



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 04:53 PM EST

PDB ID : 6ZUZ
BMRB ID : 34536
Title : TFIIS N-terminal domain (TND) from human Elongin-A
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

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

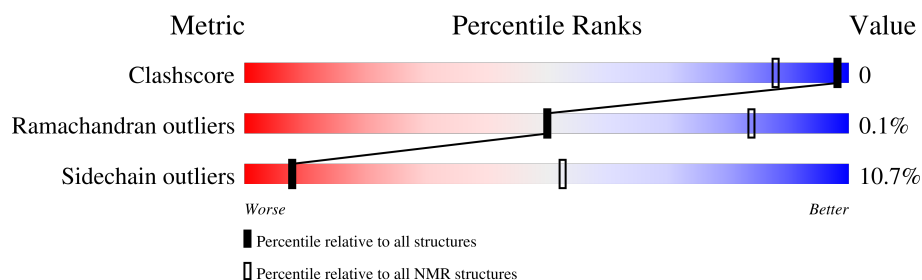
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	

2 Ensemble composition and analysis

This entry contains 40 models. Model 4 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:32-A:102 (71)	0.24	4

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1410 atoms, of which 728 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Elongin-A.

Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1410	431	728	124	126	1	

There are 7 discrepancies between the modelled and reference sequences:

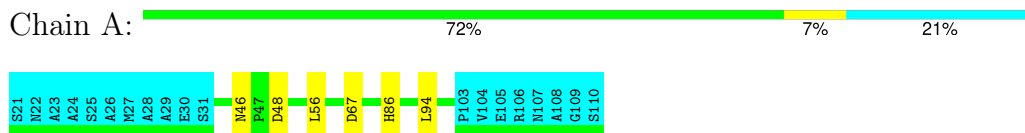
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	SER	-	expression tag	UNP Q14241
A	22	ASN	-	expression tag	UNP Q14241
A	23	ALA	-	expression tag	UNP Q14241
A	24	ALA	-	expression tag	UNP Q14241
A	25	SER	-	expression tag	UNP Q14241
A	109	GLY	-	expression tag	UNP Q14241
A	110	SER	-	expression tag	UNP Q14241

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: Elongin-A

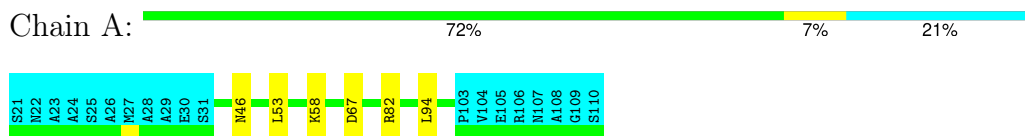


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

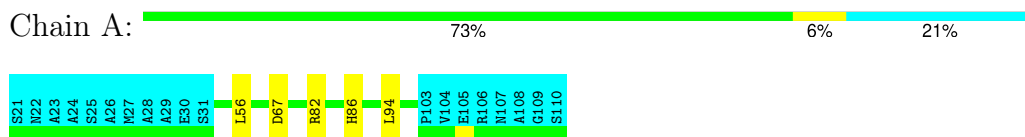
4.2.1 Score per residue for model 1

- Molecule 1: Elongin-A



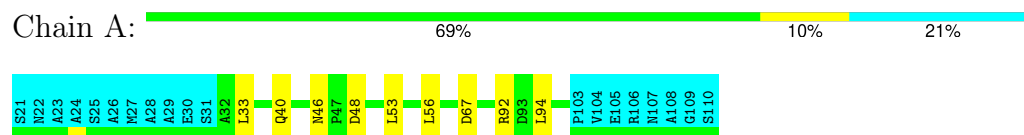
4.2.2 Score per residue for model 2

- Molecule 1: Elongin-A



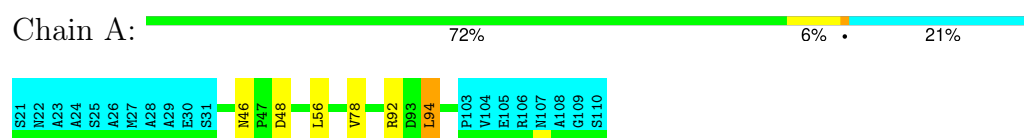
4.2.3 Score per residue for model 3

- Molecule 1: Elongin-A



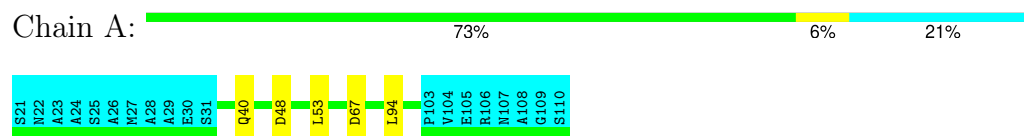
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Elongin-A



