33
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	23	0.33

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	23	0.33
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	23	0.33
(1,1434)	1:29:A:MET:HG2	1:70:A:LEU:HD11	47	0.33
(1,1434)	1:29:A:MET:HG2	1:70:A:LEU:HD12	47	0.33
(1,1434)	1:29:A:MET:HG2	1:70:A:LEU:HD13	47	0.33
(1,1434)	1:29:A:MET:HG2	1:70:A:LEU:HD21	47	0.33
(1,1434)	1:29:A:MET:HG2	1:70:A:LEU:HD22	47	0.33
(1,1434)	1:29:A:MET:HG2	1:70:A:LEU:HD23	47	0.33
(1,1434)	1:29:A:MET:HG3	1:70:A:LEU:HD11	47	0.33
(1,1434)	1:29:A:MET:HG3	1:70:A:LEU:HD12	47	0.33
(1,1434)	1:29:A:MET:HG3	1:70:A:LEU:HD13	47	0.33
(1,1434)	1:29:A:MET:HG3	1:70:A:LEU:HD21	47	0.33
(1,1434)	1:29:A:MET:HG3	1:70:A:LEU:HD22	47	0.33
(1,1434)	1:29:A:MET:HG3	1:70:A:LEU:HD23	47	0.33
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	43	0.33
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	43	0.33
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	43	0.33
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	27	0.33
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	27	0.33
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	27	0.33
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	29	0.33
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	29	0.33
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	29	0.33
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	43	0.33
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	43	0.33
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	43	0.33
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	43	0.33
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	43	0.33
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	43	0.33
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	43	0.33
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	43	0.33
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	43	0.33
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	48	0.33
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	48	0.33
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	48	0.33
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	48	0.33
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	48	0.33
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	48	0.33
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	48	0.33
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	48	0.33
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	48	0.33
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	37	0.33

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	37	0.33
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	37	0.33
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	32	0.33
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	32	0.33
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	32	0.33
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	38	0.33
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	38	0.33
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	38	0.33
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	38	0.33
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	38	0.33
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	38	0.33
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	38	0.33
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	38	0.33
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	38	0.33
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	32	0.32
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	32	0.32
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	32	0.32
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	32	0.32
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	32	0.32
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	32	0.32
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	47	0.32
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	18	0.32
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	18	0.32
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	18	0.32
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	5	0.32
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	5	0.32
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	5	0.32
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	5	0.32
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	5	0.32
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	5	0.32
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	5	0.32
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	5	0.32
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	5	0.32
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	37	0.32
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	37	0.32
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	37	0.32
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	37	0.32
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	37	0.32
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	37	0.32
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	37	0.32
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	37	0.32
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	37	0.32

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	40	0.32
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	40	0.32
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	40	0.32
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	4	0.32
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	4	0.32
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	4	0.32
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	4	0.32
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	4	0.32
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	4	0.32
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	4	0.32
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	4	0.32
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	4	0.32
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	35	0.32
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	35	0.32
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	35	0.32
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	35	0.32
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	35	0.32
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	35	0.32
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	35	0.32
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	35	0.32
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	35	0.32
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	14	0.31
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	14	0.31
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	14	0.31
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	14	0.31
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	14	0.31
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	14	0.31
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	26	0.31
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	26	0.31
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	26	0.31
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	46	0.31
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	46	0.31
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	46	0.31
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	46	0.31
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	46	0.31
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	46	0.31
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	46	0.31
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	46	0.31
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	46	0.31
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	49	0.31
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	49	0.31
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	49	0.31

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	49	0.31
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	49	0.31
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	49	0.31
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	49	0.31
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	49	0.31
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	49	0.31
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	27	0.31
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	27	0.31
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	27	0.31
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	45	0.31
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	45	0.31
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	45	0.31
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	20	0.31
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	20	0.31
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	20	0.31
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	20	0.31
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	20	0.31
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	20	0.31
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	20	0.31
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	20	0.31
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	20	0.31
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	3	0.3
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	3	0.3
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	3	0.3
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	3	0.3
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	3	0.3
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	3	0.3
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD11	47	0.3
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD12	47	0.3
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD13	47	0.3
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD21	47	0.3
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD22	47	0.3
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD23	47	0.3
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD11	47	0.3
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD12	47	0.3
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD13	47	0.3
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD21	47	0.3
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD22	47	0.3
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD23	47	0.3
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	37	0.3
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	37	0.3
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	37	0.3

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	37	0.3
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	37	0.3
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	37	0.3
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE1	44	0.3
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE2	44	0.3
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE1	44	0.3
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE2	44	0.3
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE1	44	0.3
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE2	44	0.3
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD11	43	0.3
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD12	43	0.3
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD13	43	0.3
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	31	0.3
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	31	0.3
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	31	0.3
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	35	0.3
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	35	0.3
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	35	0.3
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	28	0.3
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	28	0.3
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	28	0.3
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	40	0.3
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	40	0.3
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	40	0.3
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	4	0.3
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	4	0.3
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	4	0.3
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	23	0.3
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	23	0.3
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	23	0.3
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	30	0.3
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	30	0.3
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	30	0.3
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	18	0.3
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	18	0.3
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	18	0.3
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	18	0.3
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	18	0.3
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	18	0.3
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	18	0.3
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	18	0.3
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	18	0.3

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:7:A:ALA:HB1	1:42:A:TYR:HE1	40	0.3
(1,370)	1:7:A:ALA:HB1	1:42:A:TYR:HE2	40	0.3
(1,370)	1:7:A:ALA:HB2	1:42:A:TYR:HE1	40	0.3
(1,370)	1:7:A:ALA:HB2	1:42:A:TYR:HE2	40	0.3
(1,370)	1:7:A:ALA:HB3	1:42:A:TYR:HE1	40	0.3
(1,370)	1:7:A:ALA:HB3	1:42:A:TYR:HE2	40	0.3
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	40	0.29
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	40	0.29
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	40	0.29
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	40	0.29
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	40	0.29
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	40	0.29
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	40	0.29
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	40	0.29
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	40	0.29
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	40	0.29
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	40	0.29
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	40	0.29
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	40	0.29
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	40	0.29
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	40	0.29
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	40	0.29
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	40	0.29
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	40	0.29
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	15	0.29
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	15	0.29
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	15	0.29
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	15	0.29
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	15	0.29
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	15	0.29
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	34	0.29
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	34	0.29
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	34	0.29
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	34	0.29
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	34	0.29
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	34	0.29
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	45	0.29
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	45	0.29
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	45	0.29
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	45	0.29
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	45	0.29
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	45	0.29

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD11	22	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD12	22	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD13	22	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD21	22	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD22	22	0.29
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD23	22	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD11	22	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD12	22	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD13	22	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD21	22	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD22	22	0.29
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD23	22	0.29
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG11	40	0.29
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG12	40	0.29
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG13	40	0.29
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG21	40	0.29
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG22	40	0.29
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG23	40	0.29
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG11	40	0.29
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG12	40	0.29
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG13	40	0.29
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG21	40	0.29
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG22	40	0.29
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG23	40	0.29
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	21	0.29
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	21	0.29
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	21	0.29
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	21	0.29
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	21	0.29
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	21	0.29
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	49	0.29
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	49	0.29
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	49	0.29
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	49	0.29
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	49	0.29
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	49	0.29
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	41	0.29
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	41	0.29
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	41	0.29
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	41	0.29
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	41	0.29
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	41	0.29

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE1	43	0.29
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE2	43	0.29
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE1	43	0.29
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE2	43	0.29
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE1	43	0.29
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE2	43	0.29
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	15	0.29
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	15	0.29
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	15	0.29
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	44	0.29
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	44	0.29
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	44	0.29
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	38	0.29
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	38	0.29
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	38	0.29
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	38	0.29
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	38	0.29
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	38	0.29
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	38	0.29
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	38	0.29
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	38	0.29
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	14	0.29
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	14	0.29
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	14	0.29
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	14	0.29
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	14	0.29
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	14	0.29
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	14	0.29
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	14	0.29
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	14	0.29
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	33	0.29
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	33	0.29
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	33	0.29
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	47	0.29
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	47	0.29
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	47	0.29
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	29	0.29
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	29	0.29
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	29	0.29
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	44	0.29
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	44	0.29
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	44	0.29

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	44	0.29
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	44	0.29
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	44	0.29
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	44	0.29
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	44	0.29
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	44	0.29
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	14	0.29
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	14	0.29
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	14	0.29
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	14	0.29
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	14	0.29
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	14	0.29
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	14	0.29
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	14	0.29
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	14	0.29
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	32	0.29
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	32	0.29
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	32	0.29
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	32	0.29
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	32	0.29
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	32	0.29
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	32	0.29
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	32	0.29
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	32	0.29
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	41	0.29
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	41	0.29
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	41	0.29
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	41	0.29
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	41	0.29
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	41	0.29
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	41	0.29
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	41	0.29
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	41	0.29
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	33	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	33	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	33	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	33	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	33	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	33	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	33	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	33	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	33	0.28

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	33	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	33	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	33	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	33	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	33	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	33	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	33	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	33	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	33	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	41	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	41	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	41	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	41	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	41	0.28
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	41	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	41	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	41	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	41	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	41	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	41	0.28
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	41	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	41	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	41	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	41	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	41	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	41	0.28
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	41	0.28
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	50	0.28
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	19	0.28
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	19	0.28
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	19	0.28
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	45	0.28
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	45	0.28
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	45	0.28
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	16	0.28
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	16	0.28
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	16	0.28
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	16	0.28
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	16	0.28
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	16	0.28
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	24	0.28
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	24	0.28

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	24	0.28
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	42	0.28
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	42	0.28
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	42	0.28
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD11	10	0.28
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD12	10	0.28
(1,510)	1:49:A:LEU:HD21	1:84:A:LEU:HD13	10	0.28
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD11	10	0.28
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD12	10	0.28
(1,510)	1:49:A:LEU:HD22	1:84:A:LEU:HD13	10	0.28
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD11	10	0.28
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD12	10	0.28
(1,510)	1:49:A:LEU:HD23	1:84:A:LEU:HD13	10	0.28
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	26	0.28
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	26	0.28
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	26	0.28
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	26	0.28
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	26	0.28
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	26	0.28
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	26	0.28
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	26	0.28
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	26	0.28
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	26	0.28
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	26	0.28
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	26	0.28
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	34	0.28
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	34	0.28
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	34	0.28
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	48	0.28
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	48	0.28
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	48	0.28
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	17	0.28
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	17	0.28
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	17	0.28
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	36	0.28
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	36	0.28
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	36	0.28
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	25	0.28
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	25	0.28
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	25	0.28
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	25	0.28
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	25	0.28

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	25	0.28
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	25	0.28
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	25	0.28
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	25	0.28
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	29	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	29	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	29	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	29	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	29	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	29	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	32	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	32	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	32	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	32	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	32	0.27
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	32	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	17	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	17	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	17	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	17	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	17	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	17	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	17	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	17	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	17	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	17	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	17	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	17	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	17	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	17	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	17	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	17	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	17	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	17	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	46	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	46	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	46	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	46	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	46	0.27
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	46	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	46	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	46	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	46	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	46	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	46	0.27
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	46	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	46	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	46	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	46	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	46	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	46	0.27
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	46	0.27
(1,1527)	1:39:A:LEU:HD11	1:44:A:ILE:H	49	0.27
(1,1527)	1:39:A:LEU:HD12	1:44:A:ILE:H	49	0.27
(1,1527)	1:39:A:LEU:HD13	1:44:A:ILE:H	49	0.27
(1,1527)	1:39:A:LEU:HD21	1:44:A:ILE:H	49	0.27
(1,1527)	1:39:A:LEU:HD22	1:44:A:ILE:H	49	0.27
(1,1527)	1:39:A:LEU:HD23	1:44:A:ILE:H	49	0.27
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	42	0.27
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	42	0.27
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	42	0.27
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	42	0.27
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	42	0.27
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	42	0.27
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	45	0.27
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	45	0.27
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	45	0.27
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	45	0.27
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	45	0.27
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	45	0.27
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	46	0.27
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	46	0.27
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	46	0.27
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	46	0.27
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	46	0.27
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	46	0.27
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	48	0.27
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	48	0.27
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	48	0.27
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	48	0.27
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	48	0.27
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	48	0.27
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	48	0.27
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	48	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	48	0.27
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	48	0.27
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	48	0.27
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	48	0.27
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	49	0.27
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	49	0.27
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	49	0.27
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	48	0.27
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	29	0.27
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	29	0.27
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	29	0.27
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	36	0.27
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	36	0.27
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	36	0.27
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	36	0.27
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	36	0.27
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	36	0.27
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	19	0.27
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	19	0.27
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	19	0.27
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	2	0.27
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	2	0.27
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	2	0.27
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	2	0.27
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	2	0.27
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	2	0.27
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	2	0.27
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	2	0.27
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	2	0.27
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	45	0.27
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	45	0.27
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	45	0.27
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	45	0.27
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	45	0.27
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	45	0.27
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	45	0.27
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	45	0.27
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	45	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	19	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	19	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	19	0.27
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	19	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	19	0.27
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	19	0.27
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	19	0.27
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	19	0.27
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	19	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	29	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	29	0.27
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	29	0.27
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	29	0.27
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	29	0.27
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	29	0.27
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	29	0.27
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	29	0.27
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	29	0.27
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	15	0.27
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	15	0.27
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	15	0.27
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	15	0.27
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	15	0.27
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	15	0.27
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	37	0.27
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	37	0.27
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	37	0.27
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	41	0.27
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	41	0.27
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	41	0.27
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	38	0.27
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	38	0.27
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	38	0.27
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	49	0.27
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	49	0.27
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	49	0.27
(1,40)	1:12:A:ILE:HD11	1:39:A:LEU:HG	45	0.27
(1,40)	1:12:A:ILE:HD12	1:39:A:LEU:HG	45	0.27
(1,40)	1:12:A:ILE:HD13	1:39:A:LEU:HG	45	0.27
(1,1619)	1:51:A:GLU:HG2	1:52:A:THR:HG21	14	0.26
(1,1619)	1:51:A:GLU:HG2	1:52:A:THR:HG22	14	0.26
(1,1619)	1:51:A:GLU:HG2	1:52:A:THR:HG23	14	0.26
(1,1619)	1:51:A:GLU:HG3	1:52:A:THR:HG21	14	0.26
(1,1619)	1:51:A:GLU:HG3	1:52:A:THR:HG22	14	0.26
(1,1619)	1:51:A:GLU:HG3	1:52:A:THR:HG23	14	0.26
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	8	0.26

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	8	0.26
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	8	0.26
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	8	0.26
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	8	0.26
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	8	0.26
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD11	8	0.26
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD12	8	0.26
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD13	8	0.26
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD21	8	0.26
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD22	8	0.26
(1,1433)	1:29:A:MET:HG2	1:33:A:LEU:HD23	8	0.26
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD11	8	0.26
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD12	8	0.26
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD13	8	0.26
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD21	8	0.26
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD22	8	0.26
(1,1433)	1:29:A:MET:HG3	1:33:A:LEU:HD23	8	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG11	34	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG12	34	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG13	34	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG21	34	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG22	34	0.26
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG23	34	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG11	34	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG12	34	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG13	34	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG21	34	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG22	34	0.26
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG23	34	0.26
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	27	0.26
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	27	0.26
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	27	0.26
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	27	0.26
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	27	0.26
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	27	0.26
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	28	0.26
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	28	0.26
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	28	0.26
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	28	0.26
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	28	0.26
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	28	0.26
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	49	0.26

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	49	0.26
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	49	0.26
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	49	0.26
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	49	0.26
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	49	0.26
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	40	0.26
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	40	0.26
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	40	0.26
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	38	0.26
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	38	0.26
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	38	0.26
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	4	0.26
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	4	0.26
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	4	0.26
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	38	0.26
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	38	0.26
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	38	0.26
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	18	0.26
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	18	0.26
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	18	0.26
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	18	0.26
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	18	0.26
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	18	0.26
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	18	0.26
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	18	0.26
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	18	0.26
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	18	0.26
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	18	0.26
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	18	0.26
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	21	0.26
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	21	0.26
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	21	0.26
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	48	0.26
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	48	0.26
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	48	0.26
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	25	0.26
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	25	0.26
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	25	0.26
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	40	0.26
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	40	0.26
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	40	0.26
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	16	0.26

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	16	0.26
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	16	0.26
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	33	0.26
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	33	0.26
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	33	0.26
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	4	0.26
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	4	0.26
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	4	0.26
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	4	0.26
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	4	0.26
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	4	0.26
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	4	0.26
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	4	0.26
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	4	0.26
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	25	0.26
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	25	0.26
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	25	0.26
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	34	0.26
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	34	0.26
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	34	0.26
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	47	0.26
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	47	0.26
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	47	0.26
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	47	0.26
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	47	0.26
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	47	0.26
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	47	0.26
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	47	0.26
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	47	0.26
(1,1605)	1:49:A:LEU:HD11	1:84:A:LEU:HB2	21	0.25
(1,1605)	1:49:A:LEU:HD11	1:84:A:LEU:HB3	21	0.25
(1,1605)	1:49:A:LEU:HD12	1:84:A:LEU:HB2	21	0.25
(1,1605)	1:49:A:LEU:HD12	1:84:A:LEU:HB3	21	0.25
(1,1605)	1:49:A:LEU:HD13	1:84:A:LEU:HB2	21	0.25
(1,1605)	1:49:A:LEU:HD13	1:84:A:LEU:HB3	21	0.25
(1,1605)	1:49:A:LEU:HD21	1:84:A:LEU:HB2	21	0.25
(1,1605)	1:49:A:LEU:HD21	1:84:A:LEU:HB3	21	0.25
(1,1605)	1:49:A:LEU:HD22	1:84:A:LEU:HB2	21	0.25
(1,1605)	1:49:A:LEU:HD22	1:84:A:LEU:HB3	21	0.25
(1,1605)	1:49:A:LEU:HD23	1:84:A:LEU:HB2	21	0.25
(1,1605)	1:49:A:LEU:HD23	1:84:A:LEU:HB3	21	0.25
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	41	0.25