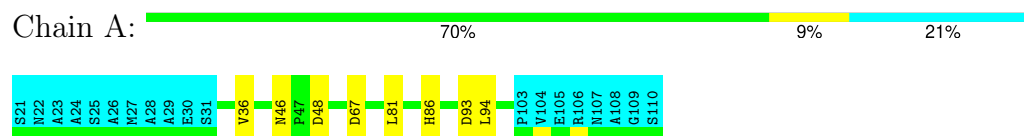
4.2.5 Score per residue for model 5

- Molecule 1: Elongin-A



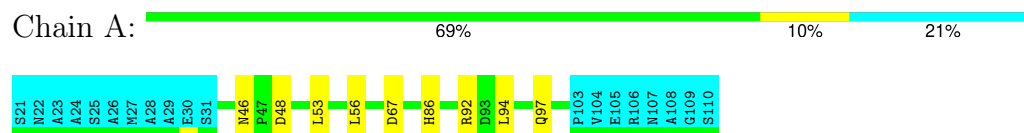
4.2.6 Score per residue for model 6

- Molecule 1: Elongin-A



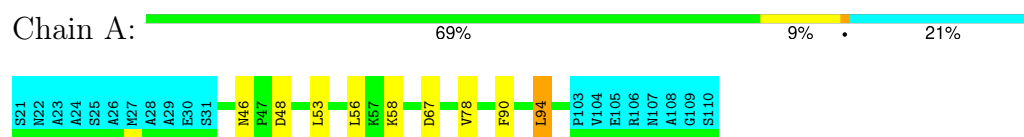
4.2.7 Score per residue for model 7

- Molecule 1: Elongin-A



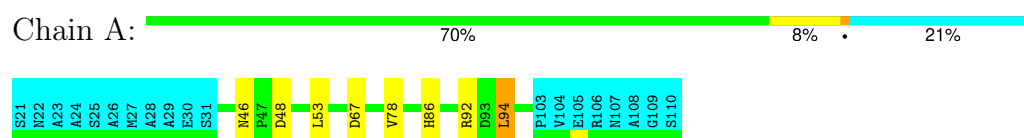
4.2.8 Score per residue for model 8

- Molecule 1: Elongin-A



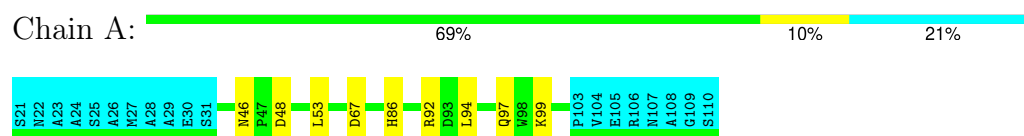
4.2.9 Score per residue for model 9

- Molecule 1: Elongin-A



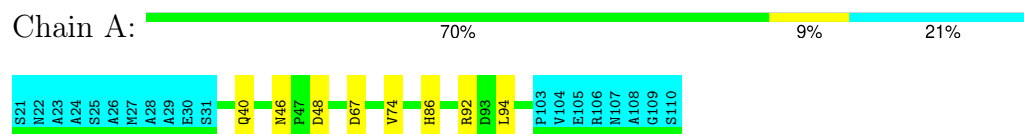
4.2.10 Score per residue for model 10

- Molecule 1: Elongin-A



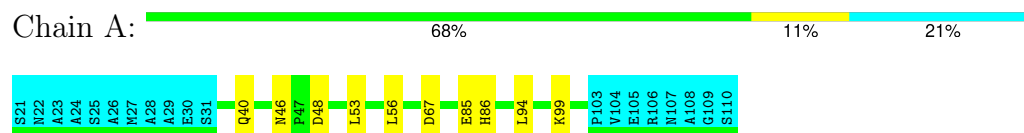
4.2.11 Score per residue for model 11

- Molecule 1: Elongin-A



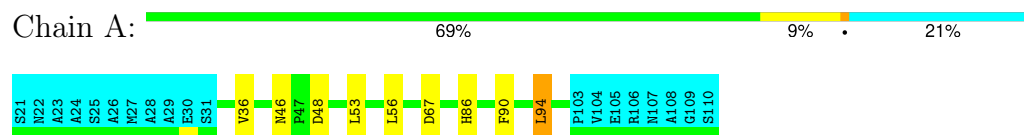
4.2.12 Score per residue for model 12

- Molecule 1: Elongin-A



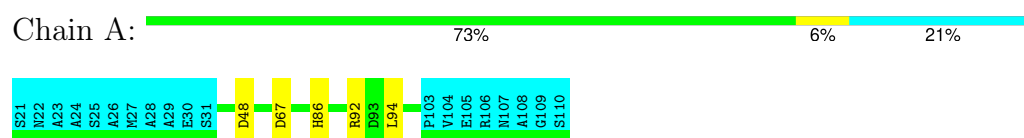
4.2.13 Score per residue for model 13

- Molecule 1: Elongin-A



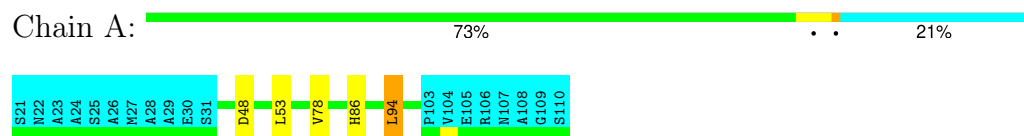
4.2.14 Score per residue for model 14

- Molecule 1: Elongin-A



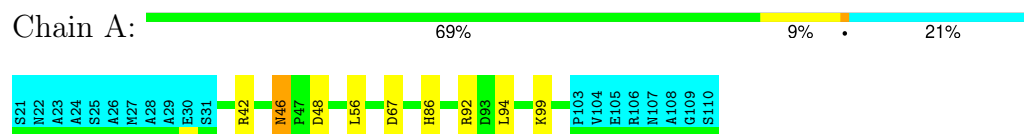
4.2.15 Score per residue for model 15

- Molecule 1: Elongin-A



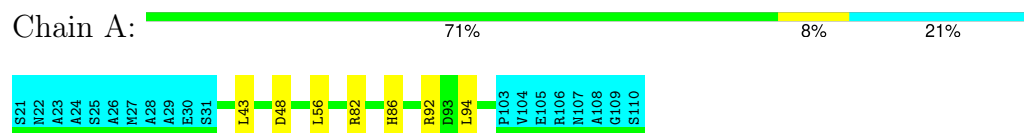
4.2.16 Score per residue for model 16

- Molecule 1: Elongin-A



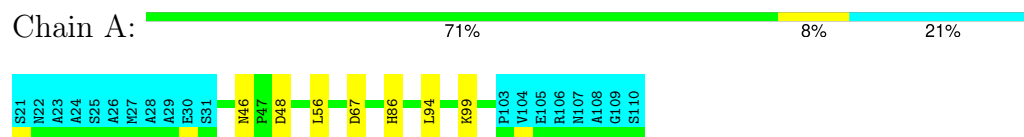
4.2.17 Score per residue for model 17

- Molecule 1: Elongin-A



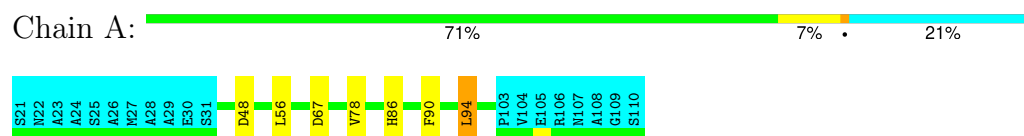
4.2.18 Score per residue for model 18

- Molecule 1: Elongin-A



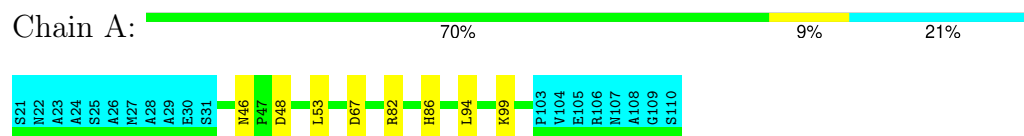
4.2.19 Score per residue for model 19

- Molecule 1: Elongin-A



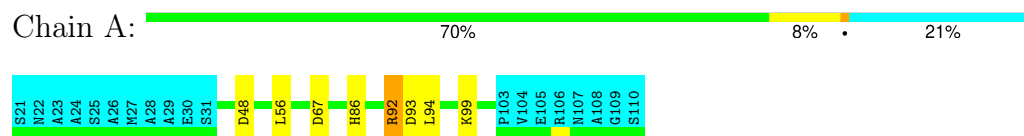
4.2.20 Score per residue for model 20

- Molecule 1: Elongin-A



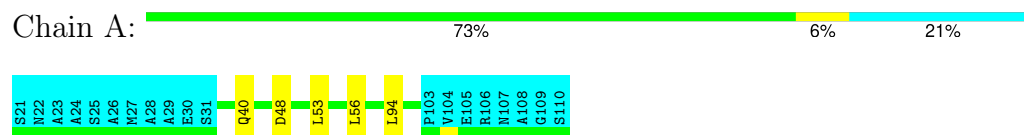
4.2.21 Score per residue for model 21

- Molecule 1: Elongin-A



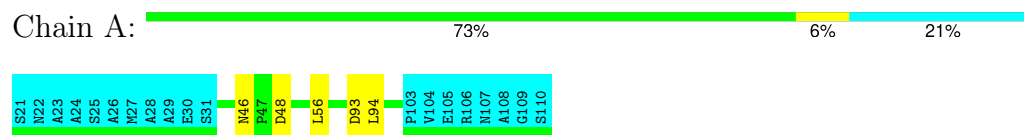
4.2.22 Score per residue for model 22

- Molecule 1: Elongin-A



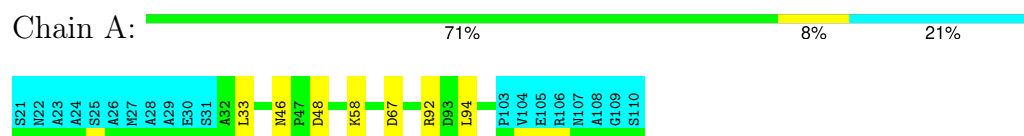
4.2.23 Score per residue for model 23

- Molecule 1: Elongin-A



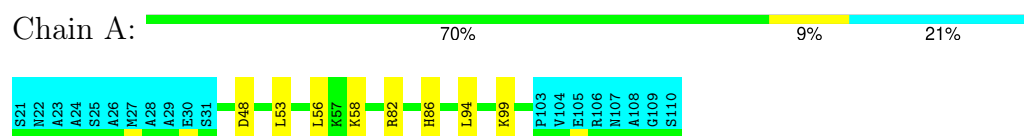
4.2.24 Score per residue for model 24

- Molecule 1: Elongin-A



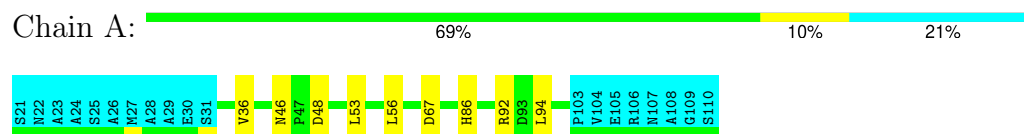
4.2.25 Score per residue for model 25

- Molecule 1: Elongin-A



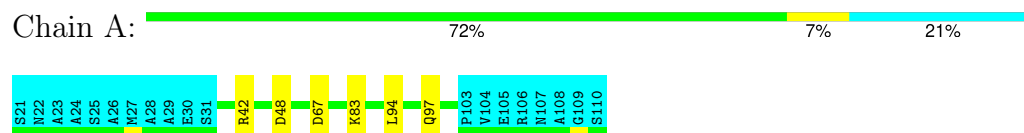
4.2.26 Score per residue for model 26

- Molecule 1: Elongin-A



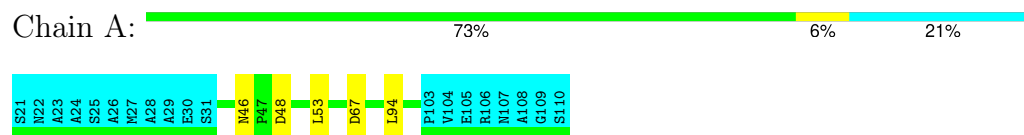
4.2.27 Score per residue for model 27

- Molecule 1: Elongin-A



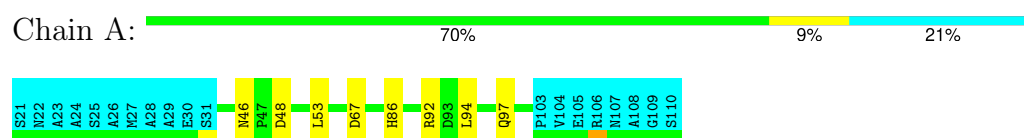
4.2.28 Score per residue for model 28

- Molecule 1: Elongin-A



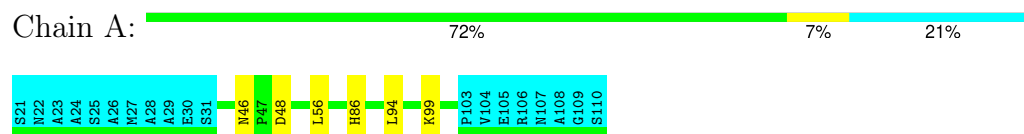
4.2.29 Score per residue for model 29

- Molecule 1: Elongin-A



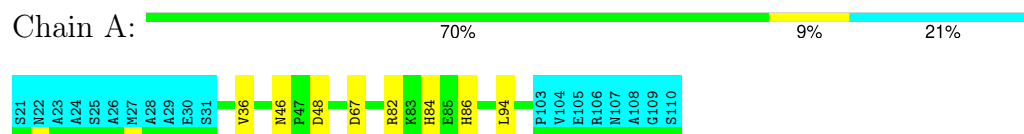
4.2.30 Score per residue for model 30

- Molecule 1: Elongin-A



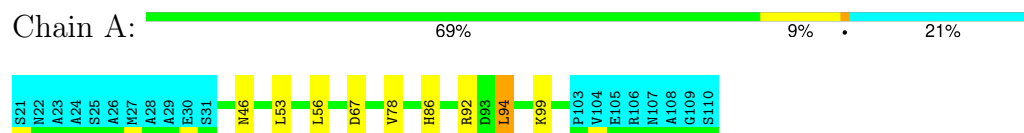
4.2.31 Score per residue for model 31

- Molecule 1: Elongin-A



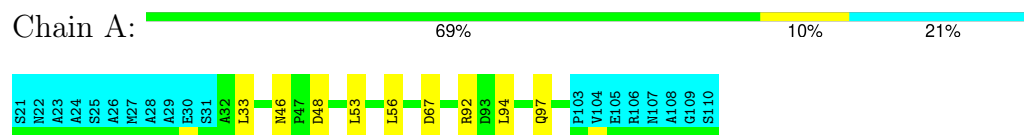
4.2.32 Score per residue for model 32

- Molecule 1: Elongin-A



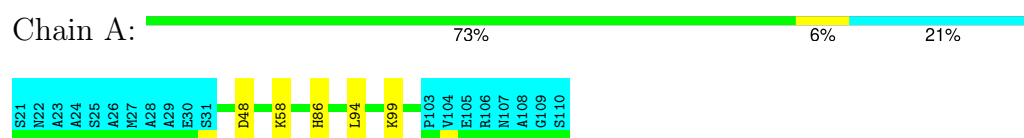
4.2.33 Score per residue for model 33

- Molecule 1: Elongin-A



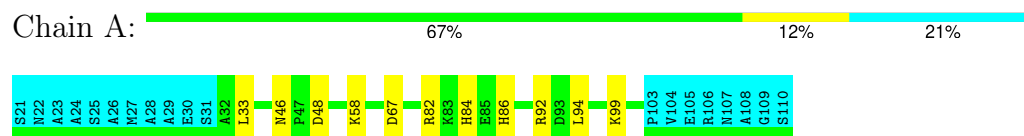
4.2.34 Score per residue for model 34

- Molecule 1: Elongin-A



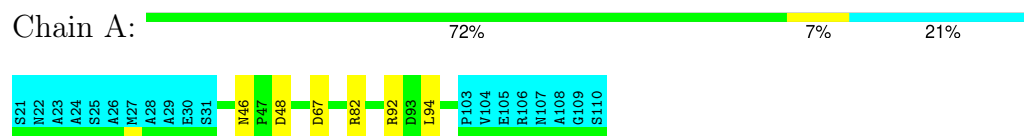
4.2.35 Score per residue for model 35

- Molecule 1: Elongin-A



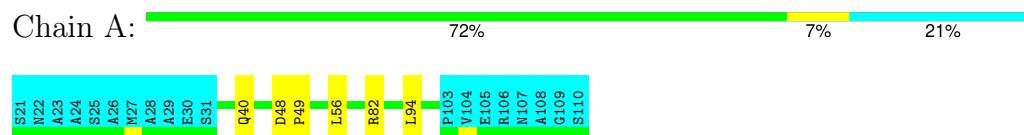
4.2.36 Score per residue for model 36

- Molecule 1: Elongin-A



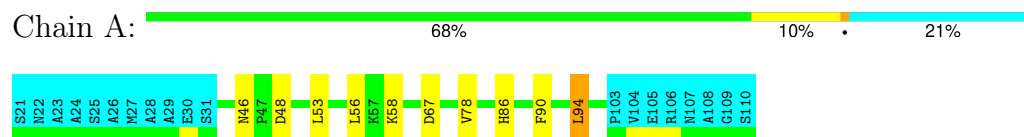
4.2.37 Score per residue for model 37

- Molecule 1: Elongin-A



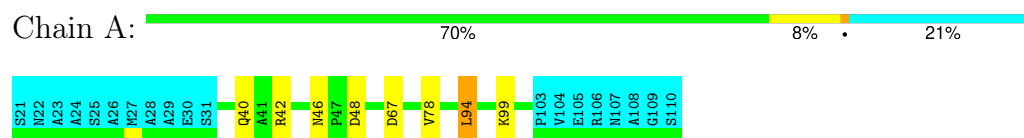
4.2.38 Score per residue for model 38

- Molecule 1: Elongin-A



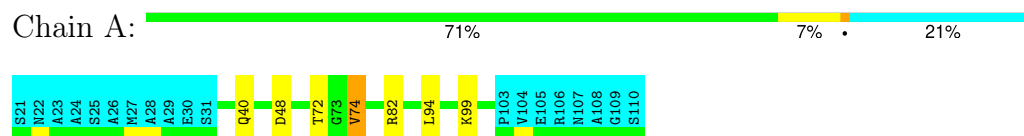
4.2.39 Score per residue for model 39

- Molecule 1: Elongin-A



4.2.40 Score per residue for model 40

- Molecule 1: Elongin-A



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
YASARA	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1140
Number of shifts mapped to atoms	1140
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.60±0.01	0±0/565 (0.0± 0.1%)	0.73±0.03	0±1/765 (0.0± 0.1%)
All	All	0.60	4/22600 (0.0%)	0.73	15/30600 (0.0%)

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	36	VAL	CB-CG2	-5.25	1.41	1.52	31	3
1	A	36	VAL	CB-CG1	-5.03	1.42	1.52	26	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	42	ARG	NE-CZ-NH1	5.90	123.25	120.30	16	3
1	A	43	LEU	CB-CG-CD1	5.68	120.66	111.00	17	1
1	A	92	ARG	NE-CZ-NH1	5.57	123.08	120.30	21	2
1	A	82	ARG	NE-CZ-NH1	5.52	123.06	120.30	37	9

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	556	611	611	0±1
All	All	22240	24440	24440	14

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:HG11	1:A:94:LEU:HB3	0.52	1.82	9	8
1:A:90:PHE:CE1	1:A:94:LEU:HD23	0.47	2.45	8	4
1:A:72:THR:OG1	1:A:74:VAL:HG22	0.44	2.13	40	1
1:A:48:ASP:CG	1:A:49:PRO:HD2	0.44	2.32	37	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	71/90 (79%)	68±1 (96±1%)	3±1 (4±1%)	0±0 (0±0%)	50	84
All	All	2840/3600 (79%)	2725 (96%)	113 (4%)	2 (0%)	50	84

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	46	ASN	2

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	61/73 (84%)	54±2 (89±3%)	7±2 (11±3%)	8	52
All	All	2440/2920 (84%)	2179 (89%)	261 (11%)	8	52

All 20 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	94	LEU	40
1	A	48	ASP	36
1	A	67	ASP	30
1	A	46	ASN	26
1	A	86	HIS	25
1	A	56	LEU	21
1	A	53	LEU	19
1	A	92	ARG	16
1	A	99	LYS	13
1	A	40	GLN	8
1	A	58	LYS	7
1	A	97	GLN	5
1	A	33	LEU	4
1	A	93	ASP	3
1	A	74	VAL	2
1	A	84	HIS	2
1	A	81	LEU	1
1	A	85	GLU	1
1	A	83	LYS	1
1	A	82	ARG	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 94% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *eloa_dep.star*

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	1140
Number of shifts mapped to atoms	1140
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	89	-0.50 ± 0.20	Should be checked
$^{13}\text{C}_\beta$	84	0.15 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	88	-0.61 ± 0.19	Should be applied
^{15}N	83	-0.04 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 961 atoms were assigned a chemical shift out of a possible 1023. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	352/352 (100%)	142/142 (100%)	142/142 (100%)	68/68 (100%)
Sidechain	575/626 (92%)	393/410 (96%)	177/192 (92%)	5/24 (21%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	34/45 (76%)	19/23 (83%)	14/19 (74%)	1/3 (33%)
Overall	961/1023 (94%)	554/575 (96%)	333/353 (94%)	74/95 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1140 atoms were assigned a chemical shift out of a possible 1228. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	436/446 (98%)	176/180 (98%)	177/180 (98%)	83/86 (97%)
Sidechain	670/737 (91%)	459/483 (95%)	204/225 (91%)	7/29 (24%)
Aromatic	34/45 (76%)	19/23 (83%)	14/19 (74%)	1/3 (33%)
Overall	1140/1228 (93%)	654/686 (95%)	395/424 (93%)	91/118 (77%)

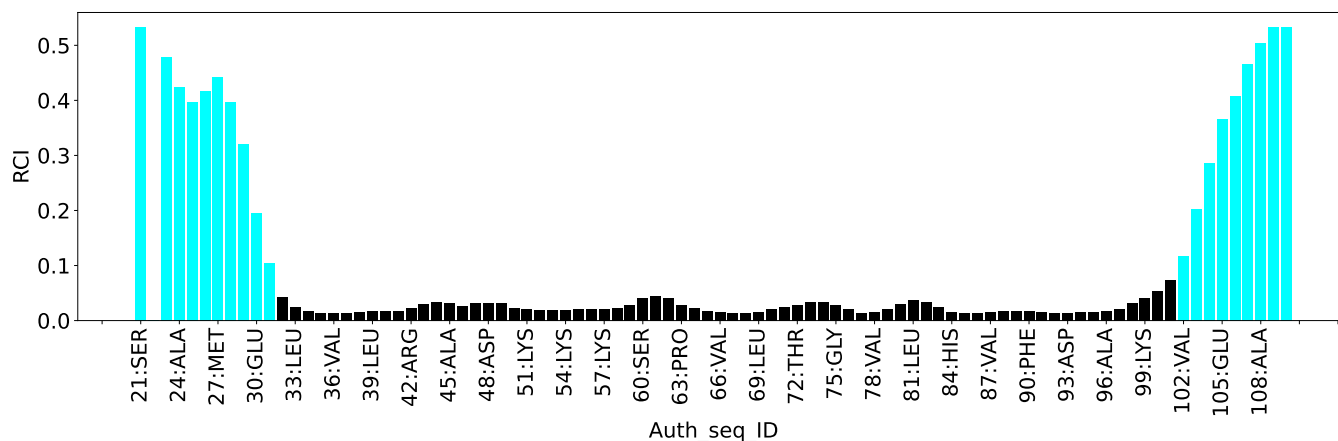
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain 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	1961
Intra-residue ($ i-j =0$)	447
Sequential ($ i-j =1$)	468
Medium range ($ i-j >1$ and $ i-j <5$)	524
Long range ($ i-j \geq 5$)	522
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	128
Number of unmapped restraints	0
Number of restraints per residue	23.2
Number of long range restraints per residue ¹	5.8

¹Long 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)	4.5	0.2
0.2-0.5 (Medium)	1.9	0.47
>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)	2.0	5.09
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

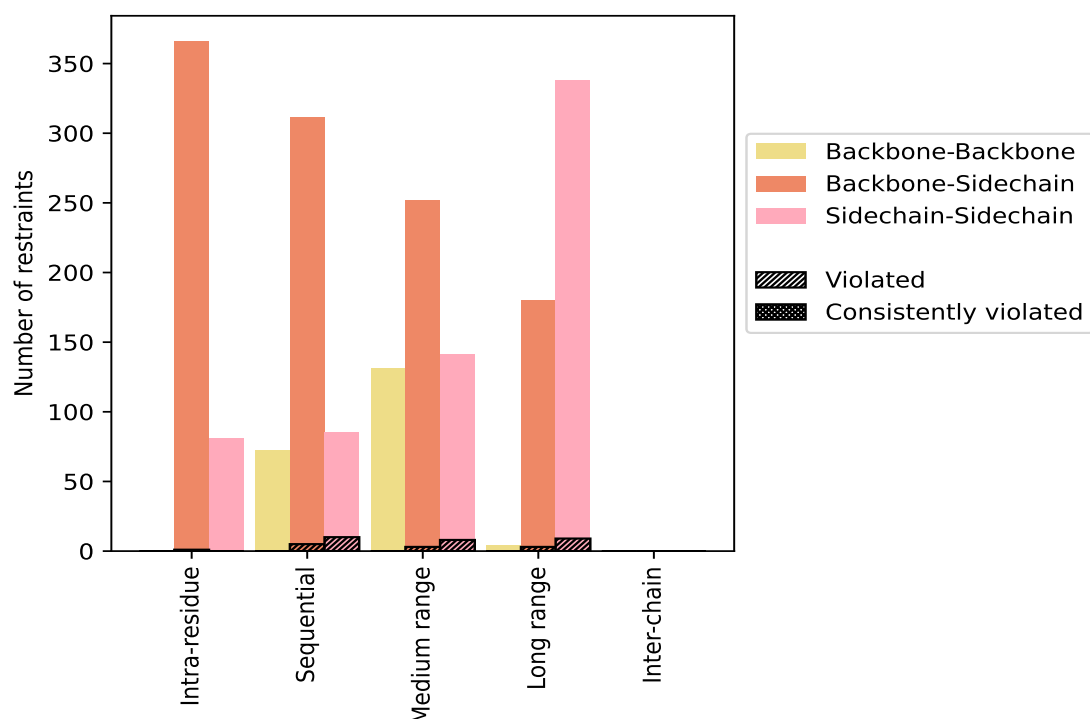
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	447	22.8	1	0.2	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	366	18.7	1	0.3	0.1	0	0.0	0.0
Sidechain-Sidechain	81	4.1	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	468	23.9	15	3.2	0.8	0	0.0	0.0
Backbone-Backbone	72	3.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	311	15.9	5	1.6	0.3	0	0.0	0.0
Sidechain-Sidechain	85	4.3	10	11.8	0.5	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	524	26.7	11	2.1	0.6	0	0.0	0.0
Backbone-Backbone	131	6.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	252	12.9	3	1.2	0.2	0	0.0	0.0
Sidechain-Sidechain	141	7.2	8	5.7	0.4	0	0.0	0.0
Long range ($i-j \geq 5$)	522	26.6	12	2.3	0.6	0	0.0	0.0
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	180	9.2	3	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	338	17.2	9	2.7	0.5	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
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
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1961	100.0	39	2.0	2.0	0	0.0	0.0
Backbone-Backbone	207	10.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1109	56.6	12	1.1	0.6	0	0.0	0.0
Sidechain-Sidechain	645	32.9	27	4.2	1.4	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	2	0	3	0	5	0.16	0.24	0.04	0.17
2	0	6	2	3	0	11	0.2	0.39	0.09	0.16
3	0	1	2	3	0	6	0.17	0.24	0.04	0.16
4	0	1	2	2	0	5	0.19	0.32	0.09	0.16
5	0	3	1	5	0	9	0.16	0.27	0.05	0.15
6	1	2	0	4	0	7	0.15	0.27	0.05	0.13
7	0	1	2	2	0	5	0.22	0.29	0.07	0.25
8	0	1	0	3	0	4	0.17	0.23	0.04	0.16
9	0	1	0	4	0	5	0.14	0.18	0.03	0.14
10	0	2	1	2	0	5	0.18	0.32	0.08	0.14

Continued on next page...

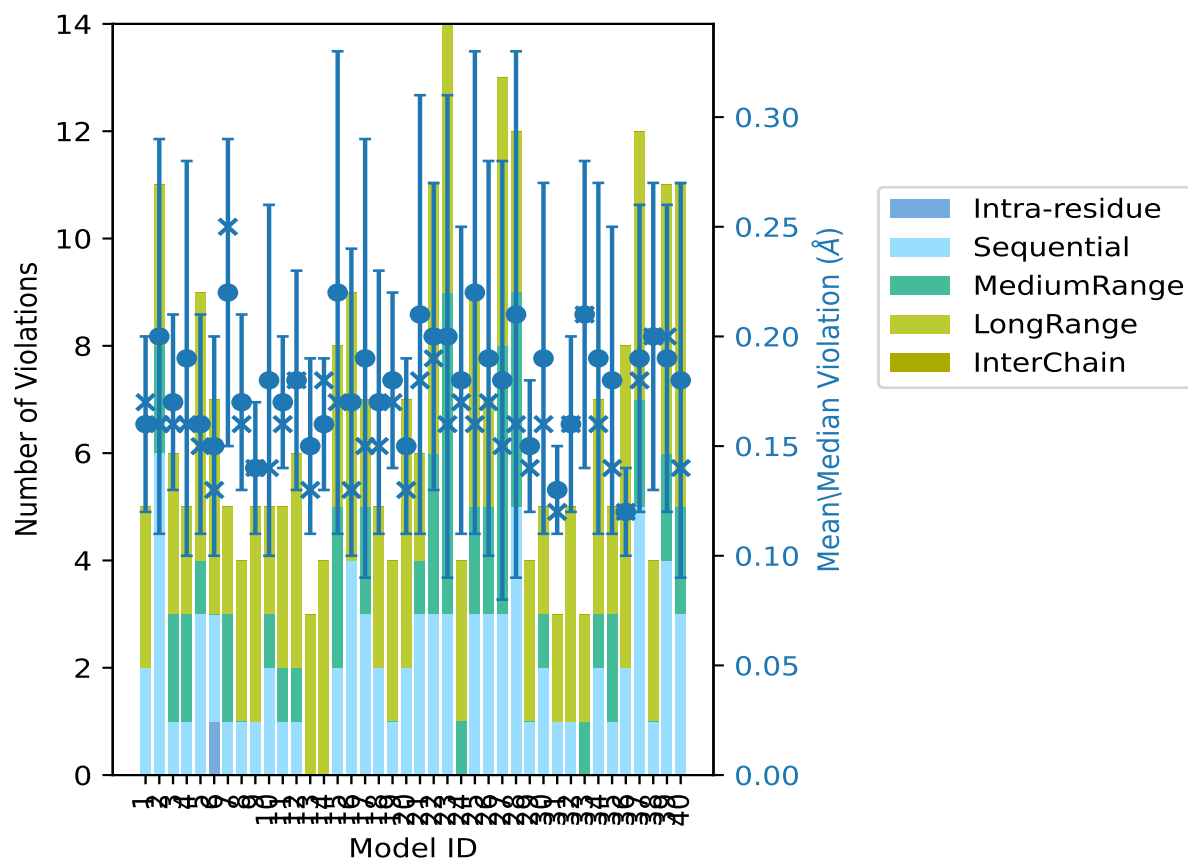
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	1	3	0	5	0.17	0.23	0.03	0.16
12	0	1	1	4	0	6	0.18	0.26	0.05	0.18
13	0	0	0	3	0	3	0.15	0.2	0.04	0.13
14	0	0	0	4	0	4	0.16	0.19	0.03	0.18
15	0	2	3	3	0	8	0.22	0.43	0.11	0.17
16	0	4	0	5	0	9	0.17	0.3	0.07	0.13
17	0	3	2	2	0	7	0.19	0.34	0.1	0.15
18	0	2	0	3	0	5	0.17	0.26	0.06	0.15
19	0	1	0	3	0	4	0.18	0.23	0.04	0.17
20	0	2	0	5	0	7	0.15	0.21	0.04	0.13
21	0	3	1	2	0	6	0.21	0.37	0.1	0.18
22	0	3	3	5	0	11	0.2	0.34	0.07	0.19
23	0	3	6	5	0	14	0.2	0.47	0.11	0.16
24	0	0	1	3	0	4	0.18	0.29	0.07	0.17
25	0	3	2	4	0	9	0.22	0.45	0.11	0.16
26	0	3	2	2	0	7	0.19	0.36	0.09	0.17
27	0	3	5	5	0	13	0.18	0.44	0.1	0.15
28	0	5	4	3	0	12	0.21	0.46	0.12	0.16
29	0	1	0	3	0	4	0.15	0.2	0.03	0.14
30	0	2	1	2	0	5	0.19	0.33	0.08	0.16
31	0	1	0	2	0	3	0.13	0.16	0.02	0.12
32	0	1	0	4	0	5	0.16	0.23	0.04	0.16
33	0	0	1	2	0	3	0.21	0.29	0.07	0.21
34	0	2	1	4	0	7	0.19	0.35	0.08	0.16
35	0	1	2	2	0	5	0.18	0.3	0.07	0.14
36	0	2	0	6	0	8	0.12	0.16	0.02	0.12
37	0	5	2	5	0	12	0.19	0.34	0.07	0.18
38	0	1	0	3	0	4	0.2	0.27	0.07	0.2
39	0	4	2	5	0	11	0.19	0.31	0.07	0.2
40	0	3	2	6	0	11	0.18	0.37	0.09	0.14