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	41	0.25
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	19	0.25
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	19	0.25
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	19	0.25
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	19	0.25
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	19	0.25
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	19	0.25
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	19	0.25
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	19	0.25
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	19	0.25
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	19	0.25
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	19	0.25
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	19	0.25
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	19	0.25
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	19	0.25
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	19	0.25
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	19	0.25
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	19	0.25
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	19	0.25
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	26	0.25
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	26	0.25
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	26	0.25
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	26	0.25
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	26	0.25
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	26	0.25
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	43	0.25
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	43	0.25
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	43	0.25
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	43	0.25
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	43	0.25
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	43	0.25
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	39	0.25
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	39	0.25
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	39	0.25
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	15	0.25
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	15	0.25
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	15	0.25
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	21	0.25
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	21	0.25
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	21	0.25
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG21	20	0.25
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG22	20	0.25

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG23	20	0.25
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG21	20	0.25
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG22	20	0.25
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG23	20	0.25
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	13	0.25
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	13	0.25
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	13	0.25
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	17	0.25
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	17	0.25
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	17	0.25
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	47	0.25
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	47	0.25
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	47	0.25
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD2	1	0.25
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD3	1	0.25
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	14	0.25
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	14	0.25
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	14	0.25
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	14	0.25
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	14	0.25
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	14	0.25
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	14	0.25
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	14	0.25
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	14	0.25
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	40	0.25
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	40	0.25
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	40	0.25
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	40	0.25
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	40	0.25
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	40	0.25
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	40	0.25
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	40	0.25
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	40	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	12	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	12	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	12	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	12	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	12	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	12	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	12	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	12	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	12	0.25

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	25	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	25	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	25	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	25	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	25	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	25	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	25	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	25	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	25	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	32	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	32	0.25
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	32	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	32	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	32	0.25
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	32	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	32	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	32	0.25
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	32	0.25
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	18	0.25
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	18	0.25
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	18	0.25
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	18	0.25
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	18	0.25
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	18	0.25
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	18	0.25
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	18	0.25
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	18	0.25
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	2	0.25
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	2	0.25
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	2	0.25
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	18	0.25
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	18	0.25
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	18	0.25
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	21	0.25
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	21	0.25
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	21	0.25
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	40	0.25
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	40	0.25
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	40	0.25
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	41	0.25
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	41	0.25
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	41	0.25

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	19	0.25
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	19	0.25
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	19	0.25
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	19	0.25
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	19	0.25
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	19	0.25
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	19	0.25
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	19	0.25
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	19	0.25
(1,192)	1:26:A:ILE:HD11	1:32:A:VAL:H	28	0.25
(1,192)	1:26:A:ILE:HD12	1:32:A:VAL:H	28	0.25
(1,192)	1:26:A:ILE:HD13	1:32:A:VAL:H	28	0.25
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	29	0.24
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	29	0.24
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	29	0.24
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	29	0.24
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	29	0.24
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	29	0.24
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	13	0.24
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	13	0.24
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	13	0.24
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	13	0.24
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	13	0.24
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	13	0.24
(1,1484)	1:35:A:VAL:HG11	1:36:A:ILE:HD11	40	0.24
(1,1484)	1:35:A:VAL:HG11	1:36:A:ILE:HD12	40	0.24
(1,1484)	1:35:A:VAL:HG11	1:36:A:ILE:HD13	40	0.24
(1,1484)	1:35:A:VAL:HG12	1:36:A:ILE:HD11	40	0.24
(1,1484)	1:35:A:VAL:HG12	1:36:A:ILE:HD12	40	0.24
(1,1484)	1:35:A:VAL:HG12	1:36:A:ILE:HD13	40	0.24
(1,1484)	1:35:A:VAL:HG13	1:36:A:ILE:HD11	40	0.24
(1,1484)	1:35:A:VAL:HG13	1:36:A:ILE:HD12	40	0.24
(1,1484)	1:35:A:VAL:HG13	1:36:A:ILE:HD13	40	0.24
(1,1484)	1:35:A:VAL:HG21	1:36:A:ILE:HD11	40	0.24
(1,1484)	1:35:A:VAL:HG21	1:36:A:ILE:HD12	40	0.24
(1,1484)	1:35:A:VAL:HG21	1:36:A:ILE:HD13	40	0.24
(1,1484)	1:35:A:VAL:HG22	1:36:A:ILE:HD11	40	0.24
(1,1484)	1:35:A:VAL:HG22	1:36:A:ILE:HD12	40	0.24
(1,1484)	1:35:A:VAL:HG22	1:36:A:ILE:HD13	40	0.24
(1,1484)	1:35:A:VAL:HG23	1:36:A:ILE:HD11	40	0.24
(1,1484)	1:35:A:VAL:HG23	1:36:A:ILE:HD12	40	0.24
(1,1484)	1:35:A:VAL:HG23	1:36:A:ILE:HD13	40	0.24

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	32	0.24
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	32	0.24
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	32	0.24
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	32	0.24
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	32	0.24
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	32	0.24
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	43	0.24
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	43	0.24
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	43	0.24
(1,652)	1:49:A:LEU:HD21	1:84:A:LEU:HD21	28	0.24
(1,652)	1:49:A:LEU:HD21	1:84:A:LEU:HD22	28	0.24
(1,652)	1:49:A:LEU:HD21	1:84:A:LEU:HD23	28	0.24
(1,652)	1:49:A:LEU:HD22	1:84:A:LEU:HD21	28	0.24
(1,652)	1:49:A:LEU:HD22	1:84:A:LEU:HD22	28	0.24
(1,652)	1:49:A:LEU:HD22	1:84:A:LEU:HD23	28	0.24
(1,652)	1:49:A:LEU:HD23	1:84:A:LEU:HD21	28	0.24
(1,652)	1:49:A:LEU:HD23	1:84:A:LEU:HD22	28	0.24
(1,652)	1:49:A:LEU:HD23	1:84:A:LEU:HD23	28	0.24
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	22	0.24
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	22	0.24
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	22	0.24
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	25	0.24
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	25	0.24
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	25	0.24
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	45	0.24
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	45	0.24
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	45	0.24
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	49	0.24
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	49	0.24
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	49	0.24
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	23	0.24
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	23	0.24
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	23	0.24
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	23	0.24
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	23	0.24
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	23	0.24
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	23	0.24
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	23	0.24
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	23	0.24
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	8	0.24
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	8	0.24
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	8	0.24

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	8	0.24
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	8	0.24
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	8	0.24
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	8	0.24
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	8	0.24
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	8	0.24
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	24	0.24
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	24	0.24
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	24	0.24
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	24	0.24
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	24	0.24
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	24	0.24
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	24	0.24
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	24	0.24
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	24	0.24
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	22	0.24
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	22	0.24
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	22	0.24
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	22	0.24
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	22	0.24
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	22	0.24
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	22	0.24
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	22	0.24
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	22	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	23	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	23	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	23	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	33	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	33	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	33	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	39	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	39	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	39	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	42	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	42	0.24
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	42	0.24
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	27	0.24
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	27	0.24
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	27	0.24
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	16	0.24
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	16	0.24
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	16	0.24

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	16	0.24
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	16	0.24
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	16	0.24
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	16	0.24
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	16	0.24
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	16	0.24
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	19	0.24
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	19	0.24
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	19	0.24
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	19	0.24
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	19	0.24
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	19	0.24
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	19	0.24
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	19	0.24
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	19	0.24
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	50	0.24
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	50	0.24
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	50	0.24
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	50	0.24
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	50	0.24
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	50	0.24
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	50	0.24
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	50	0.24
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	50	0.24
(1,1779)	1:75:A:LYS:HG2	1:79:A:ARG:HB2	18	0.23
(1,1779)	1:75:A:LYS:HG2	1:79:A:ARG:HB3	18	0.23
(1,1779)	1:75:A:LYS:HG3	1:79:A:ARG:HB2	18	0.23
(1,1779)	1:75:A:LYS:HG3	1:79:A:ARG:HB3	18	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	29	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	29	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	29	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	29	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	29	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	29	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	29	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	29	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	29	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	29	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	29	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	29	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	29	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	29	0.23

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	29	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	29	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	29	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	29	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	42	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	42	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	42	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	42	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	42	0.23
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	42	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	42	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	42	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	42	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	42	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	42	0.23
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	42	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	42	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	42	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	42	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	42	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	42	0.23
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	42	0.23
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	39	0.23
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	39	0.23
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	39	0.23
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	39	0.23
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	39	0.23
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	39	0.23
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	41	0.23
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	42	0.23
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	45	0.23
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	43	0.23
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	43	0.23
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	43	0.23
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	16	0.23
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	16	0.23
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	16	0.23
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	49	0.23
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	49	0.23
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	49	0.23
(1,474)	1:49:A:LEU:HD21	1:81:A:TRP:HD1	28	0.23
(1,474)	1:49:A:LEU:HD22	1:81:A:TRP:HD1	28	0.23

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:49:A:LEU:HD23	1:81:A:TRP:HD1	28	0.23
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	34	0.23
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	34	0.23
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	34	0.23
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	34	0.23
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	34	0.23
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	34	0.23
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	34	0.23
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	34	0.23
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	34	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	16	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	16	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	16	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	16	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	16	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	16	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	16	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	16	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	16	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	31	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	31	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	31	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	31	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	31	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	31	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	31	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	31	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	31	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	39	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	39	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	39	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	39	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	39	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	39	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	39	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	39	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	39	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	44	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	44	0.23
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	44	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	44	0.23
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	44	0.23

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	44	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	44	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	44	0.23
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	44	0.23
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	29	0.23
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	29	0.23
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	29	0.23
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	29	0.23
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	29	0.23
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	29	0.23
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	29	0.23
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	29	0.23
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	29	0.23
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	32	0.23
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	32	0.23
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	32	0.23
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	32	0.23
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	32	0.23
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	32	0.23
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	32	0.23
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	32	0.23
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	32	0.23
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	4	0.23
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	4	0.23
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	4	0.23
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	14	0.23
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	14	0.23
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	14	0.23
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	38	0.23
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	38	0.23
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	38	0.23
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	43	0.23
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	43	0.23
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	43	0.23
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	14	0.23
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	14	0.23
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	14	0.23
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	19	0.23
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	19	0.23
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	19	0.23
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	44	0.23
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	44	0.23

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	44	0.23
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	18	0.23
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	18	0.23
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	18	0.23
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	18	0.23
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	18	0.23
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	18	0.23
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	18	0.23
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	18	0.23
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	18	0.23
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	4	0.23
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	4	0.23
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	4	0.23
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	33	0.23
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	33	0.23
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	33	0.23
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	42	0.23
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	42	0.23
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	42	0.23
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	20	0.23
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	20	0.23
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	20	0.23
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	20	0.23
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	20	0.23
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	20	0.23
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	20	0.23
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	20	0.23
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	20	0.23
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	43	0.22
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	43	0.22
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	43	0.22
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	43	0.22
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	43	0.22
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	43	0.22
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	42	0.22
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	42	0.22
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	48	0.22
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	48	0.22
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	48	0.22
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	48	0.22
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	48	0.22
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	48	0.22

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:35:A:VAL:HG11	1:39:A:LEU:HG	20	0.22
(1,1488)	1:35:A:VAL:HG12	1:39:A:LEU:HG	20	0.22
(1,1488)	1:35:A:VAL:HG13	1:39:A:LEU:HG	20	0.22
(1,1488)	1:35:A:VAL:HG21	1:39:A:LEU:HG	20	0.22
(1,1488)	1:35:A:VAL:HG22	1:39:A:LEU:HG	20	0.22
(1,1488)	1:35:A:VAL:HG23	1:39:A:LEU:HG	20	0.22
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	48	0.22
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	48	0.22
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	48	0.22
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	48	0.22
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	48	0.22
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	48	0.22
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	48	0.22
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	48	0.22
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	48	0.22
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	48	0.22
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	48	0.22
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	48	0.22
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	48	0.22
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	48	0.22
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	48	0.22
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	48	0.22
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	48	0.22
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	48	0.22
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	42	0.22
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	42	0.22
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	42	0.22
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	42	0.22
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	42	0.22
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	42	0.22
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	38	0.22
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	38	0.22
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	38	0.22
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	38	0.22
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	38	0.22
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	38	0.22
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	45	0.22
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	45	0.22
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	45	0.22
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	26	0.22
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	25	0.22
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	25	0.22

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	25	0.22
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	39	0.22
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	39	0.22
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	39	0.22
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	44	0.22
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	44	0.22
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	44	0.22
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD11	11	0.22
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD12	11	0.22
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD13	11	0.22
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD11	11	0.22
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD12	11	0.22
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD13	11	0.22
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD11	11	0.22
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD12	11	0.22
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD13	11	0.22
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	21	0.22
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	21	0.22
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	21	0.22
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	8	0.22
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	8	0.22
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	8	0.22
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	39	0.22
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	39	0.22
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	39	0.22
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	39	0.22
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	39	0.22
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	39	0.22
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	39	0.22
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	39	0.22
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	39	0.22
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	25	0.22
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	25	0.22
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	25	0.22
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	25	0.22
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	25	0.22
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	25	0.22
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	25	0.22
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	25	0.22
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	25	0.22
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	18	0.22
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	18	0.22

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	18	0.22
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	42	0.22
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	42	0.22
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	42	0.22
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	31	0.22
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	31	0.22
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	31	0.22
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	31	0.22
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	31	0.22
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	31	0.22
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	31	0.22
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	31	0.22
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	31	0.22
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	2	0.22
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	2	0.22
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	2	0.22
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	2	0.22
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	2	0.22
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	2	0.22
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	2	0.22
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	2	0.22
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	2	0.22
(1,1608)	1:49:A:LEU:HD11	1:85:A:ILE:HG21	25	0.21
(1,1608)	1:49:A:LEU:HD11	1:85:A:ILE:HG22	25	0.21
(1,1608)	1:49:A:LEU:HD11	1:85:A:ILE:HG23	25	0.21
(1,1608)	1:49:A:LEU:HD12	1:85:A:ILE:HG21	25	0.21
(1,1608)	1:49:A:LEU:HD12	1:85:A:ILE:HG22	25	0.21
(1,1608)	1:49:A:LEU:HD12	1:85:A:ILE:HG23	25	0.21
(1,1608)	1:49:A:LEU:HD13	1:85:A:ILE:HG21	25	0.21
(1,1608)	1:49:A:LEU:HD13	1:85:A:ILE:HG22	25	0.21
(1,1608)	1:49:A:LEU:HD13	1:85:A:ILE:HG23	25	0.21
(1,1608)	1:49:A:LEU:HD21	1:85:A:ILE:HG21	25	0.21
(1,1608)	1:49:A:LEU:HD21	1:85:A:ILE:HG22	25	0.21
(1,1608)	1:49:A:LEU:HD21	1:85:A:ILE:HG23	25	0.21
(1,1608)	1:49:A:LEU:HD22	1:85:A:ILE:HG21	25	0.21
(1,1608)	1:49:A:LEU:HD22	1:85:A:ILE:HG22	25	0.21
(1,1608)	1:49:A:LEU:HD22	1:85:A:ILE:HG23	25	0.21
(1,1608)	1:49:A:LEU:HD23	1:85:A:ILE:HG21	25	0.21
(1,1608)	1:49:A:LEU:HD23	1:85:A:ILE:HG22	25	0.21
(1,1608)	1:49:A:LEU:HD23	1:85:A:ILE:HG23	25	0.21
(1,1505)	1:36:A:ILE:HD11	1:70:A:LEU:HD11	45	0.21
(1,1505)	1:36:A:ILE:HD11	1:70:A:LEU:HD12	45	0.21

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1505)	1:36:A:ILE:HD11	1:70:A:LEU:HD13	45	0.21
(1,1505)	1:36:A:ILE:HD11	1:70:A:LEU:HD21	45	0.21
(1,1505)	1:36:A:ILE:HD11	1:70:A:LEU:HD22	45	0.21
(1,1505)	1:36:A:ILE:HD11	1:70:A:LEU:HD23	45	0.21
(1,1505)	1:36:A:ILE:HD12	1:70:A:LEU:HD11	45	0.21
(1,1505)	1:36:A:ILE:HD12	1:70:A:LEU:HD12	45	0.21
(1,1505)	1:36:A:ILE:HD12	1:70:A:LEU:HD13	45	0.21
(1,1505)	1:36:A:ILE:HD12	1:70:A:LEU:HD21	45	0.21
(1,1505)	1:36:A:ILE:HD12	1:70:A:LEU:HD22	45	0.21
(1,1505)	1:36:A:ILE:HD12	1:70:A:LEU:HD23	45	0.21
(1,1505)	1:36:A:ILE:HD13	1:70:A:LEU:HD11	45	0.21
(1,1505)	1:36:A:ILE:HD13	1:70:A:LEU:HD12	45	0.21
(1,1505)	1:36:A:ILE:HD13	1:70:A:LEU:HD13	45	0.21
(1,1505)	1:36:A:ILE:HD13	1:70:A:LEU:HD21	45	0.21
(1,1505)	1:36:A:ILE:HD13	1:70:A:LEU:HD22	45	0.21
(1,1505)	1:36:A:ILE:HD13	1:70:A:LEU:HD23	45	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	2	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	2	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	2	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	2	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	2	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	2	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	2	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	2	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	2	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	2	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	2	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	2	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	24	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	24	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	24	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	24	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	24	0.21
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	24	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	24	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	24	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	24	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	24	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	24	0.21
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	24	0.21
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	33	0.21
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	33	0.21