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1922(IR:446, SQ:453, MR:513, LR:510, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	6	5	3	0	15	1	2.5
0	2	0	0	0	2	2	5.0
0	1	2	2	0	5	3	7.5
0	1	0	1	0	2	4	10.0
0	1	0	1	0	2	5	12.5
0	1	0	1	0	2	6	15.0

Continued on next page...

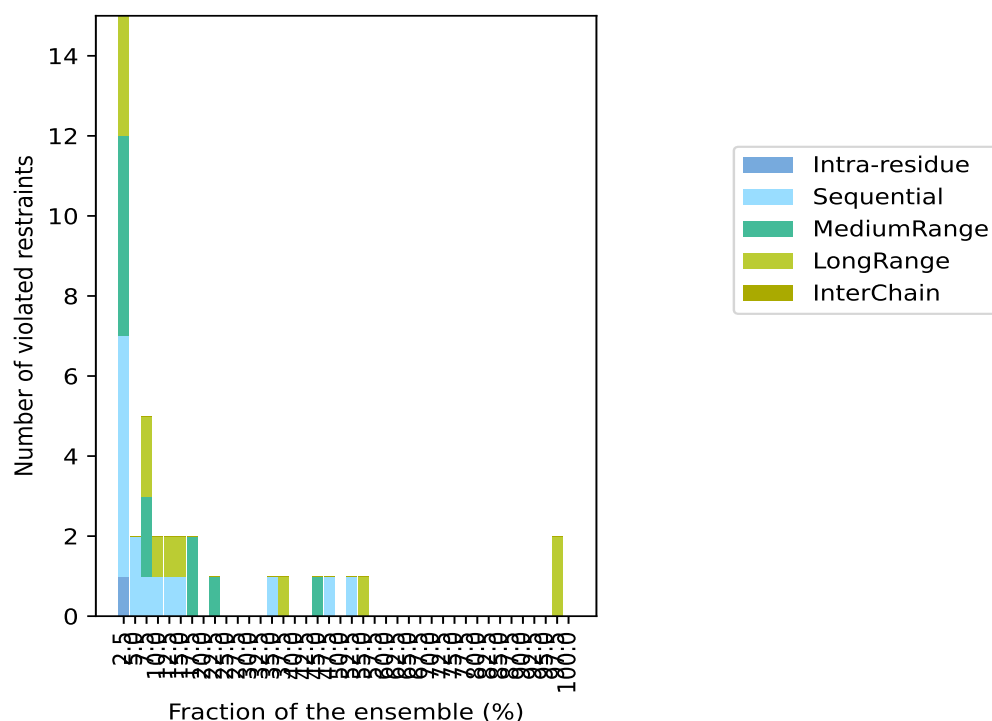
Continued from previous page...

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

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

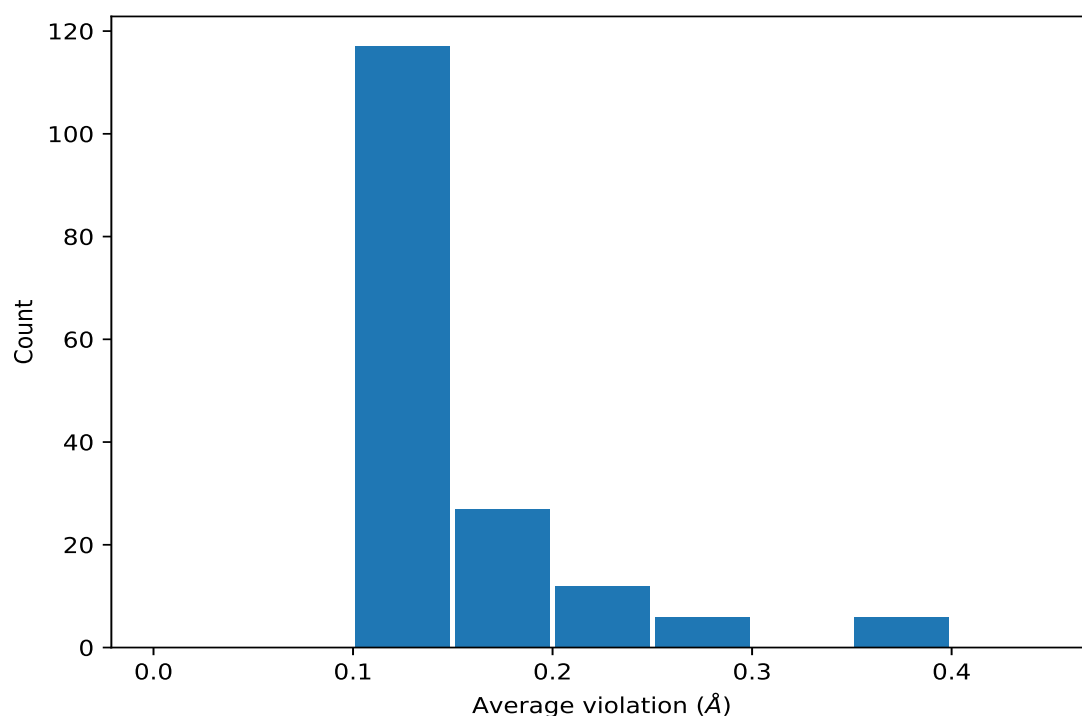
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	39	0.26	0.06	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	39	0.26	0.06	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	39	0.26	0.06	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	39	0.26	0.06	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	39	0.26	0.06	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	39	0.26	0.06	0.25
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	39	0.2	0.07	0.19
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	39	0.2	0.07	0.19
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	39	0.2	0.07	0.19
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	39	0.2	0.07	0.19
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	39	0.2	0.07	0.19
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	39	0.2	0.07	0.19
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	22	0.14	0.02	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	22	0.14	0.02	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	22	0.14	0.02	0.13
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	21	0.13	0.02	0.12
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	21	0.13	0.02	0.12
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	21	0.13	0.02	0.12
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	19	0.15	0.03	0.14
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	19	0.15	0.03	0.14
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	19	0.15	0.03	0.14
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	18	0.36	0.07	0.34
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	18	0.36	0.07	0.34
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	18	0.36	0.07	0.34
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	18	0.36	0.07	0.34
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	18	0.36	0.07	0.34
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	18	0.36	0.07	0.34
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	15	0.14	0.05	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	15	0.14	0.05	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	15	0.14	0.05	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	15	0.14	0.05	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	15	0.14	0.05	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	15	0.14	0.05	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	14	0.13	0.03	0.12
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	14	0.13	0.03	0.12
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	14	0.13	0.03	0.12
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	9	0.16	0.02	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	9	0.16	0.02	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	9	0.16	0.02	0.15
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	7	0.24	0.05	0.27
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	7	0.24	0.05	0.27
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	7	0.24	0.05	0.27
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	7	0.24	0.05	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	7	0.24	0.05	0.27
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	7	0.24	0.05	0.27
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	7	0.12	0.01	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	7	0.12	0.01	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	7	0.12	0.01	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	7	0.12	0.01	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	7	0.12	0.01	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	7	0.12	0.01	0.12
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	6	0.18	0.01	0.18
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	6	0.18	0.01	0.18
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	6	0.14	0.02	0.16
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	6	0.14	0.02	0.16
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	6	0.14	0.02	0.16
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	6	0.14	0.02	0.16
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	6	0.14	0.02	0.16
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	6	0.14	0.02	0.16
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG11	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG12	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG13	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG21	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG22	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG23	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG11	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG12	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG13	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG21	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG22	5	0.14	0.03	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG23	5	0.14	0.03	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB1	5	0.13	0.02	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB2	5	0.13	0.02	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB3	5	0.13	0.02	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB1	5	0.13	0.02	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB2	5	0.13	0.02	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB3	5	0.13	0.02	0.12
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB2	4	0.14	0.04	0.12
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB3	4	0.14	0.04	0.12
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB2	4	0.14	0.04	0.12
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB3	4	0.14	0.04	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG21	4	0.13	0.01	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG22	4	0.13	0.01	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG23	4	0.13	0.01	0.12
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG11	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG12	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG13	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG21	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG22	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG23	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG11	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG12	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG13	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG21	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG22	3	0.17	0.05	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG23	3	0.17	0.05	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG11	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG12	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG13	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG21	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG22	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG23	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG11	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG12	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG13	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG21	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG22	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG23	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG11	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG12	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG13	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG21	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG22	3	0.15	0.02	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG23	3	0.15	0.02	0.14
(1,1535)	1:48:A:ASP:HB2	1:49:A:PRO:HD3	3	0.14	0.03	0.14
(1,1535)	1:48:A:ASP:HB3	1:49:A:PRO:HD3	3	0.14	0.03	0.14
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG21	3	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

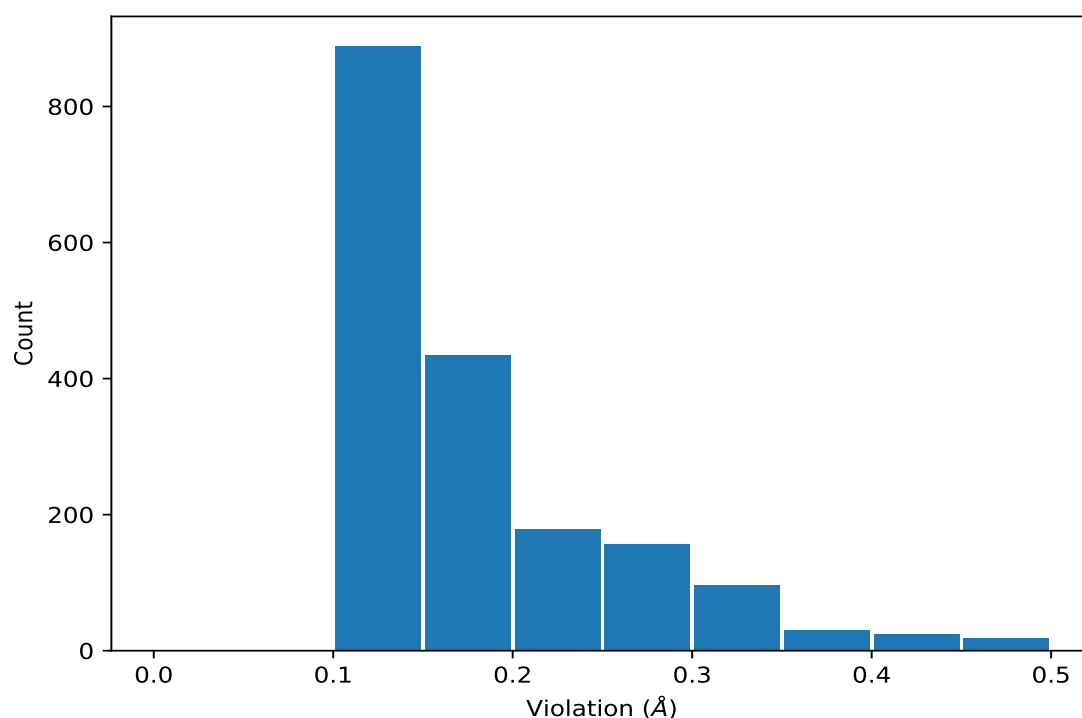
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG22	3	0.12	0.01	0.12
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG23	3	0.12	0.01	0.12
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG21	3	0.12	0.01	0.12
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG22	3	0.12	0.01	0.12
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG23	3	0.12	0.01	0.12
(1,70)	1:68:A:ILE:HG21	1:72:A:THR:HB	3	0.11	0.0	0.11
(1,70)	1:68:A:ILE:HG22	1:72:A:THR:HB	3	0.11	0.0	0.11
(1,70)	1:68:A:ILE:HG23	1:72:A:THR:HB	3	0.11	0.0	0.11
(1,1356)	1:33:A:LEU:HD11	1:34:A:GLN:HE21	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD11	1:34:A:GLN:HE22	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD12	1:34:A:GLN:HE21	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD12	1:34:A:GLN:HE22	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD13	1:34:A:GLN:HE21	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD13	1:34:A:GLN:HE22	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD21	1:34:A:GLN:HE21	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD21	1:34:A:GLN:HE22	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD22	1:34:A:GLN:HE21	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD22	1:34:A:GLN:HE22	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD23	1:34:A:GLN:HE21	2	0.14	0.01	0.14
(1,1356)	1:33:A:LEU:HD23	1:34:A:GLN:HE22	2	0.14	0.01	0.14
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG11	2	0.12	0.02	0.12
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG12	2	0.12	0.02	0.12
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG13	2	0.12	0.02	0.12
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG21	2	0.12	0.02	0.12
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG22	2	0.12	0.02	0.12
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG23	2	0.12	0.02	0.12