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	33	0.21
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	34	0.21
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	34	0.21
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	34	0.21
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	27	0.21
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	27	0.21
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	27	0.21
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	18	0.21
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	18	0.21
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	18	0.21
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	18	0.21
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	18	0.21
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	18	0.21
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	32	0.21
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	32	0.21
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	32	0.21
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	12	0.21
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	12	0.21
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	12	0.21
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	14	0.21
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	14	0.21
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	14	0.21
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	20	0.21
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	20	0.21
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	20	0.21
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	36	0.21
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	36	0.21
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	36	0.21
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	46	0.21
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	46	0.21
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	46	0.21
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	31	0.21
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	31	0.21
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	31	0.21
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	31	0.21
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	31	0.21
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	31	0.21
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	31	0.21
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	31	0.21
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	31	0.21
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	44	0.21
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	44	0.21

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	44	0.21
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	44	0.21
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	44	0.21
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	44	0.21
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	44	0.21
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	44	0.21
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	44	0.21
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	1	0.21
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	1	0.21
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	1	0.21
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	1	0.21
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	1	0.21
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	1	0.21
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	1	0.21
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	1	0.21
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	1	0.21
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	2	0.21
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	2	0.21
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	2	0.21
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	2	0.21
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	2	0.21
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	2	0.21
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	2	0.21
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	2	0.21
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	2	0.21
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	8	0.21
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	8	0.21
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	8	0.21
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	8	0.21
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	8	0.21
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	8	0.21
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	8	0.21
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	8	0.21
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	8	0.21
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	41	0.21
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	41	0.21
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	41	0.21
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	46	0.21
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	46	0.21
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	46	0.21
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	35	0.21
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	35	0.21

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	35	0.21
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	46	0.21
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	46	0.21
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	46	0.21
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	29	0.21
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	29	0.21
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	29	0.21
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	42	0.21
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	42	0.21
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	42	0.21
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	42	0.21
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	42	0.21
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	42	0.21
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	42	0.21
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	42	0.21
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	42	0.21
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	39	0.21
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	39	0.21
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	39	0.21
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	39	0.21
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	39	0.21
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	39	0.21
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	39	0.21
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	39	0.21
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	39	0.21
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	32	0.2
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	32	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	6	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	6	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	6	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	6	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	6	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	6	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	6	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	6	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	6	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	6	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	6	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	6	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	6	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	6	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	6	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	6	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	6	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	6	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	15	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	15	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	15	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	15	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	15	0.2
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	15	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	15	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	15	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	15	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	15	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	15	0.2
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	15	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	15	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	15	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	15	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	15	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	15	0.2
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	15	0.2
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	43	0.2
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	43	0.2
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	43	0.2
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	43	0.2
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	43	0.2
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	43	0.2
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG11	36	0.2
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG12	36	0.2
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG13	36	0.2
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG21	36	0.2
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG22	36	0.2
(1,1418)	1:26:A:ILE:HG12	1:32:A:VAL:HG23	36	0.2
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG11	36	0.2
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG12	36	0.2
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG13	36	0.2
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG21	36	0.2
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG22	36	0.2
(1,1418)	1:26:A:ILE:HG13	1:32:A:VAL:HG23	36	0.2
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	34	0.2
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	34	0.2
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	34	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	34	0.2
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	34	0.2
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	34	0.2
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	50	0.2
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	50	0.2
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	50	0.2
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	50	0.2
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	50	0.2
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	50	0.2
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	19	0.2
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	32	0.2
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	34	0.2
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	34	0.2
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	34	0.2
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	38	0.2
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	43	0.2
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	2	0.2
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	2	0.2
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	2	0.2
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	24	0.2
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	24	0.2
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	24	0.2
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	9	0.2
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	9	0.2
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	9	0.2
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	9	0.2
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	9	0.2
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	9	0.2
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	48	0.2
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	48	0.2
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	48	0.2
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB2	44	0.2
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB3	44	0.2
(1,482)	1:10:A:GLN:HG2	1:52:A:THR:HG21	21	0.2
(1,482)	1:10:A:GLN:HG2	1:52:A:THR:HG22	21	0.2
(1,482)	1:10:A:GLN:HG2	1:52:A:THR:HG23	21	0.2
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	41	0.2
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	41	0.2
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	41	0.2
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	4	0.2
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	4	0.2
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	4	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	4	0.2
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	4	0.2
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	4	0.2
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	4	0.2
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	4	0.2
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	4	0.2
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	48	0.2
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	48	0.2
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	48	0.2
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	48	0.2
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	48	0.2
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	48	0.2
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	48	0.2
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	48	0.2
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	48	0.2
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	33	0.2
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	33	0.2
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	33	0.2
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	33	0.2
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	33	0.2
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	33	0.2
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	33	0.2
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	33	0.2
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	33	0.2
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	11	0.2
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	11	0.2
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	11	0.2
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	11	0.2
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	11	0.2
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	11	0.2
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	11	0.2
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	11	0.2
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	11	0.2
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	13	0.2
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	13	0.2
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	13	0.2
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	13	0.2
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	13	0.2
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	13	0.2
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	13	0.2
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	13	0.2
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	13	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	27	0.2
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	27	0.2
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	27	0.2
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	27	0.2
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	27	0.2
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	27	0.2
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	27	0.2
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	27	0.2
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	27	0.2
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	13	0.2
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	13	0.2
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	13	0.2
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	20	0.2
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	20	0.2
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	20	0.2
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	17	0.2
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	17	0.2
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	17	0.2
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	5	0.2
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	5	0.2
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	5	0.2
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	12	0.2
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	12	0.2
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	12	0.2
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	37	0.2
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	37	0.2
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	37	0.2
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	39	0.2
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	39	0.2
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	39	0.2
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	39	0.2
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	39	0.2
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	39	0.2
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	39	0.2
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	39	0.2
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	39	0.2
(1,379)	1:44:A:ILE:HB	1:81:A:TRP:HE1	38	0.2
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	28	0.19
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	28	0.19
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	28	0.19
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	28	0.19
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	28	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	28	0.19
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	42	0.19
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	42	0.19
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	42	0.19
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	42	0.19
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	42	0.19
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	42	0.19
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	42	0.19
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	42	0.19
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	42	0.19
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	42	0.19
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	42	0.19
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	42	0.19
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG11	33	0.19
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG12	33	0.19
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG13	33	0.19
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG21	33	0.19
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG22	33	0.19
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG23	33	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	2	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	2	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	2	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	2	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	2	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	2	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	2	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	2	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	2	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	2	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	2	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	2	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	2	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	2	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	2	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	2	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	2	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	2	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	5	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	5	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	5	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	5	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	5	0.19

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	5	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	5	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	5	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	5	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	5	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	5	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	5	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	5	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	5	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	5	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	5	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	5	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	5	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	12	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	12	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	12	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	12	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	12	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	12	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	12	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	12	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	12	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	12	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	12	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	12	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	12	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	12	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	12	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	12	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	12	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	12	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	37	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	37	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	37	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	37	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	37	0.19
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	37	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	37	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	37	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	37	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	37	0.19
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	37	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	37	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	37	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	37	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	37	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	37	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	37	0.19
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	37	0.19
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	22	0.19
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	22	0.19
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	22	0.19
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	22	0.19
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	22	0.19
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	22	0.19
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	35	0.19
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	35	0.19
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	35	0.19
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	35	0.19
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	35	0.19
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	35	0.19
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	49	0.19
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	49	0.19
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	49	0.19
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	49	0.19
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	49	0.19
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	49	0.19
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	44	0.19
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	44	0.19
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	44	0.19
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	44	0.19
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	44	0.19
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	44	0.19
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	44	0.19
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	44	0.19
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	44	0.19
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	44	0.19
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	44	0.19
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	44	0.19
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	44	0.19
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	44	0.19
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	44	0.19
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	44	0.19
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	44	0.19

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	44	0.19
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	48	0.19
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	48	0.19
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	48	0.19
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	48	0.19
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	48	0.19
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	48	0.19
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	48	0.19
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	48	0.19
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	48	0.19
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	48	0.19
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	50	0.19
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	50	0.19
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	50	0.19
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	50	0.19
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	50	0.19
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	50	0.19
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	27	0.19
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	27	0.19
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	27	0.19
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	27	0.19
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	27	0.19
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	27	0.19
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	36	0.19
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	36	0.19
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	36	0.19
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	36	0.19
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	36	0.19
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	36	0.19
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	36	0.19
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	36	0.19
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	36	0.19
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	36	0.19
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	36	0.19
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	36	0.19
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	39	0.19
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	48	0.19
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	48	0.19
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	48	0.19
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	41	0.19
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	41	0.19
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	41	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	37	0.19
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	37	0.19
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	37	0.19
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	27	0.19
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	47	0.19
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD11	7	0.19
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD12	7	0.19
(1,625)	1:65:A:THR:HG21	1:70:A:LEU:HD13	7	0.19
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD11	7	0.19
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD12	7	0.19
(1,625)	1:65:A:THR:HG22	1:70:A:LEU:HD13	7	0.19
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD11	7	0.19
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD12	7	0.19
(1,625)	1:65:A:THR:HG23	1:70:A:LEU:HD13	7	0.19
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	26	0.19
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	26	0.19
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	26	0.19
(1,500)	1:49:A:LEU:HD11	1:54:A:LEU:HB2	43	0.19
(1,500)	1:49:A:LEU:HD12	1:54:A:LEU:HB2	43	0.19
(1,500)	1:49:A:LEU:HD13	1:54:A:LEU:HB2	43	0.19
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD21	38	0.19
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD22	38	0.19
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD23	38	0.19
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	26	0.19
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	26	0.19
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	26	0.19
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	28	0.19
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	28	0.19
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	28	0.19
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	28	0.19
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	28	0.19
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	28	0.19
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	28	0.19
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	28	0.19
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	28	0.19
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	38	0.19
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	38	0.19
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	38	0.19
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	38	0.19
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	38	0.19
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	38	0.19
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	38	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	38	0.19
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	38	0.19
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	14	0.19
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	14	0.19
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	14	0.19
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	14	0.19
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	14	0.19
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	14	0.19
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	14	0.19
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	14	0.19
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	14	0.19
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	26	0.19
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	26	0.19
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	26	0.19
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	26	0.19
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	26	0.19
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	26	0.19
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	26	0.19
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	26	0.19
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	26	0.19
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	2	0.19
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	2	0.19
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	2	0.19
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	11	0.19
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	11	0.19
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	11	0.19
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	32	0.19
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	32	0.19
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	32	0.19
(1,411)	1:44:A:ILE:HG21	1:84:A:LEU:HD21	38	0.19
(1,411)	1:44:A:ILE:HG21	1:84:A:LEU:HD22	38	0.19
(1,411)	1:44:A:ILE:HG21	1:84:A:LEU:HD23	38	0.19
(1,411)	1:44:A:ILE:HG22	1:84:A:LEU:HD21	38	0.19
(1,411)	1:44:A:ILE:HG22	1:84:A:LEU:HD22	38	0.19
(1,411)	1:44:A:ILE:HG22	1:84:A:LEU:HD23	38	0.19
(1,411)	1:44:A:ILE:HG23	1:84:A:LEU:HD21	38	0.19
(1,411)	1:44:A:ILE:HG23	1:84:A:LEU:HD22	38	0.19
(1,411)	1:44:A:ILE:HG23	1:84:A:LEU:HD23	38	0.19
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	47	0.19
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	47	0.19
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	47	0.19
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	47	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	47	0.19
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	47	0.19
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	47	0.19
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	47	0.19
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	47	0.19
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	23	0.19
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	23	0.19
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	23	0.19
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	26	0.19
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	26	0.19
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	26	0.19
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	45	0.19
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	45	0.19
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	45	0.19
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	45	0.19
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	45	0.19
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	45	0.19
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	45	0.19
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	45	0.19
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	45	0.19
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	50	0.19
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	50	0.19
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	50	0.19
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	50	0.19
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	50	0.19
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	50	0.19
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	50	0.19
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	50	0.19
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	50	0.19
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	47	0.19
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	47	0.19
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	47	0.19
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	2	0.18
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	2	0.18
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	2	0.18
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	2	0.18
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	2	0.18
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	2	0.18
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	38	0.18
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	38	0.18
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	38	0.18
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	38	0.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	38	0.18
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	38	0.18
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	38	0.18
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	38	0.18
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	38	0.18
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	38	0.18
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	38	0.18
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	38	0.18
(1,1737)	1:68:A:GLU:HG2	1:69:A:GLU:H	27	0.18
(1,1737)	1:68:A:GLU:HG3	1:69:A:GLU:H	27	0.18
(1,1605)	1:49:A:LEU:HD11	1:84:A:LEU:HB2	24	0.18
(1,1605)	1:49:A:LEU:HD11	1:84:A:LEU:HB3	24	0.18
(1,1605)	1:49:A:LEU:HD12	1:84:A:LEU:HB2	24	0.18
(1,1605)	1:49:A:LEU:HD12	1:84:A:LEU:HB3	24	0.18
(1,1605)	1:49:A:LEU:HD13	1:84:A:LEU:HB2	24	0.18
(1,1605)	1:49:A:LEU:HD13	1:84:A:LEU:HB3	24	0.18
(1,1605)	1:49:A:LEU:HD21	1:84:A:LEU:HB2	24	0.18
(1,1605)	1:49:A:LEU:HD21	1:84:A:LEU:HB3	24	0.18
(1,1605)	1:49:A:LEU:HD22	1:84:A:LEU:HB2	24	0.18
(1,1605)	1:49:A:LEU:HD22	1:84:A:LEU:HB3	24	0.18
(1,1605)	1:49:A:LEU:HD23	1:84:A:LEU:HB2	24	0.18
(1,1605)	1:49:A:LEU:HD23	1:84:A:LEU:HB3	24	0.18
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	17	0.18
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	17	0.18
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	40	0.18
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	40	0.18
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	45	0.18
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	45	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	1	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	1	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	1	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	1	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	1	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	1	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	1	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	1	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	1	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	1	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	1	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	1	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	1	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	1	0.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	1	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	1	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	1	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	1	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	9	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	9	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	9	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	9	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	9	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	9	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	9	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	9	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	9	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	9	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	9	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	9	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	9	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	9	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	9	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	9	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	9	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	9	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	36	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	36	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	36	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	36	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	36	0.18
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	36	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	36	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	36	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	36	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	36	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	36	0.18
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	36	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	36	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	36	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	36	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	36	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	36	0.18
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	36	0.18
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	12	0.18
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	12	0.18

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	12	0.18
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	12	0.18
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	12	0.18
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	12	0.18
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	18	0.18
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	18	0.18
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	18	0.18
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	18	0.18
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	18	0.18
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	18	0.18
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	35	0.18
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	35	0.18
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	35	0.18
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	35	0.18
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	35	0.18
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	35	0.18
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD11	34	0.18
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD12	34	0.18
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD13	34	0.18
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD11	34	0.18
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD12	34	0.18
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD13	34	0.18
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	8	0.18
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	8	0.18
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	8	0.18
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	8	0.18
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	8	0.18
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	8	0.18
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	25	0.18
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	25	0.18
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	25	0.18
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	25	0.18
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	25	0.18
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	25	0.18
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	25	0.18
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	49	0.18
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	49	0.18
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	49	0.18
(1,1063)	1:54:A:LEU:H	1:57:A:LEU:HG	26	0.18
(1,701)	1:74:A:ALA:HA	1:77:A:LEU:HB3	41	0.18
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	43	0.18
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	43	0.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	43	0.18
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	11	0.18
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	11	0.18
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	11	0.18
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	21	0.18
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	21	0.18
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	21	0.18
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD2	17	0.18
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD3	17	0.18
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD21	50	0.18
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD22	50	0.18
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD23	50	0.18
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	48	0.18
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	48	0.18
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	48	0.18
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	48	0.18
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	48	0.18
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	48	0.18
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	48	0.18
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	48	0.18
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	48	0.18
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	3	0.18
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	3	0.18
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	3	0.18
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	3	0.18
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	3	0.18
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	3	0.18
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	3	0.18
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	3	0.18
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	3	0.18
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	22	0.18
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	22	0.18
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	22	0.18
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	22	0.18
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	22	0.18
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	22	0.18
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	22	0.18
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	22	0.18
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	22	0.18
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	16	0.18
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	16	0.18
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	16	0.18

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	22	0.18
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	22	0.18
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	22	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	14	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	14	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	14	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	27	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	27	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	27	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	44	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	44	0.18
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	44	0.18
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	7	0.18
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	7	0.18
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	7	0.18
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD21	24	0.18
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD22	24	0.18
(1,407)	1:44:A:ILE:HG21	1:49:A:LEU:HD23	24	0.18
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD21	24	0.18
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD22	24	0.18
(1,407)	1:44:A:ILE:HG22	1:49:A:LEU:HD23	24	0.18
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD21	24	0.18
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD22	24	0.18
(1,407)	1:44:A:ILE:HG23	1:49:A:LEU:HD23	24	0.18
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	21	0.18
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	21	0.18
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	21	0.18
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	21	0.18
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	21	0.18
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	21	0.18
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	21	0.18
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	21	0.18
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	21	0.18
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	5	0.18
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	5	0.18
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	5	0.18
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	5	0.18
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	5	0.18
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	5	0.18
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	5	0.18
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	5	0.18
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	5	0.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	13	0.18
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	13	0.18
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	13	0.18
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	13	0.18
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	13	0.18
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	13	0.18
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	13	0.18
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	13	0.18
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	13	0.18
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	33	0.18
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	33	0.18
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	33	0.18
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	42	0.17
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	42	0.17
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	42	0.17
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	42	0.17
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	42	0.17
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	42	0.17
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	28	0.17
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	28	0.17
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	28	0.17
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	28	0.17
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	28	0.17
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	28	0.17
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	28	0.17
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	28	0.17
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	28	0.17
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	28	0.17
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	28	0.17
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	28	0.17
(1,1737)	1:68:A:GLU:HG2	1:69:A:GLU:H	32	0.17
(1,1737)	1:68:A:GLU:HG3	1:69:A:GLU:H	32	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	50	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	50	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	50	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	50	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	50	0.17
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	50	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	8	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	8	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	8	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	8	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	8	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	8	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	20	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	20	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	20	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	20	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	20	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	20	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	50	0.17
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	50	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	50	0.17
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	50	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	50	0.17
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	50	0.17
(1,1462)	1:32:A:VAL:HG11	1:36:A:ILE:HD11	45	0.17
(1,1462)	1:32:A:VAL:HG11	1:36:A:ILE:HD12	45	0.17
(1,1462)	1:32:A:VAL:HG11	1:36:A:ILE:HD13	45	0.17
(1,1462)	1:32:A:VAL:HG12	1:36:A:ILE:HD11	45	0.17
(1,1462)	1:32:A:VAL:HG12	1:36:A:ILE:HD12	45	0.17
(1,1462)	1:32:A:VAL:HG12	1:36:A:ILE:HD13	45	0.17
(1,1462)	1:32:A:VAL:HG13	1:36:A:ILE:HD11	45	0.17
(1,1462)	1:32:A:VAL:HG13	1:36:A:ILE:HD12	45	0.17
(1,1462)	1:32:A:VAL:HG13	1:36:A:ILE:HD13	45	0.17
(1,1462)	1:32:A:VAL:HG21	1:36:A:ILE:HD11	45	0.17
(1,1462)	1:32:A:VAL:HG21	1:36:A:ILE:HD12	45	0.17
(1,1462)	1:32:A:VAL:HG21	1:36:A:ILE:HD13	45	0.17
(1,1462)	1:32:A:VAL:HG22	1:36:A:ILE:HD11	45	0.17
(1,1462)	1:32:A:VAL:HG22	1:36:A:ILE:HD12	45	0.17
(1,1462)	1:32:A:VAL:HG22	1:36:A:ILE:HD13	45	0.17
(1,1462)	1:32:A:VAL:HG23	1:36:A:ILE:HD11	45	0.17
(1,1462)	1:32:A:VAL:HG23	1:36:A:ILE:HD12	45	0.17
(1,1462)	1:32:A:VAL:HG23	1:36:A:ILE:HD13	45	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	42	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	42	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	42	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	42	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	42	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	42	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	42	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	42	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	42	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	42	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	42	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	42	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	42	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	42	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	42	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	42	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	42	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	42	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	45	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	45	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	45	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	45	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	45	0.17
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	45	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	45	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	45	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	45	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	45	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	45	0.17
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	45	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	45	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	45	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	45	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	45	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	45	0.17
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	45	0.17
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	23	0.17
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	23	0.17
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	23	0.17
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	23	0.17
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	23	0.17
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	23	0.17
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	23	0.17
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	23	0.17
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	23	0.17
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	23	0.17
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	4	0.17
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	4	0.17
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	4	0.17
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	4	0.17
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	4	0.17
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	4	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	4	0.17
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	4	0.17
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	4	0.17
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	4	0.17
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	4	0.17
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	4	0.17
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	31	0.17
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	18	0.17
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	18	0.17
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	18	0.17
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	42	0.17
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	42	0.17
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	42	0.17
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	44	0.17
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	26	0.17
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	26	0.17
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	26	0.17
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE2	38	0.17
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE3	38	0.17
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE2	45	0.17
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE3	45	0.17
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD11	41	0.17
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD12	41	0.17
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD13	41	0.17
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD11	41	0.17
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD12	41	0.17
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD13	41	0.17
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD11	41	0.17
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD12	41	0.17
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD13	41	0.17
(1,678)	1:62:A:ARG:HG2	1:74:A:ALA:HB1	43	0.17
(1,678)	1:62:A:ARG:HG2	1:74:A:ALA:HB2	43	0.17
(1,678)	1:62:A:ARG:HG2	1:74:A:ALA:HB3	43	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	29	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	29	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	29	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	29	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	29	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	29	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	32	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	32	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	32	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	32	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	32	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	32	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	34	0.17
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	34	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	34	0.17
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	34	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	34	0.17
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	34	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	28	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	28	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	28	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	49	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	49	0.17
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	49	0.17
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	9	0.17
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	9	0.17
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	9	0.17
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	32	0.17
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	32	0.17
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	32	0.17
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	33	0.17
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	33	0.17
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	33	0.17
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD21	36	0.17
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD22	36	0.17
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD23	36	0.17
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD21	36	0.17
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD22	36	0.17
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD23	36	0.17
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD21	36	0.17
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD22	36	0.17
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD23	36	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	16	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	16	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	16	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	16	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	16	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	16	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	16	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	16	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	16	0.17

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	19	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	19	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	19	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	19	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	19	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	19	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	19	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	19	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	19	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	21	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	21	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	21	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	21	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	21	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	21	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	21	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	21	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	21	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	29	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	29	0.17
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	29	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	29	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	29	0.17
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	29	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	29	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	29	0.17
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	29	0.17
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	8	0.17
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	8	0.17
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	8	0.17
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	8	0.17
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	8	0.17
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	8	0.17
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	8	0.17
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	8	0.17
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	8	0.17
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	22	0.17
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	22	0.17
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	22	0.17
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	22	0.17
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	22	0.17
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	22	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	22	0.17
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	22	0.17
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	22	0.17
(1,427)	1:45:A:THR:HG21	1:46:A:LYS:H	23	0.17
(1,427)	1:45:A:THR:HG22	1:46:A:LYS:H	23	0.17
(1,427)	1:45:A:THR:HG23	1:46:A:LYS:H	23	0.17
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	3	0.17
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	3	0.17
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	3	0.17
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	8	0.17
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	8	0.17
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	8	0.17
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	34	0.17
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	34	0.17
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	34	0.17
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	49	0.17
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	49	0.17
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	49	0.17
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	15	0.17
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	15	0.17
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	15	0.17
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	17	0.17
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	17	0.17
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	17	0.17
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	32	0.17
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	32	0.17
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	32	0.17
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	24	0.17
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	24	0.17
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	24	0.17
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	24	0.17
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	24	0.17
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	24	0.17
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	24	0.17
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	24	0.17
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	24	0.17
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	50	0.17
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	16	0.17
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	16	0.17
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	16	0.17
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	16	0.17
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	16	0.17

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	16	0.17
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	16	0.17
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	16	0.17
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	16	0.17
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	22	0.17
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	22	0.17
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	22	0.17
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	30	0.16
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	30	0.16
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	30	0.16
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	30	0.16
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	30	0.16
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	30	0.16
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	40	0.16
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	40	0.16
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	40	0.16
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	40	0.16
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	40	0.16
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	40	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	36	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	36	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	36	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	36	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	36	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	36	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	48	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	48	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	48	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	48	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	48	0.16
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	48	0.16
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	20	0.16
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	20	0.16
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	20	0.16
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	20	0.16
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	20	0.16
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	20	0.16
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	20	0.16
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	20	0.16
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	20	0.16
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	20	0.16
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	20	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	20	0.16
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	48	0.16
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	48	0.16
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	48	0.16
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	48	0.16
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	48	0.16
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	48	0.16
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	48	0.16
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	48	0.16
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	48	0.16
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	48	0.16
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	48	0.16
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	48	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	22	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	22	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	22	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	22	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	22	0.16
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	22	0.16
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	22	0.16
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	22	0.16
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	22	0.16
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	22	0.16
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	22	0.16
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	22	0.16
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	22	0.16
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	22	0.16
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	22	0.16
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	22	0.16
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	22	0.16
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	22	0.16
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	49	0.16
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	49	0.16
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	49	0.16
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	49	0.16
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	49	0.16
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	49	0.16
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	39	0.16
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	39	0.16
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	39	0.16
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	39	0.16
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	39	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	39	0.16
(1,1527)	1:39:A:LEU:HD11	1:44:A:ILE:H	39	0.16
(1,1527)	1:39:A:LEU:HD12	1:44:A:ILE:H	39	0.16
(1,1527)	1:39:A:LEU:HD13	1:44:A:ILE:H	39	0.16
(1,1527)	1:39:A:LEU:HD21	1:44:A:ILE:H	39	0.16
(1,1527)	1:39:A:LEU:HD22	1:44:A:ILE:H	39	0.16
(1,1527)	1:39:A:LEU:HD23	1:44:A:ILE:H	39	0.16
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	11	0.16
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	11	0.16
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	11	0.16
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	11	0.16
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	11	0.16
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	11	0.16
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD11	33	0.16
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD12	33	0.16
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD13	33	0.16
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD11	33	0.16
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD12	33	0.16
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD13	33	0.16
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	17	0.16
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	17	0.16
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	17	0.16
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	17	0.16
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	17	0.16
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	17	0.16
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	19	0.16
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	19	0.16
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	19	0.16
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	19	0.16
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	19	0.16
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	19	0.16
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	41	0.16
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	41	0.16
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	41	0.16
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	41	0.16
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	41	0.16
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	41	0.16
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	29	0.16
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	33	0.16
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	50	0.16
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	50	0.16
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	50	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	50	0.16
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	50	0.16
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	50	0.16
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	27	0.16
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	27	0.16
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	27	0.16
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	10	0.16
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	10	0.16
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	10	0.16
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	18	0.16
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	18	0.16
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	18	0.16
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	32	0.16
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	32	0.16
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	32	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	2	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	2	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	2	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	2	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	2	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	2	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	2	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	2	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	2	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	32	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	32	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	32	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	32	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	32	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	32	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	32	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	32	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	32	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	35	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	35	0.16
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	35	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	35	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	35	0.16
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	35	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	35	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	35	0.16
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	35	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:45:A:THR:HG21	1:46:A:LYS:H	21	0.16
(1,427)	1:45:A:THR:HG22	1:46:A:LYS:H	21	0.16
(1,427)	1:45:A:THR:HG23	1:46:A:LYS:H	21	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	3	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	3	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	3	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	3	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	3	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	3	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	3	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	3	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	3	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	9	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	9	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	9	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	9	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	9	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	9	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	9	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	9	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	9	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	24	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	24	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	24	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	24	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	24	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	24	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	24	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	24	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	24	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	35	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	35	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	35	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	35	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	35	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	35	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	35	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	35	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	35	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	37	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	37	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	37	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	37	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	37	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	37	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	37	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	37	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	37	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	38	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	38	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	38	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	38	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	38	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	38	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	38	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	38	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	38	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	41	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	41	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	41	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	41	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	41	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	41	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	41	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	41	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	41	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	50	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	50	0.16
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	50	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	50	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	50	0.16
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	50	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	50	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	50	0.16
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	50	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	24	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	24	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	24	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	26	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	26	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	26	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	47	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	47	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	47	0.16

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	49	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	49	0.16
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	49	0.16
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	20	0.16
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	20	0.16
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	20	0.16
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	35	0.16
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	35	0.16
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	35	0.16
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	39	0.16
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	39	0.16
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	39	0.16
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	27	0.16
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	45	0.16
(1,335)	1:36:A:ILE:HG21	1:77:A:LEU:H	35	0.16
(1,335)	1:36:A:ILE:HG22	1:77:A:LEU:H	35	0.16
(1,335)	1:36:A:ILE:HG23	1:77:A:LEU:H	35	0.16
(1,335)	1:36:A:ILE:HG21	1:77:A:LEU:H	37	0.16
(1,335)	1:36:A:ILE:HG22	1:77:A:LEU:H	37	0.16
(1,335)	1:36:A:ILE:HG23	1:77:A:LEU:H	37	0.16
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG21	48	0.16
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG22	48	0.16
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG23	48	0.16
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG21	48	0.16
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG22	48	0.16
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG23	48	0.16
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG21	48	0.16
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG22	48	0.16
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG23	48	0.16
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	49	0.16
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	49	0.16
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	49	0.16
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	49	0.16
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	49	0.16
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	49	0.16
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	49	0.16
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	49	0.16
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	49	0.16
(1,192)	1:26:A:ILE:HD11	1:32:A:VAL:H	40	0.16
(1,192)	1:26:A:ILE:HD12	1:32:A:VAL:H	40	0.16
(1,192)	1:26:A:ILE:HD13	1:32:A:VAL:H	40	0.16
(1,1805)	1:78:A:LEU:HD11	1:81:A:TRP:HH2	32	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	1:78:A:LEU:HD12	1:81:A:TRP:HH2	32	0.15
(1,1805)	1:78:A:LEU:HD13	1:81:A:TRP:HH2	32	0.15
(1,1805)	1:78:A:LEU:HD21	1:81:A:TRP:HH2	32	0.15
(1,1805)	1:78:A:LEU:HD22	1:81:A:TRP:HH2	32	0.15
(1,1805)	1:78:A:LEU:HD23	1:81:A:TRP:HH2	32	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	17	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	17	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	17	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	17	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	17	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	17	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	20	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	20	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	20	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	20	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	20	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	20	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	27	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	27	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	27	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	27	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	27	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	27	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	27	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	27	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	27	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	27	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	27	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	27	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	27	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	27	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	27	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	27	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	27	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	27	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	34	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	34	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	34	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	34	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	34	0.15
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	34	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	34	0.15

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	34	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	34	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	34	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	34	0.15
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	34	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	34	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	34	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	34	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	34	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	34	0.15
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	34	0.15
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	17	0.15
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	17	0.15
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	17	0.15
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	17	0.15
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	17	0.15
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	17	0.15
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	30	0.15
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	30	0.15
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	30	0.15
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	30	0.15
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	30	0.15
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	30	0.15
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	39	0.15
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	39	0.15
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	39	0.15
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	39	0.15
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	39	0.15
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	39	0.15
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD11	31	0.15
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD12	31	0.15
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD13	31	0.15
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD21	31	0.15
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD22	31	0.15
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD23	31	0.15
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	27	0.15
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	27	0.15
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	27	0.15
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	27	0.15
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	27	0.15
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	27	0.15
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	27	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	27	0.15
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	27	0.15
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	27	0.15
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	27	0.15
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	27	0.15
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	27	0.15
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	27	0.15
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	27	0.15
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	27	0.15
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	27	0.15
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	27	0.15
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	22	0.15
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	22	0.15
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	22	0.15
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	22	0.15
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	22	0.15
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	22	0.15
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	47	0.15
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	47	0.15
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	47	0.15
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	47	0.15
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	47	0.15
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	47	0.15
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	25	0.15
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	25	0.15
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	25	0.15
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	25	0.15
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	25	0.15
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	25	0.15
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	46	0.15
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	30	0.15
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	30	0.15
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	30	0.15
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	34	0.15
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	34	0.15
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	34	0.15
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	4	0.15
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	4	0.15
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	4	0.15
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	21	0.15
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	21	0.15
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	21	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	27	0.15
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	27	0.15
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	27	0.15
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	44	0.15
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	44	0.15
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	44	0.15
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	18	0.15
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	18	0.15
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	18	0.15
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	30	0.15
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	30	0.15
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	30	0.15
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	42	0.15
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	42	0.15
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	42	0.15
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	50	0.15
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	50	0.15
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	50	0.15
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	32	0.15
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	45	0.15
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD21	28	0.15
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD22	28	0.15
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD23	28	0.15
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	19	0.15
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	19	0.15
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	19	0.15
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB2	26	0.15
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB3	26	0.15
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	2	0.15
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	2	0.15
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	2	0.15
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	3	0.15
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	3	0.15
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	3	0.15
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	42	0.15
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	42	0.15
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	42	0.15
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	28	0.15
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	28	0.15
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	28	0.15
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	37	0.15
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	37	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	37	0.15
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD2	4	0.15
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD3	4	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	12	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	12	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	12	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	12	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	12	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	12	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	12	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	12	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	12	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	16	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	16	0.15
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	16	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	16	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	16	0.15
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	16	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	16	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	16	0.15
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	16	0.15
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	33	0.15
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	33	0.15
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	33	0.15
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	40	0.15
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	40	0.15
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	40	0.15
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	42	0.15
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	42	0.15
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	42	0.15
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	42	0.15
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	42	0.15
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	42	0.15
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	42	0.15
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	42	0.15
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	42	0.15
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	10	0.15
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	10	0.15
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	10	0.15
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	10	0.15
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	10	0.15
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	10	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	10	0.15
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	10	0.15
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	10	0.15
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	21	0.15
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	21	0.15
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	21	0.15
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	21	0.15
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	21	0.15
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	21	0.15
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	21	0.15
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	21	0.15
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	21	0.15
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	34	0.15
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	34	0.15
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	34	0.15
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	34	0.15
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	34	0.15
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	34	0.15
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	34	0.15
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	34	0.15
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	34	0.15
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	12	0.15
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	12	0.15
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	12	0.15
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	21	0.15
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	21	0.15
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	21	0.15
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	1	0.15
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	1	0.15
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	1	0.15
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	26	0.15
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	26	0.15
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	26	0.15
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	8	0.15
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	8	0.15
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	8	0.15
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	18	0.15
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	18	0.15
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	18	0.15
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	28	0.15
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	28	0.15
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	28	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	7	0.15
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	7	0.15
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	7	0.15
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	7	0.15
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	7	0.15
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	7	0.15
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	7	0.15
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	7	0.15
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	7	0.15
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	12	0.15
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	12	0.15
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	12	0.15
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	12	0.15
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	12	0.15
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	12	0.15
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	12	0.15
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	12	0.15
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	12	0.15
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	26	0.15
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	43	0.15
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	43	0.15
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	43	0.15
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	43	0.15
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	43	0.15
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	43	0.15
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	43	0.15
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	43	0.15
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	43	0.15
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	44	0.14
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	44	0.14
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	44	0.14
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	44	0.14
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	44	0.14
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	44	0.14
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	39	0.14
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	39	0.14
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	39	0.14
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	39	0.14
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	39	0.14
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	39	0.14
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	39	0.14
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	39	0.14