¹Number of violated models, ²Standard 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)
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	23	0.47
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	23	0.47
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	23	0.47
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	23	0.47
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	23	0.47
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	23	0.47
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	28	0.46
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	28	0.46
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	28	0.46
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	28	0.46
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	28	0.46
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	28	0.46
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	25	0.45
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	25	0.45
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	25	0.45
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	25	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	25	0.45
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	25	0.45
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	27	0.44
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	27	0.44
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	27	0.44
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	27	0.44
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	27	0.44
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	27	0.44
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	15	0.43
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	15	0.43
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	15	0.43
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	15	0.43
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	15	0.43
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	15	0.43
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	28	0.41
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	28	0.41
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	28	0.41
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	28	0.41
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	28	0.41
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	28	0.41
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	23	0.4
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	23	0.4
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	23	0.4
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	23	0.4
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	23	0.4
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	23	0.4
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	2	0.39
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	2	0.39
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	2	0.39
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	2	0.39
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	2	0.39
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	2	0.39
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	21	0.37
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	21	0.37
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	21	0.37
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	21	0.37
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	21	0.37
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	21	0.37
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	40	0.37
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	40	0.37
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	40	0.37
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	40	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	40	0.37
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	40	0.37
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	2	0.37
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	2	0.37
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	2	0.37
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	2	0.37
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	2	0.37
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	2	0.37
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	26	0.36
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	26	0.36
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	26	0.36
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	26	0.36
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	26	0.36
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	26	0.36
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	34	0.35
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	34	0.35
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	34	0.35
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	34	0.35
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	34	0.35
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	34	0.35
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	23	0.34
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	23	0.34
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	23	0.34
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	23	0.34
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	23	0.34
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	23	0.34
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	17	0.34
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	17	0.34
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	17	0.34
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	17	0.34
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	17	0.34
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	17	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	22	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	22	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	22	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	22	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	22	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	22	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	27	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	27	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	27	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	27	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	27	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	27	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	37	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	37	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	37	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	37	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	37	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	37	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	40	0.34
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	40	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	40	0.34
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	40	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	40	0.34
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	40	0.34
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	17	0.33
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	17	0.33
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	17	0.33
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	17	0.33
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	17	0.33
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	17	0.33
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	30	0.33
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	30	0.33
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	30	0.33
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	30	0.33
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	30	0.33
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	30	0.33
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	15	0.33
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	15	0.33
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	15	0.33
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	15	0.33
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	15	0.33
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	15	0.33
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	4	0.32
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	4	0.32
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	4	0.32
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	4	0.32
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	4	0.32
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	4	0.32
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	10	0.32
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	10	0.32
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	10	0.32
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	10	0.32
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	10	0.32
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	22	0.31
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	22	0.31
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	22	0.31
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	22	0.31
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	22	0.31
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	22	0.31
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	28	0.31
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	28	0.31
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	28	0.31
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	28	0.31
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	28	0.31
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	28	0.31
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	25	0.31
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	25	0.31
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	25	0.31
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	25	0.31
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	25	0.31
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	25	0.31
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	39	0.31
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	39	0.31
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	39	0.31
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	39	0.31
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	39	0.31
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	39	0.31
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	37	0.3
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	37	0.3
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	37	0.3
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	37	0.3
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	37	0.3
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	37	0.3
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	35	0.3
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	35	0.3
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	35	0.3
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	35	0.3
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	35	0.3
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	35	0.3
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	16	0.3
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	16	0.3
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	16	0.3
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	16	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	16	0.3
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	16	0.3
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	7	0.29
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	7	0.29
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	7	0.29
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	7	0.29
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	7	0.29
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	7	0.29
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	22	0.29
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	22	0.29
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	22	0.29
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	22	0.29
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	22	0.29
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	22	0.29
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	24	0.29
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	24	0.29
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	24	0.29
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	24	0.29
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	24	0.29
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	24	0.29
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	33	0.29
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	33	0.29
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	33	0.29
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	33	0.29
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	33	0.29
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	33	0.29
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	21	0.29
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	21	0.29
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	21	0.29
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	21	0.29
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	21	0.29
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	21	0.29
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	39	0.28
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	39	0.28
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	39	0.28
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	39	0.28
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	39	0.28
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	39	0.28
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	16	0.28
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	16	0.28
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	16	0.28
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	16	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	16	0.28
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	16	0.28
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	25	0.28
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	25	0.28
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	25	0.28
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	25	0.28
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	25	0.28
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	25	0.28
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	7	0.28
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	7	0.28
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	7	0.28
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	7	0.28
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	7	0.28
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	7	0.28
(1,1830)	1:81:A:LEU:HA	1:81:A:LEU:HD11	6	0.27
(1,1830)	1:81:A:LEU:HA	1:81:A:LEU:HD12	6	0.27
(1,1830)	1:81:A:LEU:HA	1:81:A:LEU:HD13	6	0.27
(1,1830)	1:81:A:LEU:HA	1:81:A:LEU:HD21	6	0.27
(1,1830)	1:81:A:LEU:HA	1:81:A:LEU:HD22	6	0.27
(1,1830)	1:81:A:LEU:HA	1:81:A:LEU:HD23	6	0.27
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	37	0.27
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	37	0.27
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	37	0.27
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	37	0.27
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	37	0.27
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	37	0.27
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	15	0.27
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	15	0.27
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	15	0.27
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	15	0.27
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	15	0.27
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	15	0.27
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	5	0.27
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	5	0.27
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	5	0.27
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	5	0.27
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	5	0.27
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	5	0.27
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	38	0.27
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	38	0.27
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	38	0.27
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	38	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	38	0.27
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	38	0.27
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	39	0.26
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	39	0.26
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	39	0.26
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	39	0.26
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	39	0.26
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	39	0.26
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	12	0.26
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	12	0.26
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	12	0.26
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	12	0.26
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	12	0.26
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	12	0.26
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	18	0.26
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	18	0.26
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	18	0.26
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	18	0.26
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	18	0.26
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	18	0.26
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	26	0.26
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	26	0.26
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	26	0.26
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	26	0.26
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	26	0.26
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	26	0.26
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	25	0.25
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	25	0.25
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	25	0.25
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	25	0.25
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	25	0.25
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	25	0.25
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	38	0.25
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	38	0.25
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	38	0.25
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	38	0.25
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	38	0.25
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	38	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	4	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	4	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	4	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	4	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	4	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	4	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	7	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	7	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	7	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	7	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	7	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	7	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	34	0.25
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	34	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	34	0.25
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	34	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	34	0.25
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	34	0.25
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	40	0.24
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	40	0.24
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	40	0.24
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	40	0.24
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	40	0.24
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	40	0.24
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	39	0.24
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	39	0.24
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	39	0.24
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	39	0.24
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	39	0.24
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	39	0.24
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG11	34	0.24
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG12	34	0.24
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG13	34	0.24
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG21	34	0.24
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG22	34	0.24
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG23	34	0.24
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG11	34	0.24
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG12	34	0.24
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG13	34	0.24
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG21	34	0.24
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG22	34	0.24
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG23	34	0.24
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	1	0.24
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	1	0.24
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	1	0.24
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	1	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	1	0.24
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	1	0.24
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	3	0.24
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	3	0.24
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	3	0.24
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	3	0.24
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	3	0.24
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	3	0.24
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	30	0.24
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	30	0.24
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	30	0.24
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	30	0.24
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	30	0.24
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	30	0.24
(1,1357)	1:33:A:LEU:HD11	1:36:A:VAL:HB	11	0.23
(1,1357)	1:33:A:LEU:HD12	1:36:A:VAL:HB	11	0.23
(1,1357)	1:33:A:LEU:HD13	1:36:A:VAL:HB	11	0.23
(1,1357)	1:33:A:LEU:HD21	1:36:A:VAL:HB	11	0.23
(1,1357)	1:33:A:LEU:HD22	1:36:A:VAL:HB	11	0.23
(1,1357)	1:33:A:LEU:HD23	1:36:A:VAL:HB	11	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	8	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	8	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	8	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	8	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	8	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	8	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	10	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	10	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	10	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	10	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	10	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	10	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	19	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	19	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	19	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	19	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	19	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	19	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	32	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	32	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	32	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	32	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	32	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	32	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	35	0.23
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	35	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	35	0.23
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	35	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	35	0.23
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	35	0.23
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	21	0.22
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	21	0.22
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	21	0.22
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	21	0.22
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	21	0.22
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	21	0.22
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	27	0.22
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	27	0.22
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	27	0.22
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	27	0.22
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	27	0.22
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	27	0.22
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	16	0.22
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	16	0.22
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	16	0.22
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	16	0.22
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	16	0.22
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	16	0.22
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	24	0.22
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	24	0.22
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	24	0.22
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	24	0.22
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	24	0.22
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	24	0.22
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	39	0.22
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	39	0.22
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	39	0.22
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	12	0.21
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	12	0.21
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	12	0.21
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	12	0.21
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	12	0.21
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	12	0.21
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	20	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	20	0.21
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	20	0.21
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	20	0.21
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	20	0.21
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	20	0.21
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	33	0.21
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	33	0.21
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	33	0.21