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	39	0.14
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	39	0.14
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	39	0.14
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	39	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	24	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	24	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	24	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	24	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	24	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	24	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	35	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	35	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	35	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	35	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	35	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	35	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	41	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	41	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	41	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	41	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	41	0.14
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	41	0.14
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	37	0.14
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	37	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	7	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	7	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	7	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	7	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	7	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	7	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	7	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	7	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	7	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	7	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	7	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	7	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	7	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	7	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	7	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	7	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	7	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	7	0.14

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	28	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	28	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	28	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	28	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	28	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	28	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	28	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	28	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	28	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	28	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	28	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	28	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	28	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	28	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	28	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	28	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	28	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	28	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	32	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	32	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	32	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	32	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	32	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	32	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	32	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	32	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	32	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	32	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	32	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	32	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	32	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	32	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	32	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	32	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	32	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	32	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	45	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	45	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	45	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	45	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	45	0.14
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	45	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	45	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	45	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	45	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	45	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	45	0.14
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	45	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	45	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	45	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	45	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	45	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	45	0.14
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	45	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG21	9	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG22	9	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG23	9	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG21	9	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG22	9	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG23	9	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG21	36	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG22	36	0.14
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG23	36	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG21	36	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG22	36	0.14
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG23	36	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	9	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	9	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	9	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	9	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	9	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	9	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	13	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	13	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	13	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	13	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	13	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	13	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	28	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	28	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	28	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	28	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	28	0.14
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	28	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	16	0.14
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	16	0.14
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	16	0.14
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	16	0.14
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	16	0.14
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	16	0.14
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	47	0.14
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	47	0.14
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	47	0.14
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	47	0.14
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	47	0.14
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	47	0.14
(1,1496)	1:36:A:ILE:HG21	1:37:A:SER:HB2	42	0.14
(1,1496)	1:36:A:ILE:HG21	1:37:A:SER:HB3	42	0.14
(1,1496)	1:36:A:ILE:HG22	1:37:A:SER:HB2	42	0.14
(1,1496)	1:36:A:ILE:HG22	1:37:A:SER:HB3	42	0.14
(1,1496)	1:36:A:ILE:HG23	1:37:A:SER:HB2	42	0.14
(1,1496)	1:36:A:ILE:HG23	1:37:A:SER:HB3	42	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	19	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	19	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	19	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	19	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	19	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	19	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	19	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	19	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	19	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	19	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	19	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	19	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	19	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	19	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	19	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	19	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	19	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	19	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	38	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	38	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	38	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	38	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	38	0.14
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	38	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	38	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	38	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	38	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	38	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	38	0.14
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	38	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	38	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	38	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	38	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	38	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	38	0.14
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	38	0.14
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	24	0.14
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	24	0.14
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	24	0.14
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	24	0.14
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	2	0.14
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	2	0.14
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	2	0.14
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	2	0.14
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	2	0.14
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	2	0.14
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	44	0.14
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	44	0.14
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	44	0.14
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	44	0.14
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	44	0.14
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	44	0.14
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	26	0.14
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	26	0.14
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	26	0.14
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	26	0.14
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	26	0.14
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	26	0.14
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	29	0.14
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	29	0.14
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	29	0.14
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	29	0.14
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	29	0.14
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	29	0.14
(1,1288)	1:12:A:ILE:HG12	1:42:A:TYR:HB2	25	0.14
(1,1288)	1:12:A:ILE:HG12	1:42:A:TYR:HB3	25	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:12:A:ILE:HG13	1:42:A:TYR:HB2	25	0.14
(1,1288)	1:12:A:ILE:HG13	1:42:A:TYR:HB3	25	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	17	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	17	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	17	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	26	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	26	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	26	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	31	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	31	0.14
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	31	0.14
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	3	0.14
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	3	0.14
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	3	0.14
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	13	0.14
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	13	0.14
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	13	0.14
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	19	0.14
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	19	0.14
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	19	0.14
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	38	0.14
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	38	0.14
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	38	0.14
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	46	0.14
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	46	0.14
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	46	0.14
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	41	0.14
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD11	37	0.14
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD12	37	0.14
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD13	37	0.14
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD11	37	0.14
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD12	37	0.14
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD13	37	0.14
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD11	37	0.14
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD12	37	0.14
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD13	37	0.14
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB2	45	0.14
(1,617)	1:60:A:ASP:HA	1:63:A:LYS:HB3	45	0.14
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	45	0.14
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	45	0.14
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	45	0.14
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD11	48	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD12	48	0.14
(1,601)	1:62:A:ARG:HA	1:70:A:LEU:HD13	48	0.14
(1,567)	1:58:A:ILE:HD11	1:59:A:ASN:H	34	0.14
(1,567)	1:58:A:ILE:HD12	1:59:A:ASN:H	34	0.14
(1,567)	1:58:A:ILE:HD13	1:59:A:ASN:H	34	0.14
(1,552)	1:54:A:LEU:HB3	1:58:A:ILE:HD11	45	0.14
(1,552)	1:54:A:LEU:HB3	1:58:A:ILE:HD12	45	0.14
(1,552)	1:54:A:LEU:HB3	1:58:A:ILE:HD13	45	0.14
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	23	0.14
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	23	0.14
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	23	0.14
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	32	0.14
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	32	0.14
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	32	0.14
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	29	0.14
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	29	0.14
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	29	0.14
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD2	2	0.14
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD3	2	0.14
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG21	32	0.14
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG22	32	0.14
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG23	32	0.14
(1,474)	1:49:A:LEU:HD21	1:81:A:TRP:HD1	43	0.14
(1,474)	1:49:A:LEU:HD22	1:81:A:TRP:HD1	43	0.14
(1,474)	1:49:A:LEU:HD23	1:81:A:TRP:HD1	43	0.14
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	42	0.14
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	42	0.14
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	42	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	5	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	5	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	5	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	5	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	5	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	5	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	5	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	5	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	5	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	12	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	12	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	12	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	12	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	12	0.14

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	12	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	12	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	12	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	12	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	20	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	20	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	20	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	20	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	20	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	20	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	20	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	20	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	20	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	24	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	24	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	24	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	24	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	24	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	24	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	24	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	24	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	24	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	30	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	30	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	30	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	30	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	30	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	30	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	30	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	30	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	30	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	37	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	37	0.14
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	37	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	37	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	37	0.14
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	37	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	37	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	37	0.14
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	37	0.14
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	35	0.14
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	35	0.14

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	35	0.14
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	35	0.14
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	35	0.14
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	35	0.14
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	35	0.14
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	35	0.14
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	35	0.14
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	49	0.14
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	49	0.14
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	49	0.14
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	49	0.14
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	49	0.14
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	49	0.14
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	49	0.14
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	49	0.14
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	49	0.14
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG21	13	0.14
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG22	13	0.14
(1,424)	1:44:A:ILE:HD11	1:45:A:THR:HG23	13	0.14
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG21	13	0.14
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG22	13	0.14
(1,424)	1:44:A:ILE:HD12	1:45:A:THR:HG23	13	0.14
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG21	13	0.14
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG22	13	0.14
(1,424)	1:44:A:ILE:HD13	1:45:A:THR:HG23	13	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	11	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	11	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	11	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	11	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	11	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	11	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	11	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	11	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	11	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	19	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	19	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	19	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	19	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	19	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	19	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	19	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	19	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	19	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	46	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	46	0.14
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	46	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	46	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	46	0.14
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	46	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	46	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	46	0.14
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	46	0.14
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	1	0.14
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	1	0.14
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	1	0.14
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	15	0.14
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	15	0.14
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	15	0.14
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	45	0.14
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	45	0.14
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	45	0.14
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	19	0.14
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	19	0.14
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	19	0.14
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	47	0.14
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	47	0.14
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	47	0.14
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG21	44	0.14
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG22	44	0.14
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG23	44	0.14
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG21	44	0.14
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG22	44	0.14
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG23	44	0.14
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG21	44	0.14
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG22	44	0.14
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG23	44	0.14
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	27	0.14
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	27	0.14
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	27	0.14
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	27	0.14
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	27	0.14
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	27	0.14
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	27	0.14
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	27	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	27	0.14
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	42	0.14
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	42	0.14
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	42	0.14
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	42	0.14
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	42	0.14
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	42	0.14
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	42	0.14
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	42	0.14
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	42	0.14
(1,169)	1:23:A:GLN:HB3	1:25:A:ASN:HD22	40	0.14
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	31	0.14
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	31	0.14
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	31	0.14
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	46	0.14
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	46	0.14
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	46	0.14
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD11	44	0.14
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD12	44	0.14
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD13	44	0.14
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	34	0.13
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	34	0.13
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	34	0.13
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	34	0.13
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	34	0.13
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	34	0.13
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	47	0.13
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	47	0.13
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	47	0.13
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	47	0.13
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	47	0.13
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	47	0.13
(1,1737)	1:68:A:GLU:HG2	1:69:A:GLU:H	28	0.13
(1,1737)	1:68:A:GLU:HG3	1:69:A:GLU:H	28	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	18	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	18	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	18	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	18	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	18	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	18	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	28	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	28	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	28	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	28	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	28	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	28	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	49	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	49	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	49	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	49	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	49	0.13
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	49	0.13
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	10	0.13
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	10	0.13
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	10	0.13
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	10	0.13
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	10	0.13
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	10	0.13
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	10	0.13
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	10	0.13
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	10	0.13
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	10	0.13
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	10	0.13
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	10	0.13
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	10	0.13
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	10	0.13
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	10	0.13
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	10	0.13
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	10	0.13
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	10	0.13
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	45	0.13
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	45	0.13
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	45	0.13
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	45	0.13
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	45	0.13
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	45	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	24	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	24	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	24	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	24	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	24	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	24	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	24	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	24	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	24	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	24	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	24	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	24	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	24	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	24	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	24	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	24	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	24	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	24	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	32	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	32	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	32	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	32	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	32	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	32	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	32	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	32	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	32	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	32	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	32	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	32	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	32	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	32	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	32	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	32	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	32	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	32	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	41	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	41	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	41	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	41	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	41	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	41	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	41	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	41	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	41	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	41	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	41	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	41	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	41	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	41	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	41	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	41	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	41	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	41	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG11	49	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG12	49	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG13	49	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG21	49	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG22	49	0.13
(1,1435)	1:29:A:MET:HE1	1:32:A:VAL:HG23	49	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG11	49	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG12	49	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG13	49	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG21	49	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG22	49	0.13
(1,1435)	1:29:A:MET:HE2	1:32:A:VAL:HG23	49	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG11	49	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG12	49	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG13	49	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG21	49	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG22	49	0.13
(1,1435)	1:29:A:MET:HE3	1:32:A:VAL:HG23	49	0.13
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	30	0.13
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	30	0.13
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	30	0.13
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	30	0.13
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	35	0.13
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	35	0.13
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	35	0.13
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	35	0.13
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD11	17	0.13
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD12	17	0.13
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD13	17	0.13
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD11	17	0.13
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD12	17	0.13
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD13	17	0.13
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	20	0.13
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	20	0.13
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	20	0.13
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	20	0.13
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	20	0.13
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	20	0.13

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	26	0.13
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	26	0.13
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	26	0.13
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	26	0.13
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	26	0.13
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	26	0.13
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	31	0.13
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	31	0.13
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	31	0.13
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	31	0.13
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	31	0.13
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	31	0.13
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	21	0.13
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	28	0.13
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	28	0.13
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	28	0.13
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	33	0.13
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	33	0.13
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	33	0.13
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	9	0.13
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	9	0.13
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	9	0.13
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	34	0.13
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	37	0.13
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	37	0.13
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	37	0.13
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	45	0.13
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	45	0.13
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	45	0.13
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	46	0.13
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	46	0.13
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	46	0.13
(1,942)	1:33:A:LEU:HG	1:34:A:GLU:H	38	0.13
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	22	0.13
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	22	0.13
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	22	0.13
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	31	0.13
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	37	0.13
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE2	50	0.13
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE3	50	0.13
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE1	34	0.13
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE2	34	0.13

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE1	34	0.13
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE2	34	0.13
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE1	34	0.13
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE2	34	0.13
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	31	0.13
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	31	0.13
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	31	0.13
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	31	0.13
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	31	0.13
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	31	0.13
(1,567)	1:58:A:ILE:HD11	1:59:A:ASN:H	47	0.13
(1,567)	1:58:A:ILE:HD12	1:59:A:ASN:H	47	0.13
(1,567)	1:58:A:ILE:HD13	1:59:A:ASN:H	47	0.13
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	5	0.13
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	5	0.13
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	5	0.13
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	38	0.13
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	38	0.13
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	38	0.13
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	17	0.13
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	17	0.13
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	17	0.13
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	47	0.13
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	47	0.13
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	47	0.13
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG21	17	0.13
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG22	17	0.13
(1,491)	1:51:A:GLU:H	1:52:A:THR:HG23	17	0.13
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	22	0.13
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	22	0.13
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	22	0.13
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	43	0.13
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	43	0.13
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	43	0.13
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	5	0.13
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	5	0.13
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	5	0.13
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	5	0.13
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	5	0.13
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	5	0.13
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	5	0.13
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	5	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	5	0.13
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD11	25	0.13
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD12	25	0.13
(1,456)	1:49:A:LEU:HD11	1:85:A:ILE:HD13	25	0.13
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD11	25	0.13
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD12	25	0.13
(1,456)	1:49:A:LEU:HD12	1:85:A:ILE:HD13	25	0.13
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD11	25	0.13
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD12	25	0.13
(1,456)	1:49:A:LEU:HD13	1:85:A:ILE:HD13	25	0.13
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	36	0.13
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	36	0.13
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	36	0.13
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	46	0.13
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	46	0.13
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	46	0.13
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	25	0.13
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	25	0.13
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	25	0.13
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	25	0.13
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	25	0.13
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	25	0.13
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	25	0.13
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	25	0.13
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	25	0.13
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	27	0.13
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	27	0.13
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	27	0.13
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	27	0.13
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	27	0.13
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	27	0.13
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	27	0.13
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	27	0.13
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	27	0.13
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	20	0.13
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	20	0.13
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	20	0.13
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	20	0.13
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	20	0.13
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	20	0.13
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	20	0.13
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	20	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	20	0.13
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	39	0.13
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	39	0.13
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	39	0.13
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	39	0.13
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	39	0.13
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	39	0.13
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	39	0.13
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	39	0.13
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	39	0.13
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	5	0.13
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	5	0.13
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	5	0.13
(1,414)	1:44:A:ILE:HG21	1:52:A:THR:HB	12	0.13
(1,414)	1:44:A:ILE:HG22	1:52:A:THR:HB	12	0.13
(1,414)	1:44:A:ILE:HG23	1:52:A:THR:HB	12	0.13
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	22	0.13
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	22	0.13
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	22	0.13
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	30	0.13
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	30	0.13
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	30	0.13
(1,410)	1:44:A:ILE:HG21	1:49:A:LEU:HG	50	0.13
(1,410)	1:44:A:ILE:HG22	1:49:A:LEU:HG	50	0.13
(1,410)	1:44:A:ILE:HG23	1:49:A:LEU:HG	50	0.13
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	45	0.13
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	45	0.13
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	45	0.13
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	46	0.13
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	46	0.13
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	46	0.13
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	5	0.13
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	5	0.13
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	5	0.13
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	5	0.13
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	5	0.13
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	5	0.13
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	5	0.13
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	5	0.13
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	5	0.13
(1,370)	1:7:A:ALA:HB1	1:42:A:TYR:HE1	18	0.13
(1,370)	1:7:A:ALA:HB1	1:42:A:TYR:HE2	18	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:7:A:ALA:HB2	1:42:A:TYR:HE1	18	0.13
(1,370)	1:7:A:ALA:HB2	1:42:A:TYR:HE2	18	0.13
(1,370)	1:7:A:ALA:HB3	1:42:A:TYR:HE1	18	0.13
(1,370)	1:7:A:ALA:HB3	1:42:A:TYR:HE2	18	0.13
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	40	0.13
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG21	49	0.13
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG22	49	0.13
(1,259)	1:29:A:MET:HE1	1:32:A:VAL:HG23	49	0.13
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG21	49	0.13
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG22	49	0.13
(1,259)	1:29:A:MET:HE2	1:32:A:VAL:HG23	49	0.13
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG21	49	0.13
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG22	49	0.13
(1,259)	1:29:A:MET:HE3	1:32:A:VAL:HG23	49	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	15	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	15	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	15	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	15	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	15	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	15	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	15	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	15	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	15	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	20	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	20	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	20	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	20	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	20	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	20	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	20	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	20	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	20	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	48	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	48	0.13
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	48	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	48	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	48	0.13
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	48	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	48	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	48	0.13
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	48	0.13
(1,40)	1:12:A:ILE:HD11	1:39:A:LEU:HG	20	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:12:A:ILE:HD12	1:39:A:LEU:HG	20	0.13
(1,40)	1:12:A:ILE:HD13	1:39:A:LEU:HG	20	0.13
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	26	0.12
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	26	0.12
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	26	0.12
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	26	0.12
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	26	0.12
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	26	0.12
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	37	0.12
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	37	0.12
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	37	0.12
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	37	0.12
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	37	0.12
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	37	0.12
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	39	0.12
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	39	0.12
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	39	0.12
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	39	0.12
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	39	0.12
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	39	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	3	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	3	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	3	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	3	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	3	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	3	0.12
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB2	17	0.12
(1,1748)	1:70:A:LEU:HD11	1:73:A:ARG:HB3	17	0.12
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB2	17	0.12
(1,1748)	1:70:A:LEU:HD12	1:73:A:ARG:HB3	17	0.12
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB2	17	0.12
(1,1748)	1:70:A:LEU:HD13	1:73:A:ARG:HB3	17	0.12
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB2	17	0.12
(1,1748)	1:70:A:LEU:HD21	1:73:A:ARG:HB3	17	0.12
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB2	17	0.12
(1,1748)	1:70:A:LEU:HD22	1:73:A:ARG:HB3	17	0.12
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB2	17	0.12
(1,1748)	1:70:A:LEU:HD23	1:73:A:ARG:HB3	17	0.12
(1,1737)	1:68:A:GLU:HG2	1:69:A:GLU:H	8	0.12
(1,1737)	1:68:A:GLU:HG3	1:69:A:GLU:H	8	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	21	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	21	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	21	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	21	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	21	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	21	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	31	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	31	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	31	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	31	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	31	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	31	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	36	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	36	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	36	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	36	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	36	0.12
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	36	0.12
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG21	7	0.12
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG22	7	0.12
(1,1576)	1:46:A:LYS:HB2	1:85:A:ILE:HG23	7	0.12
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG21	7	0.12
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG22	7	0.12
(1,1576)	1:46:A:LYS:HB3	1:85:A:ILE:HG23	7	0.12
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	3	0.12
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	3	0.12
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	3	0.12
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	3	0.12
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	3	0.12
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	3	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	18	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	18	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	18	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	18	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	18	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	18	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	19	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	19	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	19	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	19	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	19	0.12
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	19	0.12
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	3	0.12
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	3	0.12

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	3	0.12
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	3	0.12
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	3	0.12
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	3	0.12
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	31	0.12
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	31	0.12
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	31	0.12
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	31	0.12
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	31	0.12
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	31	0.12
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	36	0.12
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	36	0.12
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	36	0.12
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	36	0.12
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	36	0.12
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	36	0.12
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD11	49	0.12
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD12	49	0.12
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD13	49	0.12
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD21	49	0.12
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD22	49	0.12
(1,1451)	1:32:A:VAL:HB	1:33:A:LEU:HD23	49	0.12
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	15	0.12
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	15	0.12
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	15	0.12
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	15	0.12
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	34	0.12
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	34	0.12
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	34	0.12
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	34	0.12
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	40	0.12
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	40	0.12
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	40	0.12
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	40	0.12
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD11	36	0.12
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD12	36	0.12
(1,1387)	1:20:A:ILE:HG12	1:26:A:ILE:HD13	36	0.12
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD11	36	0.12
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD12	36	0.12
(1,1387)	1:20:A:ILE:HG13	1:26:A:ILE:HD13	36	0.12
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	36	0.12
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	36	0.12

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	36	0.12
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	36	0.12
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	36	0.12
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	36	0.12
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	33	0.12
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	33	0.12
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	33	0.12
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	33	0.12
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	33	0.12
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	33	0.12
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	45	0.12
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	45	0.12
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	45	0.12
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	45	0.12
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	45	0.12
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	45	0.12
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD11	46	0.12
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD12	46	0.12
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD13	46	0.12
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD21	46	0.12
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD22	46	0.12
(1,1309)	1:13:A:ARG:HD2	1:57:A:LEU:HD23	46	0.12
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD11	46	0.12
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD12	46	0.12
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD13	46	0.12
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD21	46	0.12
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD22	46	0.12
(1,1309)	1:13:A:ARG:HD3	1:57:A:LEU:HD23	46	0.12
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	18	0.12
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	27	0.12
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	46	0.12
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	46	0.12
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	46	0.12
(1,1067)	1:49:A:LEU:HD11	1:54:A:LEU:H	8	0.12
(1,1067)	1:49:A:LEU:HD12	1:54:A:LEU:H	8	0.12
(1,1067)	1:49:A:LEU:HD13	1:54:A:LEU:H	8	0.12
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	36	0.12
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	49	0.12
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	49	0.12
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	49	0.12
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	33	0.12
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	36	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	42	0.12
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	50	0.12
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE1	48	0.12
(1,773)	1:5:A:ALA:HB1	1:42:A:TYR:HE2	48	0.12
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE1	48	0.12
(1,773)	1:5:A:ALA:HB2	1:42:A:TYR:HE2	48	0.12
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE1	48	0.12
(1,773)	1:5:A:ALA:HB3	1:42:A:TYR:HE2	48	0.12
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD11	23	0.12
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD12	23	0.12
(1,749)	1:49:A:LEU:HD11	1:84:A:LEU:HD13	23	0.12
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD11	23	0.12
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD12	23	0.12
(1,749)	1:49:A:LEU:HD12	1:84:A:LEU:HD13	23	0.12
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD11	23	0.12
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD12	23	0.12
(1,749)	1:49:A:LEU:HD13	1:84:A:LEU:HD13	23	0.12
(1,740)	1:81:A:TRP:HD1	1:84:A:LEU:HG	25	0.12
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE2	3	0.12
(1,663)	1:71:A:ALA:HB1	1:72:A:LYS:HE3	3	0.12
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE2	3	0.12
(1,663)	1:71:A:ALA:HB2	1:72:A:LYS:HE3	3	0.12
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE2	3	0.12
(1,663)	1:71:A:ALA:HB3	1:72:A:LYS:HE3	3	0.12
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD21	38	0.12
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD22	38	0.12
(1,655)	1:81:A:TRP:HD1	1:84:A:LEU:HD23	38	0.12
(1,567)	1:58:A:ILE:HD11	1:59:A:ASN:H	19	0.12
(1,567)	1:58:A:ILE:HD12	1:59:A:ASN:H	19	0.12
(1,567)	1:58:A:ILE:HD13	1:59:A:ASN:H	19	0.12
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	1	0.12
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	1	0.12
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	1	0.12
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	21	0.12
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	21	0.12
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	21	0.12
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	37	0.12
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	37	0.12
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	37	0.12
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	41	0.12
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	41	0.12
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	41	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	44	0.12
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	44	0.12
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	44	0.12
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	26	0.12
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	26	0.12
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	26	0.12
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	38	0.12
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	38	0.12
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	38	0.12
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD21	31	0.12
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD22	31	0.12
(1,477)	1:49:A:LEU:H	1:49:A:LEU:HD23	31	0.12
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	34	0.12
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	34	0.12
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	34	0.12
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	17	0.12
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	17	0.12
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	17	0.12
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	7	0.12
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	7	0.12
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	7	0.12
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	7	0.12
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	7	0.12
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	7	0.12
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	7	0.12
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	7	0.12
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	7	0.12
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	50	0.12
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	50	0.12
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	50	0.12
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	50	0.12
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	50	0.12
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	50	0.12
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	50	0.12
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	50	0.12
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	50	0.12
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	26	0.12
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	26	0.12
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	26	0.12
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	26	0.12
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	26	0.12
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	26	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	26	0.12
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	26	0.12
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	26	0.12
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	40	0.12
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	40	0.12
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	40	0.12
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	40	0.12
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	40	0.12
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	40	0.12
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	40	0.12
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	40	0.12
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	40	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	10	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	10	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	10	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	10	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	10	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	10	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	10	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	10	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	10	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	15	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	15	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	15	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	15	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	15	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	15	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	15	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	15	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	15	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	21	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	21	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	21	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	21	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	21	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	21	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	21	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	21	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	21	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	47	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	47	0.12
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	47	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	47	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	47	0.12
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	47	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	47	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	47	0.12
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	47	0.12
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	28	0.12
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	28	0.12
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	28	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	8	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	8	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	8	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	35	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	35	0.12
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	35	0.12
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	2	0.12
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	2	0.12
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	2	0.12
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	12	0.12
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	12	0.12
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	12	0.12
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	1	0.12
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	1	0.12
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	1	0.12
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	1	0.12
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	1	0.12
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	1	0.12
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	1	0.12
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	1	0.12
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	1	0.12
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD1	30	0.12
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD2	30	0.12
(1,359)	1:39:A:LEU:HA	1:42:A:TYR:HB3	32	0.12
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE1	33	0.12
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE2	33	0.12
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE3	33	0.12
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	38	0.12
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	38	0.12
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	38	0.12
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	38	0.12
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	38	0.12
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	38	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	38	0.12
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	38	0.12
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	38	0.12
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	39	0.12
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	39	0.12
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	39	0.12
(1,40)	1:12:A:ILE:HD11	1:39:A:LEU:HG	42	0.12
(1,40)	1:12:A:ILE:HD12	1:39:A:LEU:HG	42	0.12
(1,40)	1:12:A:ILE:HD13	1:39:A:LEU:HG	42	0.12
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	4	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	4	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	4	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	4	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	4	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	4	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	38	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	38	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	38	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	38	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	38	0.11
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	38	0.11
(1,1737)	1:68:A:GLU:HG2	1:69:A:GLU:H	7	0.11
(1,1737)	1:68:A:GLU:HG3	1:69:A:GLU:H	7	0.11
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG11	26	0.11
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG12	26	0.11
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG13	26	0.11
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG21	26	0.11
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG22	26	0.11
(1,1657)	1:57:A:LEU:HA	1:61:A:VAL:HG23	26	0.11
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	26	0.11
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	26	0.11
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	26	0.11
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	26	0.11
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	26	0.11
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	26	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	14	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	14	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	14	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	14	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	14	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	14	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	14	0.11

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	14	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	14	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	14	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	14	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	14	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	14	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	14	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	14	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	14	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	14	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	14	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD11	49	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD12	49	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD13	49	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	49	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	49	0.11
(1,1582)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	49	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD11	49	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD12	49	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD13	49	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	49	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	49	0.11
(1,1582)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	49	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD11	49	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD12	49	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD13	49	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	49	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	49	0.11
(1,1582)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	49	0.11
(1,1562)	1:44:A:ILE:HG21	1:84:A:LEU:HB2	3	0.11
(1,1562)	1:44:A:ILE:HG21	1:84:A:LEU:HB3	3	0.11
(1,1562)	1:44:A:ILE:HG22	1:84:A:LEU:HB2	3	0.11
(1,1562)	1:44:A:ILE:HG22	1:84:A:LEU:HB3	3	0.11
(1,1562)	1:44:A:ILE:HG23	1:84:A:LEU:HB2	3	0.11
(1,1562)	1:44:A:ILE:HG23	1:84:A:LEU:HB3	3	0.11
(1,1562)	1:44:A:ILE:HG21	1:84:A:LEU:HB2	38	0.11
(1,1562)	1:44:A:ILE:HG21	1:84:A:LEU:HB3	38	0.11
(1,1562)	1:44:A:ILE:HG22	1:84:A:LEU:HB2	38	0.11
(1,1562)	1:44:A:ILE:HG22	1:84:A:LEU:HB3	38	0.11
(1,1562)	1:44:A:ILE:HG23	1:84:A:LEU:HB2	38	0.11
(1,1562)	1:44:A:ILE:HG23	1:84:A:LEU:HB3	38	0.11
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	10	0.11

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	10	0.11
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	10	0.11
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	10	0.11
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	10	0.11
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	10	0.11
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	32	0.11
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	32	0.11
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	32	0.11
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	32	0.11
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	32	0.11
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	32	0.11
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	40	0.11
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	40	0.11
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	40	0.11
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	40	0.11
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	40	0.11
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	40	0.11
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG12	42	0.11
(1,1498)	1:36:A:ILE:HG21	1:58:A:ILE:HG13	42	0.11
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG12	42	0.11
(1,1498)	1:36:A:ILE:HG22	1:58:A:ILE:HG13	42	0.11
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG12	42	0.11
(1,1498)	1:36:A:ILE:HG23	1:58:A:ILE:HG13	42	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	20	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	20	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	20	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	20	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	21	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	21	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	21	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	21	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	26	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	26	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	26	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	26	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	31	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	31	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	31	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	31	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	33	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	33	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	33	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	33	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	38	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	38	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	38	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	38	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	45	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	45	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	45	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	45	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	49	0.11
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	49	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	49	0.11
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	49	0.11
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	5	0.11
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	5	0.11
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	5	0.11
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	5	0.11
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	5	0.11
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	5	0.11
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	14	0.11
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	14	0.11
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	14	0.11
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	14	0.11
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	14	0.11
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	14	0.11
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	30	0.11
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	30	0.11
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	30	0.11
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	30	0.11
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	30	0.11
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	30	0.11
(1,1345)	1:16:A:LEU:HD11	1:33:A:LEU:H	35	0.11
(1,1345)	1:16:A:LEU:HD12	1:33:A:LEU:H	35	0.11
(1,1345)	1:16:A:LEU:HD13	1:33:A:LEU:H	35	0.11
(1,1345)	1:16:A:LEU:HD21	1:33:A:LEU:H	35	0.11
(1,1345)	1:16:A:LEU:HD22	1:33:A:LEU:H	35	0.11
(1,1345)	1:16:A:LEU:HD23	1:33:A:LEU:H	35	0.11
(1,1340)	1:16:A:LEU:HD11	1:20:A:ILE:H	37	0.11
(1,1340)	1:16:A:LEU:HD12	1:20:A:ILE:H	37	0.11
(1,1340)	1:16:A:LEU:HD13	1:20:A:ILE:H	37	0.11
(1,1340)	1:16:A:LEU:HD21	1:20:A:ILE:H	37	0.11
(1,1340)	1:16:A:LEU:HD22	1:20:A:ILE:H	37	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:16:A:LEU:HD23	1:20:A:ILE:H	37	0.11
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	1	0.11
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	24	0.11
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	37	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	29	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	29	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	29	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	37	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	37	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	37	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	38	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	38	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	38	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG21	43	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG22	43	0.11
(1,1111)	1:62:A:ARG:H	1:65:A:THR:HG23	43	0.11
(1,1069)	1:55:A:GLY:H	1:56:A:LYS:HB2	41	0.11
(1,1069)	1:55:A:GLY:H	1:56:A:LYS:HB3	41	0.11
(1,1016)	1:46:A:LYS:H	1:84:A:LEU:HG	5	0.11
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	32	0.11
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	32	0.11
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	32	0.11
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	48	0.11
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	48	0.11
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	48	0.11
(1,973)	1:39:A:LEU:H	1:39:A:LEU:HG	44	0.11
(1,934)	1:29:A:MET:HE1	1:33:A:LEU:H	11	0.11
(1,934)	1:29:A:MET:HE2	1:33:A:LEU:H	11	0.11
(1,934)	1:29:A:MET:HE3	1:33:A:LEU:H	11	0.11
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	38	0.11
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	48	0.11
(1,873)	1:16:A:LEU:HA	1:20:A:ILE:H	49	0.11
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD11	8	0.11
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD12	8	0.11
(1,750)	1:46:A:LYS:HA	1:84:A:LEU:HD13	8	0.11
(1,639)	1:66:A:LYS:HA	1:66:A:LYS:HD2	50	0.11
(1,639)	1:66:A:LYS:HA	1:66:A:LYS:HD3	50	0.11
(1,567)	1:58:A:ILE:HD11	1:59:A:ASN:H	32	0.11
(1,567)	1:58:A:ILE:HD12	1:59:A:ASN:H	32	0.11
(1,567)	1:58:A:ILE:HD13	1:59:A:ASN:H	32	0.11
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	6	0.11
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	6	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	6	0.11
(1,565)	1:58:A:ILE:HD11	1:81:A:TRP:HE3	7	0.11
(1,565)	1:58:A:ILE:HD12	1:81:A:TRP:HE3	7	0.11
(1,565)	1:58:A:ILE:HD13	1:81:A:TRP:HE3	7	0.11
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	19	0.11
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	19	0.11
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	19	0.11
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	43	0.11
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	43	0.11
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	43	0.11
(1,542)	1:57:A:LEU:HD21	1:58:A:ILE:H	50	0.11
(1,542)	1:57:A:LEU:HD22	1:58:A:ILE:H	50	0.11
(1,542)	1:57:A:LEU:HD23	1:58:A:ILE:H	50	0.11
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD21	41	0.11
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD22	41	0.11
(1,528)	1:13:A:ARG:H	1:54:A:LEU:HD23	41	0.11
(1,484)	1:48:A:ALA:HA	1:52:A:THR:HG21	49	0.11
(1,484)	1:48:A:ALA:HA	1:52:A:THR:HG22	49	0.11
(1,484)	1:48:A:ALA:HA	1:52:A:THR:HG23	49	0.11
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	8	0.11
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	8	0.11
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	8	0.11
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD21	33	0.11
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD22	33	0.11
(1,455)	1:49:A:LEU:HD11	1:84:A:LEU:HD23	33	0.11
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD21	33	0.11
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD22	33	0.11
(1,455)	1:49:A:LEU:HD12	1:84:A:LEU:HD23	33	0.11
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD21	33	0.11
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD22	33	0.11
(1,455)	1:49:A:LEU:HD13	1:84:A:LEU:HD23	33	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	1	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	1	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	1	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	1	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	1	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	1	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	1	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	1	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	1	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	17	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	17	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	17	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	17	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	17	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	17	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	17	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	17	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	17	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	18	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	18	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	18	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	18	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	18	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	18	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	18	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	18	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	18	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	33	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	33	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	33	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	33	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	33	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	33	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	33	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	33	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	33	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD21	41	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD22	41	0.11
(1,438)	1:48:A:ALA:HB1	1:49:A:LEU:HD23	41	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD21	41	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD22	41	0.11
(1,438)	1:48:A:ALA:HB2	1:49:A:LEU:HD23	41	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD21	41	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD22	41	0.11
(1,438)	1:48:A:ALA:HB3	1:49:A:LEU:HD23	41	0.11
(1,428)	1:45:A:THR:HG21	1:47:A:GLU:H	46	0.11
(1,428)	1:45:A:THR:HG22	1:47:A:GLU:H	46	0.11
(1,428)	1:45:A:THR:HG23	1:47:A:GLU:H	46	0.11
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	1	0.11
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	1	0.11
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	1	0.11
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	1	0.11
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	1	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	1	0.11
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	1	0.11
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	1	0.11
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	1	0.11
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG21	20	0.11
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG22	20	0.11
(1,423)	1:44:A:ILE:HG21	1:45:A:THR:HG23	20	0.11
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG21	20	0.11
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG22	20	0.11
(1,423)	1:44:A:ILE:HG22	1:45:A:THR:HG23	20	0.11
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG21	20	0.11
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG22	20	0.11
(1,423)	1:44:A:ILE:HG23	1:45:A:THR:HG23	20	0.11
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG21	29	0.11
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG22	29	0.11
(1,413)	1:9:A:PRO:HA	1:44:A:ILE:HG23	29	0.11
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	36	0.11
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	36	0.11
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	36	0.11
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	50	0.11
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	50	0.11
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	50	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	6	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	6	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	6	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	6	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	6	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	6	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	6	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	6	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	6	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	27	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	27	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	27	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	27	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	27	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	27	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	27	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	27	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	27	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD21	40	0.11
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD22	40	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:44:A:ILE:HD11	1:49:A:LEU:HD23	40	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD21	40	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD22	40	0.11
(1,387)	1:44:A:ILE:HD12	1:49:A:LEU:HD23	40	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD21	40	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD22	40	0.11
(1,387)	1:44:A:ILE:HD13	1:49:A:LEU:HD23	40	0.11
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD1	18	0.11
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD2	18	0.11
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD1	44	0.11
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD2	44	0.11
(1,335)	1:36:A:ILE:HG21	1:77:A:LEU:H	26	0.11
(1,335)	1:36:A:ILE:HG22	1:77:A:LEU:H	26	0.11
(1,335)	1:36:A:ILE:HG23	1:77:A:LEU:H	26	0.11
(1,327)	1:36:A:ILE:HG21	1:40:A:GLU:HG2	31	0.11
(1,327)	1:36:A:ILE:HG22	1:40:A:GLU:HG2	31	0.11
(1,327)	1:36:A:ILE:HG23	1:40:A:GLU:HG2	31	0.11
(1,252)	1:32:A:VAL:H	1:32:A:VAL:HG11	41	0.11
(1,252)	1:32:A:VAL:H	1:32:A:VAL:HG12	41	0.11
(1,252)	1:32:A:VAL:H	1:32:A:VAL:HG13	41	0.11
(1,192)	1:26:A:ILE:HD11	1:32:A:VAL:H	25	0.11
(1,192)	1:26:A:ILE:HD12	1:32:A:VAL:H	25	0.11
(1,192)	1:26:A:ILE:HD13	1:32:A:VAL:H	25	0.11
(1,154)	1:20:A:ILE:HG21	1:29:A:MET:HA	18	0.11
(1,154)	1:20:A:ILE:HG22	1:29:A:MET:HA	18	0.11
(1,154)	1:20:A:ILE:HG23	1:29:A:MET:HA	18	0.11
(1,48)	1:12:A:ILE:HG21	1:39:A:LEU:HG	45	0.11
(1,48)	1:12:A:ILE:HG22	1:39:A:LEU:HG	45	0.11
(1,48)	1:12:A:ILE:HG23	1:39:A:LEU:HG	45	0.11
(1,40)	1:12:A:ILE:HD11	1:39:A:LEU:HG	32	0.11
(1,40)	1:12:A:ILE:HD12	1:39:A:LEU:HG	32	0.11
(1,40)	1:12:A:ILE:HD13	1:39:A:LEU:HG	32	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD11	28	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD12	28	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD13	28	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD11	30	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD12	30	0.11
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD13	30	0.11
(1,1790)	1:77:A:LEU:HD11	1:78:A:LEU:H	16	0.1
(1,1790)	1:77:A:LEU:HD12	1:78:A:LEU:H	16	0.1
(1,1790)	1:77:A:LEU:HD13	1:78:A:LEU:H	16	0.1
(1,1790)	1:77:A:LEU:HD21	1:78:A:LEU:H	16	0.1