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	33	0.21
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	33	0.21
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	33	0.21
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB2	39	0.2
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB3	39	0.2
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB2	39	0.2
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB3	39	0.2
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	3	0.2
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	3	0.2
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	3	0.2
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	3	0.2
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	3	0.2
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	3	0.2
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	18	0.2
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	18	0.2
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	18	0.2
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	18	0.2
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	18	0.2
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	18	0.2
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	19	0.2
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	19	0.2
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	19	0.2
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	19	0.2
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	19	0.2
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	19	0.2
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	20	0.2
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	20	0.2
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	20	0.2
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	20	0.2
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	20	0.2
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	20	0.2
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	20	0.2
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	20	0.2
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	20	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	20	0.2
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	20	0.2
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	20	0.2
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	13	0.2
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	13	0.2
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	13	0.2
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	13	0.2
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	13	0.2
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	13	0.2
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	29	0.2
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	29	0.2
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	29	0.2
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	29	0.2
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	29	0.2
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	29	0.2
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	28	0.2
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	28	0.2
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	28	0.2
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	2	0.2
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	2	0.2
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	2	0.2
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	37	0.2
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	37	0.2
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	37	0.2
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	22	0.19
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	22	0.19
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	22	0.19
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	22	0.19
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	22	0.19
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	22	0.19
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	22	0.19
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	22	0.19
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	22	0.19
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	22	0.19
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	22	0.19
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	22	0.19
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	22	0.19
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	22	0.19
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	22	0.19
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	22	0.19
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	22	0.19
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	22	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	3	0.19
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	3	0.19
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	3	0.19
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	3	0.19
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	3	0.19
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	3	0.19
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	5	0.19
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	5	0.19
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	5	0.19
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	5	0.19
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	5	0.19
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	5	0.19
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	12	0.19
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	12	0.19
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	12	0.19
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	12	0.19
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	12	0.19
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	12	0.19
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	26	0.19
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	26	0.19
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	26	0.19
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	26	0.19
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	26	0.19
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	26	0.19
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	22	0.19
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	22	0.19
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	22	0.19
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	22	0.19
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	22	0.19
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	22	0.19
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	22	0.19
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	22	0.19
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	22	0.19
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	22	0.19
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	22	0.19
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	22	0.19
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	27	0.19
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	27	0.19
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	27	0.19
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	27	0.19
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	27	0.19
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	27	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	27	0.19
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	27	0.19
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	27	0.19
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	27	0.19
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	27	0.19
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	27	0.19
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	14	0.19
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	14	0.19
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	14	0.19
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	14	0.19
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	14	0.19
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	14	0.19
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	22	0.19
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	22	0.19
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	22	0.19
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	28	0.19
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	28	0.19
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	28	0.19
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	5	0.18
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	5	0.18
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	5	0.18
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	5	0.18
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	5	0.18
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	5	0.18
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	5	0.18
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	5	0.18
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	5	0.18
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	5	0.18
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	5	0.18
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	5	0.18
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	5	0.18
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	5	0.18
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	5	0.18
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	5	0.18
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	5	0.18
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	5	0.18
(1,1535)	1:48:A:ASP:HB2	1:49:A:PRO:HD3	37	0.18
(1,1535)	1:48:A:ASP:HB3	1:49:A:PRO:HD3	37	0.18
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	8	0.18
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	8	0.18
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	8	0.18
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	8	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	8	0.18
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	8	0.18
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	9	0.18
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	9	0.18
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	9	0.18
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	9	0.18
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	9	0.18
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	9	0.18
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	9	0.18
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	9	0.18
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	9	0.18
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	9	0.18
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	9	0.18
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	9	0.18
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	14	0.18
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	14	0.18
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	14	0.18
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	14	0.18
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	14	0.18
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	14	0.18
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	14	0.18
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	14	0.18
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	14	0.18
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	14	0.18
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	14	0.18
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	14	0.18
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG11	37	0.18
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG12	37	0.18
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG13	37	0.18
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG21	37	0.18
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG22	37	0.18
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG23	37	0.18
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG11	37	0.18
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG12	37	0.18
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG13	37	0.18
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG21	37	0.18
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG22	37	0.18
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG23	37	0.18
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	9	0.18
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	9	0.18
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	9	0.18
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	9	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	9	0.18
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	9	0.18
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	11	0.18
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	11	0.18
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	11	0.18
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	11	0.18
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	11	0.18
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	11	0.18
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	15	0.18
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	15	0.18
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	15	0.18
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	23	0.18
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	23	0.18
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	23	0.18
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	28	0.18
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	28	0.18
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	28	0.18
(1,1859)	1:84:A:HIS:HE1	1:87:A:VAL:HG11	22	0.17
(1,1859)	1:84:A:HIS:HE1	1:87:A:VAL:HG12	22	0.17
(1,1859)	1:84:A:HIS:HE1	1:87:A:VAL:HG13	22	0.17
(1,1859)	1:84:A:HIS:HE1	1:87:A:VAL:HG21	22	0.17
(1,1859)	1:84:A:HIS:HE1	1:87:A:VAL:HG22	22	0.17
(1,1859)	1:84:A:HIS:HE1	1:87:A:VAL:HG23	22	0.17
(1,1779)	1:74:A:VAL:HG11	1:78:A:VAL:H	5	0.17
(1,1779)	1:74:A:VAL:HG12	1:78:A:VAL:H	5	0.17
(1,1779)	1:74:A:VAL:HG13	1:78:A:VAL:H	5	0.17
(1,1779)	1:74:A:VAL:HG21	1:78:A:VAL:H	5	0.17
(1,1779)	1:74:A:VAL:HG22	1:78:A:VAL:H	5	0.17
(1,1779)	1:74:A:VAL:HG23	1:78:A:VAL:H	5	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	1	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	1	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	1	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	1	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	1	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	1	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	1	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	1	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	1	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	1	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	1	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	1	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	1	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	1	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	1	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	1	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	1	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	12	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	12	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	12	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	12	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	12	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	12	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	12	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	12	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	12	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	12	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	12	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	12	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	12	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	12	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	12	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	12	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	12	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	12	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	14	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	14	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	14	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	14	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	14	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	14	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	14	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	14	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	14	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	14	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	14	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	14	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	14	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	14	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	14	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	14	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	14	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	14	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	37	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	37	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	37	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	37	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	37	0.17
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	37	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	37	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	37	0.17
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	37	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	37	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	37	0.17
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	37	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	37	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	37	0.17
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	37	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	37	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	37	0.17
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	37	0.17
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	1	0.17
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	1	0.17
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	1	0.17
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	1	0.17
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	1	0.17
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	1	0.17
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	7	0.17
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	7	0.17
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	7	0.17
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	7	0.17
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	7	0.17
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	7	0.17
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	20	0.17
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	20	0.17
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	20	0.17
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	20	0.17
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	20	0.17
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	20	0.17
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	32	0.17
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	32	0.17
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	32	0.17
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	32	0.17
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	32	0.17
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	32	0.17
(1,1494)	1:42:A:ARG:HB2	1:43:A:LEU:HD11	17	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	1:42:A:ARG:HB2	1:43:A:LEU:HD12	17	0.17
(1,1494)	1:42:A:ARG:HB2	1:43:A:LEU:HD13	17	0.17
(1,1494)	1:42:A:ARG:HB2	1:43:A:LEU:HD21	17	0.17
(1,1494)	1:42:A:ARG:HB2	1:43:A:LEU:HD22	17	0.17
(1,1494)	1:42:A:ARG:HB2	1:43:A:LEU:HD23	17	0.17
(1,1494)	1:42:A:ARG:HB3	1:43:A:LEU:HD11	17	0.17
(1,1494)	1:42:A:ARG:HB3	1:43:A:LEU:HD12	17	0.17
(1,1494)	1:42:A:ARG:HB3	1:43:A:LEU:HD13	17	0.17
(1,1494)	1:42:A:ARG:HB3	1:43:A:LEU:HD21	17	0.17
(1,1494)	1:42:A:ARG:HB3	1:43:A:LEU:HD22	17	0.17
(1,1494)	1:42:A:ARG:HB3	1:43:A:LEU:HD23	17	0.17
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG11	2	0.17
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG12	2	0.17
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG13	2	0.17
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG21	2	0.17
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG22	2	0.17
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG23	2	0.17
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG11	2	0.17
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG12	2	0.17
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG13	2	0.17
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG21	2	0.17
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG22	2	0.17
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG23	2	0.17
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG11	26	0.17
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG12	26	0.17
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG13	26	0.17
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG21	26	0.17
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG22	26	0.17
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG23	26	0.17
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG11	26	0.17
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG12	26	0.17
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG13	26	0.17
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG21	26	0.17
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG22	26	0.17
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG23	26	0.17
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG11	26	0.17
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG12	26	0.17
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG13	26	0.17
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG21	26	0.17
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG22	26	0.17
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG23	26	0.17
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	2	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	2	0.17
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	2	0.17
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	2	0.17
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	2	0.17
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	2	0.17
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	6	0.17
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	6	0.17
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	6	0.17
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	6	0.17
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	6	0.17
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	6	0.17
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	23	0.17
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	23	0.17
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	23	0.17
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	12	0.17
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	12	0.17
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	12	0.17
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	16	0.17
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	16	0.17
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	16	0.17
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	23	0.17
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	23	0.17
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	23	0.17
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	2	0.16
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	2	0.16
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	2	0.16
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	2	0.16
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	2	0.16
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	2	0.16
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	2	0.16
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	2	0.16
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	2	0.16
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	2	0.16
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	2	0.16
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	2	0.16
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	2	0.16
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	2	0.16
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	2	0.16
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	2	0.16
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	2	0.16
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	2	0.16
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	4	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	4	0.16
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	4	0.16
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	4	0.16
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	4	0.16
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	4	0.16
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	30	0.16
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	30	0.16
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	30	0.16
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	30	0.16
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	30	0.16
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	30	0.16
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	34	0.16
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	34	0.16
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	34	0.16
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	34	0.16
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	34	0.16
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	34	0.16
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD2	32	0.16
(1,1465)	1:39:A:LEU:HD11	1:58:A:LYS:HD3	32	0.16
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD2	32	0.16
(1,1465)	1:39:A:LEU:HD12	1:58:A:LYS:HD3	32	0.16
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD2	32	0.16
(1,1465)	1:39:A:LEU:HD13	1:58:A:LYS:HD3	32	0.16
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD2	32	0.16
(1,1465)	1:39:A:LEU:HD21	1:58:A:LYS:HD3	32	0.16
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD2	32	0.16
(1,1465)	1:39:A:LEU:HD22	1:58:A:LYS:HD3	32	0.16
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD2	32	0.16
(1,1465)	1:39:A:LEU:HD23	1:58:A:LYS:HD3	32	0.16
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	11	0.16
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	11	0.16
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	11	0.16
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	11	0.16
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	11	0.16
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	11	0.16
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	23	0.16
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	23	0.16
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	23	0.16