*Continued on next page...*



*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1790)	1:77:A:LEU:HD22	1:78:A:LEU:H	16	0.1
(1,1790)	1:77:A:LEU:HD23	1:78:A:LEU:H	16	0.1
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD11	19	0.1
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD12	19	0.1
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD13	19	0.1
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD21	19	0.1
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD22	19	0.1
(1,1763)	1:73:A:ARG:HA	1:77:A:LEU:HD23	19	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	3	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	3	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	3	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	3	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	3	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	3	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD11	46	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD12	46	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD13	46	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD21	46	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD22	46	0.1
(1,1625)	1:53:A:ARG:HA	1:54:A:LEU:HD23	46	0.1
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	2	0.1
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	2	0.1
(1,1588)	1:49:A:LEU:HB2	1:53:A:ARG:H	12	0.1
(1,1588)	1:49:A:LEU:HB3	1:53:A:ARG:H	12	0.1
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD11	8	0.1
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD12	8	0.1
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD13	8	0.1
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD21	8	0.1
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD22	8	0.1
(1,1557)	1:44:A:ILE:HB	1:49:A:LEU:HD23	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	8	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	37	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	37	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	37	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	37	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	37	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	37	0.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD11	42	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD12	42	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD13	42	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD21	42	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD22	42	0.1
(1,1555)	1:44:A:ILE:H	1:54:A:LEU:HD23	42	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	4	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	4	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	4	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	4	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	14	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	14	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	14	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	14	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	36	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	36	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	36	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	36	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD2	41	0.1
(1,1394)	1:21:A:ASP:HB2	1:22:A:PRO:HD3	41	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD2	41	0.1
(1,1394)	1:21:A:ASP:HB3	1:22:A:PRO:HD3	41	0.1
(1,1242)	1:84:A:LEU:H	1:84:A:LEU:HG	40	0.1
(1,1233)	1:82:A:GLN:H	1:82:A:GLN:HG2	38	0.1
(1,993)	1:36:A:ILE:HD11	1:40:A:GLU:H	18	0.1
(1,993)	1:36:A:ILE:HD12	1:40:A:GLU:H	18	0.1
(1,993)	1:36:A:ILE:HD13	1:40:A:GLU:H	18	0.1
(1,838)	1:15:A:ARG:H	1:35:A:VAL:HG11	45	0.1
(1,838)	1:15:A:ARG:H	1:35:A:VAL:HG12	45	0.1
(1,838)	1:15:A:ARG:H	1:35:A:VAL:HG13	45	0.1
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE2	33	0.1
(1,775)	1:64:A:LYS:H	1:64:A:LYS:HE3	33	0.1
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG21	33	0.1
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG22	33	0.1
(1,764)	1:46:A:LYS:HE2	1:85:A:ILE:HG23	33	0.1
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG21	33	0.1
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG22	33	0.1
(1,764)	1:46:A:LYS:HE3	1:85:A:ILE:HG23	33	0.1
(1,701)	1:74:A:ALA:HA	1:77:A:LEU:HB3	26	0.1
(1,674)	1:73:A:ARG:H	1:73:A:ARG:HD3	21	0.1
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG21	34	0.1
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG22	34	0.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:63:A:LYS:HA	1:65:A:THR:HG23	34	0.1
(1,567)	1:58:A:ILE:HD11	1:59:A:ASN:H	37	0.1
(1,567)	1:58:A:ILE:HD12	1:59:A:ASN:H	37	0.1
(1,567)	1:58:A:ILE:HD13	1:59:A:ASN:H	37	0.1
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD2	18	0.1
(1,495)	1:53:A:ARG:HA	1:53:A:ARG:HD3	18	0.1
(1,469)	1:49:A:LEU:HD21	1:54:A:LEU:HB2	36	0.1
(1,469)	1:49:A:LEU:HD22	1:54:A:LEU:HB2	36	0.1
(1,469)	1:49:A:LEU:HD23	1:54:A:LEU:HB2	36	0.1
(1,463)	1:49:A:LEU:HD11	1:55:A:GLY:H	13	0.1
(1,463)	1:49:A:LEU:HD12	1:55:A:GLY:H	13	0.1
(1,463)	1:49:A:LEU:HD13	1:55:A:GLY:H	13	0.1
(1,454)	1:49:A:LEU:HG	1:55:A:GLY:HA3	26	0.1
(1,454)	1:49:A:LEU:HG	1:55:A:GLY:HA3	28	0.1
(1,454)	1:49:A:LEU:HG	1:55:A:GLY:HA3	34	0.1
(1,451)	1:44:A:ILE:HD11	1:49:A:LEU:HG	15	0.1
(1,451)	1:44:A:ILE:HD12	1:49:A:LEU:HG	15	0.1
(1,451)	1:44:A:ILE:HD13	1:49:A:LEU:HG	15	0.1
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB1	18	0.1
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB2	18	0.1
(1,435)	1:44:A:ILE:HG21	1:48:A:ALA:HB3	18	0.1
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB1	18	0.1
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB2	18	0.1
(1,435)	1:44:A:ILE:HG22	1:48:A:ALA:HB3	18	0.1
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB1	18	0.1
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB2	18	0.1
(1,435)	1:44:A:ILE:HG23	1:48:A:ALA:HB3	18	0.1
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	19	0.1
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	19	0.1
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	19	0.1
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD11	20	0.1
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD12	20	0.1
(1,404)	1:44:A:ILE:H	1:44:A:ILE:HD13	20	0.1
(1,402)	1:44:A:ILE:HD11	1:45:A:THR:H	13	0.1
(1,402)	1:44:A:ILE:HD12	1:45:A:THR:H	13	0.1
(1,402)	1:44:A:ILE:HD13	1:45:A:THR:H	13	0.1
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD1	31	0.1
(1,360)	1:38:A:SER:H	1:42:A:TYR:HD2	31	0.1
(1,240)	1:28:A:ASN:HB2	1:31:A:ALA:HB1	37	0.1
(1,240)	1:28:A:ASN:HB2	1:31:A:ALA:HB2	37	0.1
(1,240)	1:28:A:ASN:HB2	1:31:A:ALA:HB3	37	0.1
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE1	40	0.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE2	40	0.1
(1,227)	1:26:A:ILE:HA	1:29:A:MET:HE3	40	0.1
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD21	14	0.1
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD22	14	0.1
(1,224)	1:29:A:MET:HE1	1:70:A:LEU:HD23	14	0.1
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD21	14	0.1
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD22	14	0.1
(1,224)	1:29:A:MET:HE2	1:70:A:LEU:HD23	14	0.1
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD21	14	0.1
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD22	14	0.1
(1,224)	1:29:A:MET:HE3	1:70:A:LEU:HD23	14	0.1
(1,222)	1:29:A:MET:HE1	1:32:A:VAL:HG11	41	0.1
(1,222)	1:29:A:MET:HE1	1:32:A:VAL:HG12	41	0.1
(1,222)	1:29:A:MET:HE1	1:32:A:VAL:HG13	41	0.1
(1,222)	1:29:A:MET:HE2	1:32:A:VAL:HG11	41	0.1
(1,222)	1:29:A:MET:HE2	1:32:A:VAL:HG12	41	0.1
(1,222)	1:29:A:MET:HE2	1:32:A:VAL:HG13	41	0.1
(1,222)	1:29:A:MET:HE3	1:32:A:VAL:HG11	41	0.1
(1,222)	1:29:A:MET:HE3	1:32:A:VAL:HG12	41	0.1
(1,222)	1:29:A:MET:HE3	1:32:A:VAL:HG13	41	0.1
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD11	15	0.1
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD12	15	0.1
(1,23)	1:9:A:PRO:HG2	1:12:A:ILE:HD13	15	0.1

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

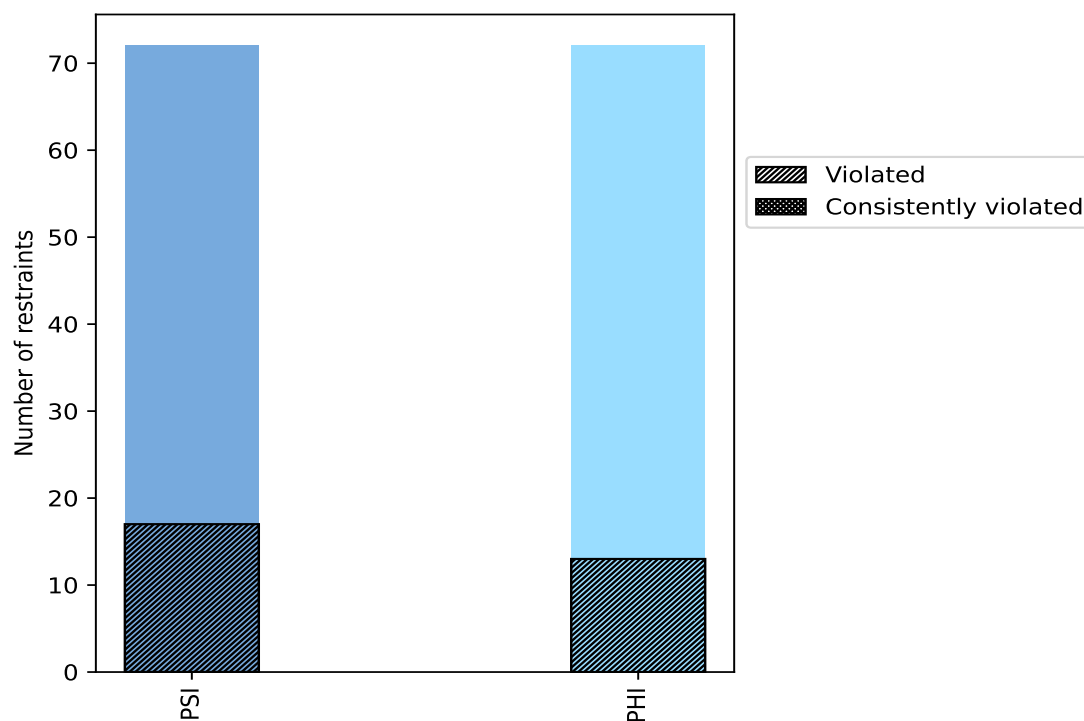
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	72	50.0	17	23.6	11.8	0	0.0	0.0
PHI	72	50.0	13	18.1	9.0	0	0.0	0.0
Total	144	100.0	30	20.8	20.8	0	0.0	0.0

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

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



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

## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

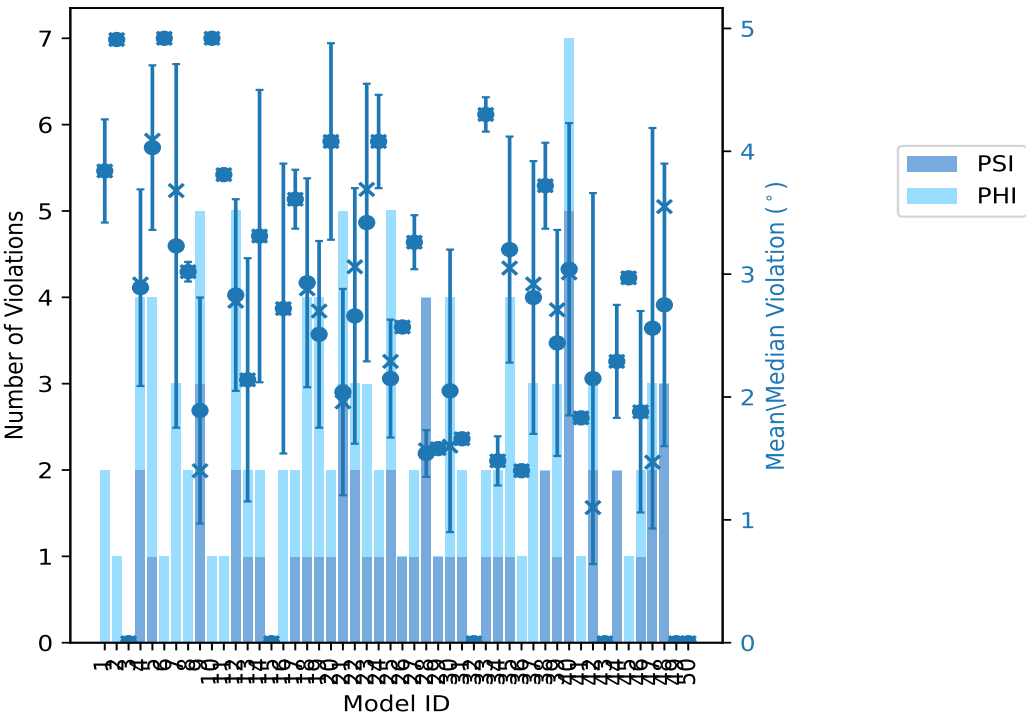
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	2	2	3.84	4.27	0.42	3.84
2	0	1	1	4.91	4.91	0.0	4.91
3	0	0	0	0.0	0.0	0.0	0.0
4	2	2	4	2.89	3.81	0.8	2.92
5	1	3	4	4.03	4.78	0.67	4.09
6	0	1	1	4.92	4.92	0.0	4.92
7	0	3	3	3.23	4.78	1.48	3.68
8	0	2	2	3.02	3.1	0.08	3.02
9	3	2	5	1.89	3.63	0.92	1.4
10	0	1	1	4.92	4.92	0.0	4.92
11	0	1	1	3.81	3.81	0.0	3.81
12	2	3	5	2.83	3.85	0.78	2.78
13	1	1	2	2.14	3.13	0.99	2.14
14	1	1	2	3.31	4.5	1.19	3.31
15	0	0	0	0.0	0.0	0.0	0.0
16	0	2	2	2.72	3.9	1.18	2.72
17	1	1	2	3.61	3.85	0.24	3.61
18	1	3	4	2.93	4.13	0.85	2.88
19	1	3	4	2.51	3.33	0.76	2.7
20	1	1	2	4.08	4.89	0.8	4.08
21	3	2	5	2.04	3.29	0.84	1.96
22	2	1	3	2.66	3.68	1.04	3.06
23	1	2	3	3.42	4.66	1.13	3.69
24	1	1	2	4.08	4.47	0.38	4.08
25	2	3	5	2.15	2.66	0.48	2.29
26	1	0	1	2.57	2.57	0.0	2.57
27	1	1	2	3.26	3.48	0.22	3.26
28	4	0	4	1.54	1.78	0.19	1.57
29	1	0	1	1.58	1.58	0.0	1.58
30	1	3	4	2.05	4.0	1.15	1.6
31	1	1	2	1.66	1.7	0.04	1.66
32	0	0	0	0.0	0.0	0.0	0.0
33	1	1	2	4.3	4.44	0.14	4.3
34	1	1	2	1.48	1.68	0.2	1.48
35	1	3	4	3.2	4.44	0.92	3.05
36	0	1	1	1.4	1.4	0.0	1.4
37	0	3	3	2.81	4.12	1.11	2.92
38	2	0	2	3.72	4.07	0.35	3.72

*Continued on next page...*

Continued from previous page...