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	23	0.16
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	23	0.16
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	23	0.16
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	40	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	40	0.16
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	40	0.16
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	40	0.16
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	40	0.16
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	40	0.16
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	31	0.16
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	31	0.16
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	31	0.16
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	31	0.16
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	31	0.16
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	31	0.16
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE1	36	0.16
(1,737)	1:43:A:LEU:HD11	1:55:A:TYR:HE2	36	0.16
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE1	36	0.16
(1,737)	1:43:A:LEU:HD12	1:55:A:TYR:HE2	36	0.16
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE1	36	0.16
(1,737)	1:43:A:LEU:HD13	1:55:A:TYR:HE2	36	0.16
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	2	0.16
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	2	0.16
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	2	0.16
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB1	40	0.16
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB2	40	0.16
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB3	40	0.16
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB1	40	0.16
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB2	40	0.16
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB3	40	0.16
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	25	0.16
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	25	0.16
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	25	0.16
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	27	0.16
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	27	0.16
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	27	0.16
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	15	0.16
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	15	0.16
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	15	0.16
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	27	0.16
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	27	0.16
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	27	0.16
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	8	0.15
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	8	0.15
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	8	0.15
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	8	0.15
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	8	0.15
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	8	0.15
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	8	0.15
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	8	0.15
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	8	0.15
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	8	0.15
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	8	0.15
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	8	0.15
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	8	0.15
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	8	0.15
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	8	0.15
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	8	0.15
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	8	0.15
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	18	0.15
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	18	0.15
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	18	0.15
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	18	0.15
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	18	0.15
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	18	0.15
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	18	0.15
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	18	0.15
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	18	0.15
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	18	0.15
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	18	0.15
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	18	0.15
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	18	0.15
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	18	0.15
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	18	0.15
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	18	0.15
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	18	0.15
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	18	0.15
(1,1533)	1:48:A:ASP:HB2	1:49:A:PRO:HG2	37	0.15
(1,1533)	1:48:A:ASP:HB2	1:49:A:PRO:HG3	37	0.15
(1,1533)	1:48:A:ASP:HB3	1:49:A:PRO:HG2	37	0.15
(1,1533)	1:48:A:ASP:HB3	1:49:A:PRO:HG3	37	0.15
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	37	0.15
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	37	0.15
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	37	0.15
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	37	0.15
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	37	0.15
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	37	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1356)	1:33:A:LEU:HD11	1:34:A:GLN:HE21	2	0.15
(1,1356)	1:33:A:LEU:HD11	1:34:A:GLN:HE22	2	0.15
(1,1356)	1:33:A:LEU:HD12	1:34:A:GLN:HE21	2	0.15
(1,1356)	1:33:A:LEU:HD12	1:34:A:GLN:HE22	2	0.15
(1,1356)	1:33:A:LEU:HD13	1:34:A:GLN:HE21	2	0.15
(1,1356)	1:33:A:LEU:HD13	1:34:A:GLN:HE22	2	0.15
(1,1356)	1:33:A:LEU:HD21	1:34:A:GLN:HE21	2	0.15
(1,1356)	1:33:A:LEU:HD21	1:34:A:GLN:HE22	2	0.15
(1,1356)	1:33:A:LEU:HD22	1:34:A:GLN:HE21	2	0.15
(1,1356)	1:33:A:LEU:HD22	1:34:A:GLN:HE22	2	0.15
(1,1356)	1:33:A:LEU:HD23	1:34:A:GLN:HE21	2	0.15
(1,1356)	1:33:A:LEU:HD23	1:34:A:GLN:HE22	2	0.15
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	11	0.15
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	11	0.15
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	11	0.15
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	11	0.15
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	11	0.15
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	11	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	17	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	17	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	17	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	27	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	27	0.15
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	27	0.15
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	5	0.15
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	5	0.15
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	5	0.15
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	2	0.15
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	2	0.15
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	2	0.15
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	15	0.15
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	15	0.15
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	15	0.15
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG21	23	0.15
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG22	23	0.15
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG23	23	0.15
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	25	0.15
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	25	0.15
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	25	0.15
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG11	28	0.14
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG12	28	0.14
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG13	28	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG21	28	0.14
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG22	28	0.14
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG23	28	0.14
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	19	0.14
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	19	0.14
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	19	0.14
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	19	0.14
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	19	0.14
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	19	0.14
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	19	0.14
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	19	0.14
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	19	0.14
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	19	0.14
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	19	0.14
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	19	0.14
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	19	0.14
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	19	0.14
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	19	0.14
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	19	0.14
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	19	0.14
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	19	0.14
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	23	0.14
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	23	0.14
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	23	0.14
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	23	0.14
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	23	0.14
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	23	0.14
(1,1535)	1:48:A:ASP:HB2	1:49:A:PRO:HD3	28	0.14
(1,1535)	1:48:A:ASP:HB3	1:49:A:PRO:HD3	28	0.14
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	9	0.14
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	9	0.14
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	9	0.14
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	9	0.14
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	9	0.14
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	9	0.14
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	10	0.14
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	10	0.14
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	10	0.14
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	10	0.14
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	10	0.14
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	10	0.14
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	11	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	11	0.14
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	11	0.14
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	11	0.14
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	11	0.14
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	11	0.14
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	35	0.14
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	35	0.14
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	35	0.14
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	35	0.14
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	35	0.14
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	35	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG11	35	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG12	35	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG13	35	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG21	35	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG22	35	0.14
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG23	35	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG11	35	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG12	35	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG13	35	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG21	35	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG22	35	0.14
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG23	35	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG11	35	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG12	35	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG13	35	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG21	35	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG22	35	0.14
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG23	35	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG11	40	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG12	40	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG13	40	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG21	40	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG22	40	0.14
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG23	40	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG11	40	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG12	40	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG13	40	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG21	40	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG22	40	0.14
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG23	40	0.14
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	22	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	22	0.14
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	22	0.14
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	40	0.14
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	40	0.14
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	40	0.14
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	3	0.14
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	3	0.14
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	3	0.14
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	18	0.14
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	18	0.14
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	18	0.14
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	29	0.14
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	29	0.14
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	29	0.14
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	38	0.14
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	38	0.14
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	38	0.14
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	40	0.14
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	40	0.14
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	40	0.14
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB2	22	0.13
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB3	22	0.13
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB2	22	0.13
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB3	22	0.13
(1,1835)	1:81:A:LEU:HB2	1:87:A:VAL:HG11	6	0.13
(1,1835)	1:81:A:LEU:HB2	1:87:A:VAL:HG12	6	0.13
(1,1835)	1:81:A:LEU:HB2	1:87:A:VAL:HG13	6	0.13
(1,1835)	1:81:A:LEU:HB2	1:87:A:VAL:HG21	6	0.13
(1,1835)	1:81:A:LEU:HB2	1:87:A:VAL:HG22	6	0.13
(1,1835)	1:81:A:LEU:HB2	1:87:A:VAL:HG23	6	0.13
(1,1835)	1:81:A:LEU:HB3	1:87:A:VAL:HG11	6	0.13
(1,1835)	1:81:A:LEU:HB3	1:87:A:VAL:HG12	6	0.13
(1,1835)	1:81:A:LEU:HB3	1:87:A:VAL:HG13	6	0.13
(1,1835)	1:81:A:LEU:HB3	1:87:A:VAL:HG21	6	0.13
(1,1835)	1:81:A:LEU:HB3	1:87:A:VAL:HG22	6	0.13
(1,1835)	1:81:A:LEU:HB3	1:87:A:VAL:HG23	6	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	3	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	3	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	3	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	3	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	3	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	3	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	3	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	3	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	3	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	3	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	3	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	3	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	3	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	3	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	3	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	3	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	3	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	3	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	6	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	6	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	6	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	6	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	6	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	6	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	6	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	6	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	6	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	6	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	6	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	6	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	6	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	6	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	6	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	6	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	6	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	6	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	16	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	16	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	16	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	16	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	16	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	16	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	16	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	16	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	16	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	16	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	16	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	16	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	16	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	16	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	16	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	16	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	16	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	16	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	20	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	20	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	20	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	20	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	20	0.13
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	20	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	20	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	20	0.13
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	20	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	20	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	20	0.13
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	20	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	20	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	20	0.13
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	20	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	20	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	20	0.13
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	20	0.13
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	25	0.13
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	25	0.13
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	25	0.13
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	25	0.13
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	25	0.13
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	25	0.13
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	13	0.13
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	13	0.13
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	13	0.13
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	13	0.13
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	13	0.13
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	13	0.13
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	29	0.13
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	29	0.13
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	29	0.13
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	29	0.13
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	29	0.13
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	29	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	36	0.13
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	36	0.13
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	36	0.13
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	36	0.13
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	36	0.13
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	36	0.13
(1,1356)	1:33:A:LEU:HD11	1:34:A:GLN:HE21	26	0.13
(1,1356)	1:33:A:LEU:HD11	1:34:A:GLN:HE22	26	0.13
(1,1356)	1:33:A:LEU:HD12	1:34:A:GLN:HE21	26	0.13
(1,1356)	1:33:A:LEU:HD12	1:34:A:GLN:HE22	26	0.13
(1,1356)	1:33:A:LEU:HD13	1:34:A:GLN:HE21	26	0.13
(1,1356)	1:33:A:LEU:HD13	1:34:A:GLN:HE22	26	0.13
(1,1356)	1:33:A:LEU:HD21	1:34:A:GLN:HE21	26	0.13
(1,1356)	1:33:A:LEU:HD21	1:34:A:GLN:HE22	26	0.13
(1,1356)	1:33:A:LEU:HD22	1:34:A:GLN:HE21	26	0.13
(1,1356)	1:33:A:LEU:HD22	1:34:A:GLN:HE22	26	0.13
(1,1356)	1:33:A:LEU:HD23	1:34:A:GLN:HE21	26	0.13
(1,1356)	1:33:A:LEU:HD23	1:34:A:GLN:HE22	26	0.13
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG11	23	0.13
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG12	23	0.13
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG13	23	0.13
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG21	23	0.13
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG22	23	0.13
(1,1346)	1:32:A:ALA:HB1	1:36:A:VAL:HG23	23	0.13
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG11	23	0.13
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG12	23	0.13
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG13	23	0.13
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG21	23	0.13
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG22	23	0.13
(1,1346)	1:32:A:ALA:HB2	1:36:A:VAL:HG23	23	0.13
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG11	23	0.13
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG12	23	0.13
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG13	23	0.13
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG21	23	0.13
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG22	23	0.13
(1,1346)	1:32:A:ALA:HB3	1:36:A:VAL:HG23	23	0.13
(1,1334)	1:30:A:GLU:HG2	1:35:A:VAL:HG11	36	0.13
(1,1334)	1:30:A:GLU:HG2	1:35:A:VAL:HG12	36	0.13
(1,1334)	1:30:A:GLU:HG2	1:35:A:VAL:HG13	36	0.13
(1,1334)	1:30:A:GLU:HG2	1:35:A:VAL:HG21	36	0.13
(1,1334)	1:30:A:GLU:HG2	1:35:A:VAL:HG22	36	0.13
(1,1334)	1:30:A:GLU:HG2	1:35:A:VAL:HG23	36	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1334)	1:30:A:GLU:HG3	1:35:A:VAL:HG11	36	0.13
(1,1334)	1:30:A:GLU:HG3	1:35:A:VAL:HG12	36	0.13
(1,1334)	1:30:A:GLU:HG3	1:35:A:VAL:HG13	36	0.13
(1,1334)	1:30:A:GLU:HG3	1:35:A:VAL:HG21	36	0.13
(1,1334)	1:30:A:GLU:HG3	1:35:A:VAL:HG22	36	0.13
(1,1334)	1:30:A:GLU:HG3	1:35:A:VAL:HG23	36	0.13
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG11	36	0.13
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG12	36	0.13
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG13	36	0.13
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG21	36	0.13
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG22	36	0.13
(1,1333)	1:30:A:GLU:HB2	1:35:A:VAL:HG23	36	0.13
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG11	36	0.13
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG12	36	0.13
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG13	36	0.13
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG21	36	0.13
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG22	36	0.13
(1,1333)	1:30:A:GLU:HB3	1:35:A:VAL:HG23	36	0.13
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	27	0.13
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	27	0.13
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	27	0.13
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	27	0.13
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	27	0.13
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	27	0.13
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG21	37	0.13
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG22	37	0.13
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG23	37	0.13
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG21	37	0.13
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG22	37	0.13
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG23	37	0.13
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD21	37	0.13
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD22	37	0.13
(1,328)	1:40:A:GLN:HA	1:43:A:LEU:HD23	37	0.13
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB1	39	0.13
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB2	39	0.13
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB3	39	0.13
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB1	39	0.13
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB2	39	0.13
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB3	39	0.13
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	1	0.13
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	1	0.13
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	8	0.13
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	8	0.13
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	8	0.13
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	19	0.13
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	19	0.13
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	19	0.13
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	20	0.13
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	20	0.13
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	20	0.13
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	16	0.13
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	16	0.13
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	16	0.13
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG21	28	0.13
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG22	28	0.13
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG23	28	0.13
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	2	0.13
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	2	0.13
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	2	0.13
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	21	0.13
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	21	0.13
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	21	0.13
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	22	0.13
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	22	0.13
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	22	0.13