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	1	2	3	2.44	3.41	0.92	2.71
40	5	2	7	3.04	4.84	1.19	3.01
41	0	1	1	1.83	1.83	0.0	1.83
42	2	1	3	2.15	4.28	1.51	1.1
43	0	0	0	0.0	0.0	0.0	0.0
44	2	0	2	2.29	2.75	0.46	2.29
45	0	1	1	2.97	2.97	0.0	2.97
46	1	1	2	1.88	2.69	0.82	1.88
47	2	1	3	2.56	4.86	1.63	1.47
48	3	0	3	2.75	3.57	1.15	3.55
49	0	0	0	0.0	0.0	0.0	0.0
50	0	0	0	0.0	0.0	0.0	0.0

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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



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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
4	4	8	1	2.0
9	3	12	2	4.0
0	2	2	3	6.0
1	0	1	4	8.0
1	1	2	5	10.0
0	0	0	6	12.0
0	1	1	7	14.0
0	0	0	8	16.0
0	0	0	9	18.0
1	0	1	10	20.0
0	0	0	11	22.0
1	0	1	12	24.0
0	0	0	13	26.0
0	0	0	14	28.0
0	0	0	15	30.0
0	1	1	16	32.0
0	0	0	17	34.0
0	0	0	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	1	1	21	42.0
0	0	0	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	0	0	25	50.0
0	0	0	26	52.0
0	0	0	27	54.0
0	0	0	28	56.0
0	0	0	29	58.0
0	0	0	30	60.0
0	0	0	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
0	0	0	34	68.0
0	0	0	35	70.0
0	0	0	36	72.0
0	0	0	37	74.0

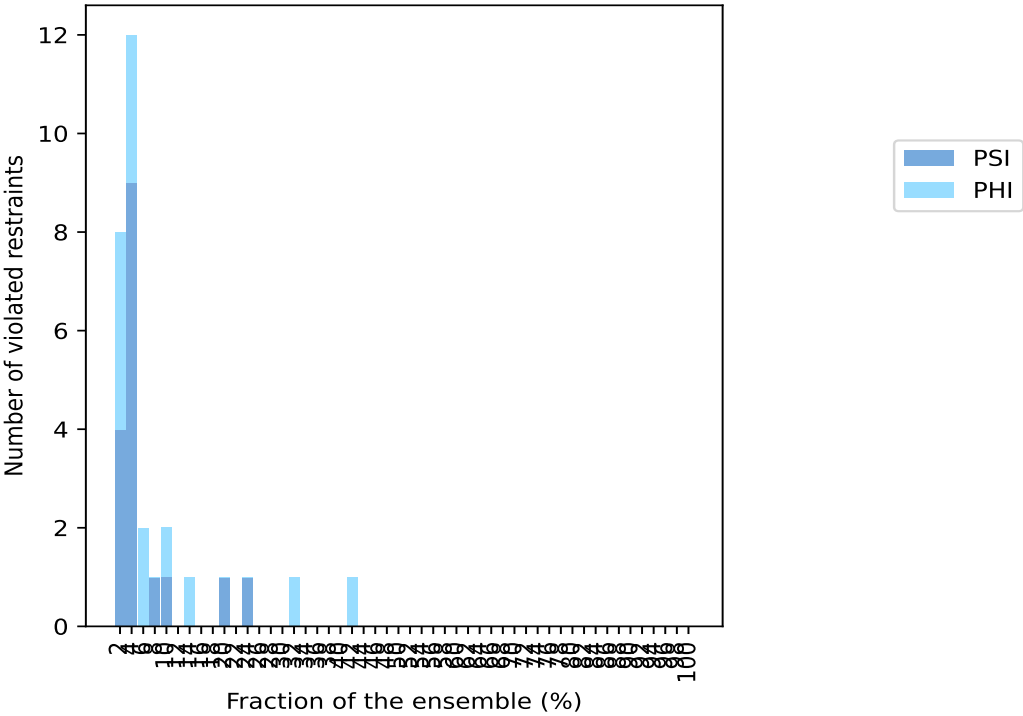
*Continued on next page...*

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
0	0	0	38	76.0
0	0	0	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
0	0	0	50	100.0

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

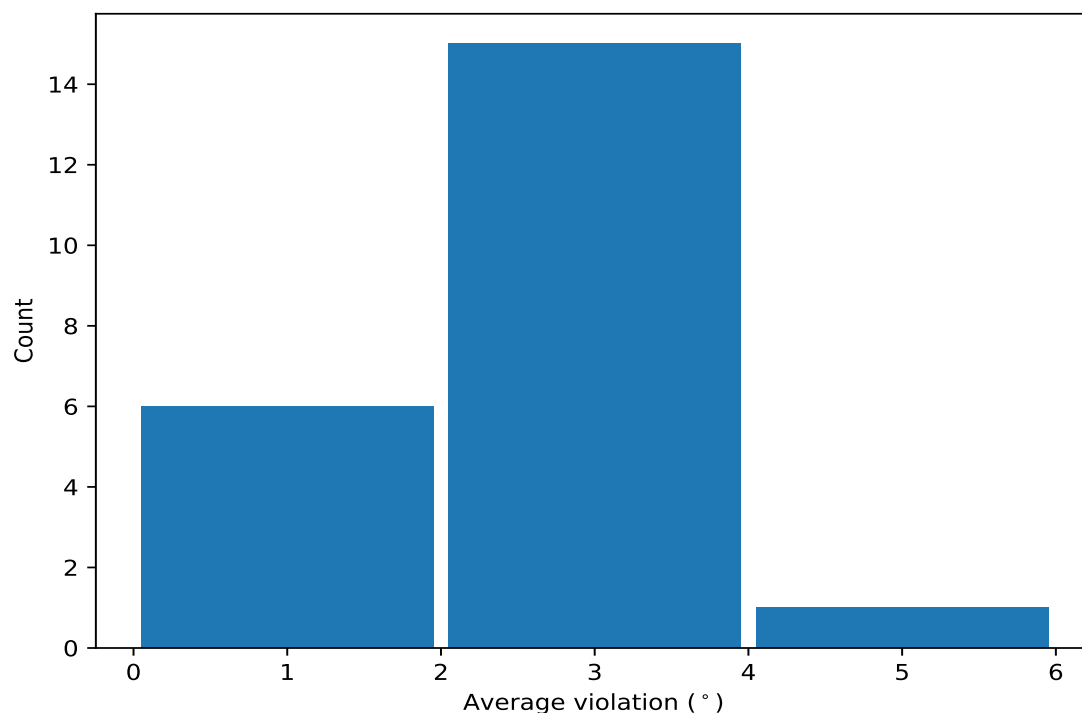
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	21	3.06	1.3	3.13
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	16	3.74	0.64	3.66
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	12	2.75	1.01	2.88
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	10	2.59	1.15	2.82
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	7	3.0	0.93	2.65
(1,7)	1:10:A:GLN:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	5	2.11	0.52	1.75
(1,144)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:GLU:N	5	1.89	0.64	1.7
(1,16)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LEU:N	4	2.22	0.84	2.12
(1,71)	1:47:A:GLU:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	3	3.37	1.68	4.44
(1,139)	1:82:A:GLN:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	3	2.43	0.92	1.83
(1,66)	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	1:46:A:LYS:N	2	4.26	0.57	4.26
(1,82)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:LEU:N	2	2.96	0.19	2.96
(1,103)	1:63:A:LYS:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	2	2.85	0.48	2.85

Continued on next page...

Continued from previous page...

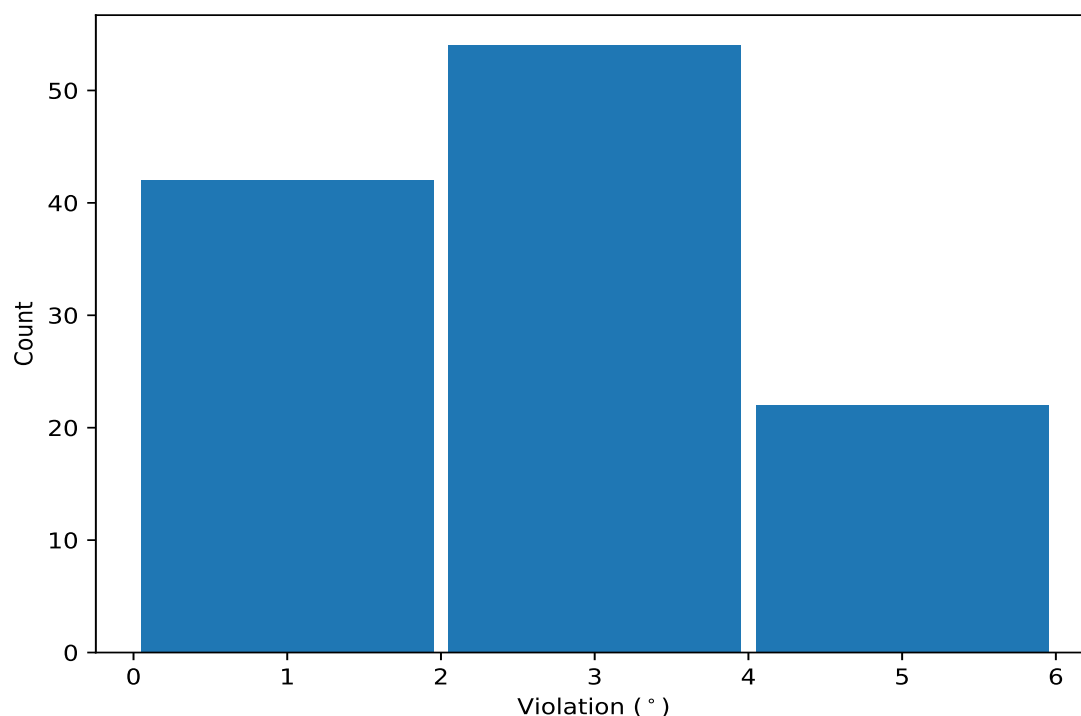
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,124)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:LYS:N	2	2.58	0.99	2.58
(1,54)	1:37:A:SER:N	1:37:A:SER:CA	1:37:A:SER:C	1:38:A:SER:N	2	2.32	1.06	2.32
(1,102)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:LYS:N	2	2.16	0.9	2.16
(1,97)	1:60:A:ASP:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	2	2.0	0.69	2.0
(1,48)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:VAL:N	2	1.85	0.72	1.85
(1,62)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:TYR:N	2	1.77	0.19	1.77
(1,143)	1:84:A:LEU:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	2	1.7	0.6	1.7
(1,106)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:ASN:N	2	1.58	0.24	1.58
(1,142)	1:84:A:LEU:N	1:84:A:LEU:CA	1:84:A:LEU:C	1:85:A:ILE:N	2	1.3	0.17	1.3

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

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

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

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



### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	6	4.92
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	10	4.92
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	2	4.91
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	20	4.89
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	47	4.86
(1,66)	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	1:46:A:LYS:N	40	4.84
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	5	4.78
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	7	4.78
(1,71)	1:47:A:GLU:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	23	4.66
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	5	4.57
(1,76)	1:50:A:GLU:N	1:50:A:GLU:CA	1:50:A:GLU:C	1:51:A:GLU:N	14	4.5
(1,141)	1:83:A:LYS:C	1:84:A:LEU:N	1:84:A:LEU:CA	1:84:A:LEU:C	40	4.48
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	24	4.47
(1,71)	1:47:A:GLU:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	33	4.44
(1,20)	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	1:18:A:GLN:N	35	4.44
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	42	4.28
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	1	4.27
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	33	4.17
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	18	4.13
(1,21)	1:17:A:LEU:C	1:18:A:GLN:N	1:18:A:GLN:CA	1:18:A:GLN:C	37	4.12
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	38	4.07
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	30	4.0
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	16	3.9
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	12	3.85
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	17	3.85
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	4	3.81
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	11	3.81
(1,139)	1:82:A:GLN:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	35	3.73
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	24	3.7
(1,66)	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	1:46:A:LYS:N	23	3.69
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	7	3.68
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	22	3.68
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	9	3.63
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	5	3.61
(1,124)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:LYS:N	48	3.57
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	4	3.55
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	48	3.55
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	12	3.5
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	27	3.48
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1	3.42
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	39	3.41
(1,54)	1:37:A:SER:N	1:37:A:SER:CA	1:37:A:SER:C	1:38:A:SER:N	38	3.38
(1,16)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LEU:N	40	3.38
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	17	3.37
(1,103)	1:63:A:LYS:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	19	3.33
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	21	3.29
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	20	3.28
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	18	3.21
(1,82)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:LEU:N	5	3.15
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	13	3.13
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	8	3.1
(1,102)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:LYS:N	22	3.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	27	3.05
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	40	3.01
(1,7)	1:10:A:GLN:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	45	2.97
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	8	2.94
(1,144)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:GLU:N	19	2.93
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	37	2.92
(1,82)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:LEU:N	12	2.78
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	44	2.75
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	39	2.71
(1,97)	1:60:A:ASP:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	46	2.69
(1,16)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LEU:N	25	2.66
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	21	2.65
(1,1)	1:6:A:PRO:C	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	25	2.61
(1,48)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:VAL:N	26	2.57
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	18	2.55
(1,7)	1:10:A:GLN:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	19	2.46
(1,103)	1:63:A:LYS:C	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	35	2.37
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	12	2.31
(1,143)	1:84:A:LEU:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	25	2.29
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	35	2.28
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	4	2.28
(1,144)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:GLU:N	40	2.24
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	14	2.12
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	9	2.03
(1,62)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:TYR:N	21	1.96
(1,87)	1:55:A:GLY:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	4	1.93
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	23	1.92
(1,139)	1:82:A:GLN:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	41	1.83
(1,106)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:ASN:N	44	1.83
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	18	1.83
(1,104)	1:64:A:LYS:N	1:64:A:LYS:CA	1:64:A:LYS:C	1:65:A:THR:N	28	1.78
(1,7)	1:10:A:GLN:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	25	1.75
(1,139)	1:82:A:GLN:C	1:83:A:LYS:N	1:83:A:LYS:CA	1:83:A:LYS:C	40	1.73
(1,144)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:GLU:N	12	1.7
(1,7)	1:10:A:GLN:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	31	1.7
(1,7)	1:10:A:GLN:C	1:11:A:GLN:N	1:11:A:GLN:CA	1:11:A:GLN:C	34	1.68
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	28	1.62
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	31	1.62
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	30	1.61
(1,124)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:LYS:N	29	1.58
(1,62)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:TYR:N	40	1.58
(1,16)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LEU:N	30	1.58
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	16	1.54
(1,144)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:GLU:N	28	1.52
(1,142)	1:84:A:LEU:N	1:84:A:LEU:CA	1:84:A:LEU:C	1:85:A:ILE:N	47	1.47
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	25	1.43
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	9	1.4
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	37	1.4
(1,65)	1:44:A:ILE:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	36	1.4
(1,106)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:ASN:N	47	1.34
(1,97)	1:60:A:ASP:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	19	1.31

Continued on next page...

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LEU:N	9	1.28
(1,6)	1:10:A:GLN:N	1:10:A:GLN:CA	1:10:A:GLN:C	1:11:A:GLN:N	34	1.28
(1,102)	1:63:A:LYS:N	1:63:A:LYS:CA	1:63:A:LYS:C	1:64:A:LYS:N	28	1.25
(1,54)	1:37:A:SER:N	1:37:A:SER:CA	1:37:A:SER:C	1:38:A:SER:N	21	1.25
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	22	1.24
(1,67)	1:45:A:THR:C	1:46:A:LYS:N	1:46:A:LYS:CA	1:46:A:LYS:C	7	1.23
(1,95)	1:59:A:ASN:C	1:60:A:ASP:N	1:60:A:ASP:CA	1:60:A:ASP:C	39	1.21
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	13	1.15
(1,48)	1:34:A:GLU:N	1:34:A:GLU:CA	1:34:A:GLU:C	1:35:A:VAL:N	9	1.13
(1,142)	1:84:A:LEU:N	1:84:A:LEU:CA	1:84:A:LEU:C	1:85:A:ILE:N	48	1.12
(1,143)	1:84:A:LEU:C	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	42	1.1
(1,72)	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	1:49:A:LEU:N	42	1.07
(1,144)	1:85:A:ILE:N	1:85:A:ILE:CA	1:85:A:ILE:C	1:86:A:GLU:N	46	1.06
(1,32)	1:24:A:SER:N	1:24:A:SER:CA	1:24:A:SER:C	1:25:A:ASN:N	21	1.05
(1,71)	1:47:A:GLU:C	1:48:A:ALA:N	1:48:A:ALA:CA	1:48:A:ALA:C	30	1.0