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	13	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	13	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	13	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	13	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	13	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	13	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	13	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	13	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	13	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	13	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	13	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	13	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	13	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	13	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	13	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	13	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	13	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	13	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	29	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	29	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	29	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	29	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	29	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	29	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	29	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	29	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	29	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	29	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	29	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	29	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	29	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	29	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	29	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	29	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	29	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	29	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	31	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	31	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	31	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	31	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	31	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	31	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	31	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	31	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	31	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	31	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	31	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	31	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	31	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	31	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	31	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	31	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	31	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	31	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	32	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	32	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	32	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	32	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	32	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	32	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	32	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	32	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	32	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	32	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	32	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	32	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	32	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	32	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	32	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	32	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	32	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	32	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	38	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	38	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	38	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	38	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	38	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	38	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	38	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	38	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	38	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	38	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	38	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	38	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	38	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	38	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	38	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	38	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	38	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	38	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	39	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	39	0.12
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	39	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	39	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	39	0.12
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	39	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	39	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	39	0.12
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	39	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	39	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	39	0.12
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	39	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	39	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	39	0.12
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	39	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	39	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	39	0.12
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	39	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	27	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	27	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	27	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	27	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	27	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	27	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	28	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	28	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	28	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	28	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	28	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	28	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	39	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	39	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	39	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	39	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	39	0.12
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	39	0.12
(1,1537)	1:48:A:ASP:HB2	1:50:A:LYS:HG2	3	0.12
(1,1537)	1:48:A:ASP:HB2	1:50:A:LYS:HG3	3	0.12
(1,1537)	1:48:A:ASP:HB3	1:50:A:LYS:HG2	3	0.12
(1,1537)	1:48:A:ASP:HB3	1:50:A:LYS:HG3	3	0.12
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	14	0.12
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	14	0.12
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	14	0.12
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	14	0.12
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	14	0.12
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	14	0.12
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	24	0.12
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	24	0.12
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	24	0.12
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	24	0.12
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	24	0.12
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	24	0.12
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	33	0.12
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	33	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	33	0.12
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	33	0.12
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	33	0.12
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	33	0.12
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	36	0.12
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	36	0.12
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	36	0.12
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	36	0.12
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	36	0.12
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	36	0.12
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	22	0.12
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	22	0.12
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	22	0.12
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	22	0.12
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	22	0.12
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	22	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG11	6	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG12	6	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG13	6	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG21	6	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG22	6	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG23	6	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG11	6	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG12	6	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG13	6	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG21	6	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG22	6	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG23	6	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG11	20	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG12	20	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG13	20	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG21	20	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG22	20	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG23	20	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG11	20	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG12	20	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG13	20	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG21	20	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG22	20	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG23	20	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG11	31	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG12	31	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG13	31	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG21	31	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG22	31	0.12
(1,1379)	1:34:A:GLN:HG2	1:35:A:VAL:HG23	31	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG11	31	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG12	31	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG13	31	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG21	31	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG22	31	0.12
(1,1379)	1:34:A:GLN:HG3	1:35:A:VAL:HG23	31	0.12
(1,744)	1:29:A:ALA:HB1	1:30:A:GLU:H	40	0.12
(1,744)	1:29:A:ALA:HB2	1:30:A:GLU:H	40	0.12
(1,744)	1:29:A:ALA:HB3	1:30:A:GLU:H	40	0.12
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG21	23	0.12
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG22	23	0.12
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG23	23	0.12
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG21	23	0.12
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG22	23	0.12
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG23	23	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB1	5	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB2	5	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB3	5	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB1	5	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB2	5	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB3	5	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB1	16	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB2	16	0.12
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB3	16	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB1	16	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB2	16	0.12
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB3	16	0.12
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	6	0.12
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	6	0.12
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	6	0.12
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	32	0.12
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	32	0.12
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	32	0.12
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	21	0.12
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	21	0.12
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	21	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG21	15	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG22	15	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG23	15	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG21	27	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG22	27	0.12
(1,72)	1:37:A:GLU:HA	1:68:A:ILE:HG23	27	0.12
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	16	0.12
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	16	0.12
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	16	0.12
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	30	0.12
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	30	0.12
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	30	0.12
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	34	0.12
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	34	0.12
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	34	0.12
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	37	0.12
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	37	0.12
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	37	0.12
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB2	1	0.11
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB3	1	0.11
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB2	1	0.11
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB3	1	0.11
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB2	5	0.11
(1,1890)	1:92:A:ARG:HG2	1:93:A:ASP:HB3	5	0.11
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB2	5	0.11
(1,1890)	1:92:A:ARG:HG3	1:93:A:ASP:HB3	5	0.11
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG11	39	0.11
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG12	39	0.11
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG13	39	0.11
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG21	39	0.11
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG22	39	0.11
(1,1864)	1:86:A:HIS:HD2	1:87:A:VAL:HG23	39	0.11
(1,1840)	1:81:A:LEU:HD11	1:84:A:HIS:HD2	27	0.11
(1,1840)	1:81:A:LEU:HD12	1:84:A:HIS:HD2	27	0.11
(1,1840)	1:81:A:LEU:HD13	1:84:A:HIS:HD2	27	0.11
(1,1840)	1:81:A:LEU:HD21	1:84:A:HIS:HD2	27	0.11
(1,1840)	1:81:A:LEU:HD22	1:84:A:HIS:HD2	27	0.11
(1,1840)	1:81:A:LEU:HD23	1:84:A:HIS:HD2	27	0.11
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	36	0.11
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	36	0.11
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	36	0.11
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	36	0.11
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	36	0.11
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	36	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	36	0.11
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	36	0.11
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	36	0.11
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	36	0.11
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	36	0.11
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	36	0.11
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	36	0.11
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	36	0.11
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	36	0.11
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	36	0.11
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	36	0.11
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	36	0.11
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	2	0.11
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	2	0.11
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	2	0.11
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	2	0.11
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	2	0.11
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	2	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	5	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	5	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	5	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	5	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	5	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	5	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	12	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	12	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	12	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	12	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	12	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	12	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	17	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	17	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	17	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	17	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	17	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	17	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	20	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	20	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	20	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	20	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	20	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	20	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	24	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	24	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	24	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	24	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	24	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	24	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	34	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	34	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	34	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	34	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	34	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	34	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	40	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	40	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	40	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	40	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	40	0.11
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	40	0.11
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB1	25	0.11
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB2	25	0.11
(1,309)	1:82:A:ARG:HG2	1:91:A:ALA:HB3	25	0.11
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB1	25	0.11
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB2	25	0.11
(1,309)	1:82:A:ARG:HG3	1:91:A:ALA:HB3	25	0.11
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	9	0.11
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	9	0.11
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	9	0.11
(1,140)	1:36:A:VAL:HG21	1:37:A:GLU:HA	36	0.11
(1,140)	1:36:A:VAL:HG22	1:37:A:GLU:HA	36	0.11
(1,140)	1:36:A:VAL:HG23	1:37:A:GLU:HA	36	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	17	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	17	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	17	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	34	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	34	0.11
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	34	0.11
(1,71)	1:32:A:ALA:HA	1:68:A:ILE:HG21	23	0.11
(1,71)	1:32:A:ALA:HA	1:68:A:ILE:HG22	23	0.11
(1,71)	1:32:A:ALA:HA	1:68:A:ILE:HG23	23	0.11
(1,70)	1:68:A:ILE:HG21	1:72:A:THR:HB	23	0.11
(1,70)	1:68:A:ILE:HG22	1:72:A:THR:HB	23	0.11
(1,70)	1:68:A:ILE:HG23	1:72:A:THR:HB	23	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:68:A:ILE:HG21	1:72:A:THR:HB	27	0.11
(1,70)	1:68:A:ILE:HG22	1:72:A:THR:HB	27	0.11
(1,70)	1:68:A:ILE:HG23	1:72:A:THR:HB	27	0.11
(1,70)	1:68:A:ILE:HG21	1:72:A:THR:HB	28	0.11
(1,70)	1:68:A:ILE:HG22	1:72:A:THR:HB	28	0.11
(1,70)	1:68:A:ILE:HG23	1:72:A:THR:HB	28	0.11
(1,35)	1:26:A:ALA:HB1	1:27:A:MET:HE1	21	0.11
(1,35)	1:26:A:ALA:HB1	1:27:A:MET:HE2	21	0.11
(1,35)	1:26:A:ALA:HB1	1:27:A:MET:HE3	21	0.11
(1,35)	1:26:A:ALA:HB2	1:27:A:MET:HE1	21	0.11
(1,35)	1:26:A:ALA:HB2	1:27:A:MET:HE2	21	0.11
(1,35)	1:26:A:ALA:HB2	1:27:A:MET:HE3	21	0.11
(1,35)	1:26:A:ALA:HB3	1:27:A:MET:HE1	21	0.11
(1,35)	1:26:A:ALA:HB3	1:27:A:MET:HE2	21	0.11
(1,35)	1:26:A:ALA:HB3	1:27:A:MET:HE3	21	0.11
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	7	0.11
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	7	0.11
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	7	0.11
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	10	0.11
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	10	0.11
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	10	0.11
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	17	0.11
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	17	0.11
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	17	0.11
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	26	0.11
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	26	0.11
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	26	0.11
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	39	0.11
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	39	0.11
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	39	0.11
(1,1916)	1:95:A:VAL:HG11	1:99:A:LYS:HG2	4	0.1
(1,1916)	1:95:A:VAL:HG11	1:99:A:LYS:HG3	4	0.1
(1,1916)	1:95:A:VAL:HG12	1:99:A:LYS:HG2	4	0.1
(1,1916)	1:95:A:VAL:HG12	1:99:A:LYS:HG3	4	0.1
(1,1916)	1:95:A:VAL:HG13	1:99:A:LYS:HG2	4	0.1
(1,1916)	1:95:A:VAL:HG13	1:99:A:LYS:HG3	4	0.1
(1,1916)	1:95:A:VAL:HG21	1:99:A:LYS:HG2	4	0.1
(1,1916)	1:95:A:VAL:HG21	1:99:A:LYS:HG3	4	0.1
(1,1916)	1:95:A:VAL:HG22	1:99:A:LYS:HG2	4	0.1
(1,1916)	1:95:A:VAL:HG22	1:99:A:LYS:HG3	4	0.1
(1,1916)	1:95:A:VAL:HG23	1:99:A:LYS:HG2	4	0.1
(1,1916)	1:95:A:VAL:HG23	1:99:A:LYS:HG3	4	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD11	9	0.1
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD12	9	0.1
(1,1685)	1:59:A:LEU:HD11	1:64:A:ILE:HD13	9	0.1
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD11	9	0.1
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD12	9	0.1
(1,1685)	1:59:A:LEU:HD12	1:64:A:ILE:HD13	9	0.1
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD11	9	0.1
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD12	9	0.1
(1,1685)	1:59:A:LEU:HD13	1:64:A:ILE:HD13	9	0.1
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD11	9	0.1
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD12	9	0.1
(1,1685)	1:59:A:LEU:HD21	1:64:A:ILE:HD13	9	0.1
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD11	9	0.1
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD12	9	0.1
(1,1685)	1:59:A:LEU:HD22	1:64:A:ILE:HD13	9	0.1
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD11	9	0.1
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD12	9	0.1
(1,1685)	1:59:A:LEU:HD23	1:64:A:ILE:HD13	9	0.1
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD11	15	0.1
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD12	15	0.1
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD13	15	0.1
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD21	15	0.1
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD22	15	0.1
(1,1661)	1:58:A:LYS:H	1:62:A:LEU:HD23	15	0.1
(1,1535)	1:48:A:ASP:HB2	1:49:A:PRO:HD3	25	0.1
(1,1535)	1:48:A:ASP:HB3	1:49:A:PRO:HD3	25	0.1
(1,1506)	1:43:A:LEU:HD11	1:55:A:TYR:HD1	6	0.1
(1,1506)	1:43:A:LEU:HD12	1:55:A:TYR:HD1	6	0.1
(1,1506)	1:43:A:LEU:HD13	1:55:A:TYR:HD1	6	0.1
(1,1506)	1:43:A:LEU:HD21	1:55:A:TYR:HD1	6	0.1
(1,1506)	1:43:A:LEU:HD22	1:55:A:TYR:HD1	6	0.1
(1,1506)	1:43:A:LEU:HD23	1:55:A:TYR:HD1	6	0.1
(1,1453)	1:39:A:LEU:HD11	1:42:A:ARG:HG3	23	0.1
(1,1453)	1:39:A:LEU:HD12	1:42:A:ARG:HG3	23	0.1
(1,1453)	1:39:A:LEU:HD13	1:42:A:ARG:HG3	23	0.1
(1,1453)	1:39:A:LEU:HD21	1:42:A:ARG:HG3	23	0.1
(1,1453)	1:39:A:LEU:HD22	1:42:A:ARG:HG3	23	0.1
(1,1453)	1:39:A:LEU:HD23	1:42:A:ARG:HG3	23	0.1
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD11	27	0.1
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD12	27	0.1
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD13	27	0.1
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD21	27	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD22	27	0.1
(1,1437)	1:38:A:LYS:H	1:59:A:LEU:HD23	27	0.1
(1,1354)	1:33:A:LEU:HD11	1:34:A:GLN:HA	16	0.1
(1,1354)	1:33:A:LEU:HD12	1:34:A:GLN:HA	16	0.1
(1,1354)	1:33:A:LEU:HD13	1:34:A:GLN:HA	16	0.1
(1,1354)	1:33:A:LEU:HD21	1:34:A:GLN:HA	16	0.1
(1,1354)	1:33:A:LEU:HD22	1:34:A:GLN:HA	16	0.1
(1,1354)	1:33:A:LEU:HD23	1:34:A:GLN:HA	16	0.1
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG2	36	0.1
(1,1328)	1:29:A:ALA:HB1	1:30:A:GLU:HG3	36	0.1
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG2	36	0.1
(1,1328)	1:29:A:ALA:HB2	1:30:A:GLU:HG3	36	0.1
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG2	36	0.1
(1,1328)	1:29:A:ALA:HB3	1:30:A:GLU:HG3	36	0.1
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG21	40	0.1
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG22	40	0.1
(1,354)	1:49:A:PRO:HG2	1:87:A:VAL:HG23	40	0.1
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG21	40	0.1
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG22	40	0.1
(1,354)	1:49:A:PRO:HG3	1:87:A:VAL:HG23	40	0.1
(1,278)	1:55:A:TYR:HB2	1:56:A:LEU:HD11	28	0.1
(1,278)	1:55:A:TYR:HB2	1:56:A:LEU:HD12	28	0.1
(1,278)	1:55:A:TYR:HB2	1:56:A:LEU:HD13	28	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	10	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	10	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	10	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	18	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	18	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	18	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	26	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	26	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	26	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG21	30	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG22	30	0.1
(1,86)	1:73:A:GLY:H	1:74:A:VAL:HG23	30	0.1
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	4	0.1
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	4	0.1
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	4	0.1
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	5	0.1
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	5	0.1
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	5	0.1
(1,8)	1:64:A:ILE:HD11	1:65:A:THR:HA	35	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:64:A:ILE:HD12	1:65:A:THR:HA	35	0.1
(1,8)	1:64:A:ILE:HD13	1:65:A:THR:HA	35	0.1

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

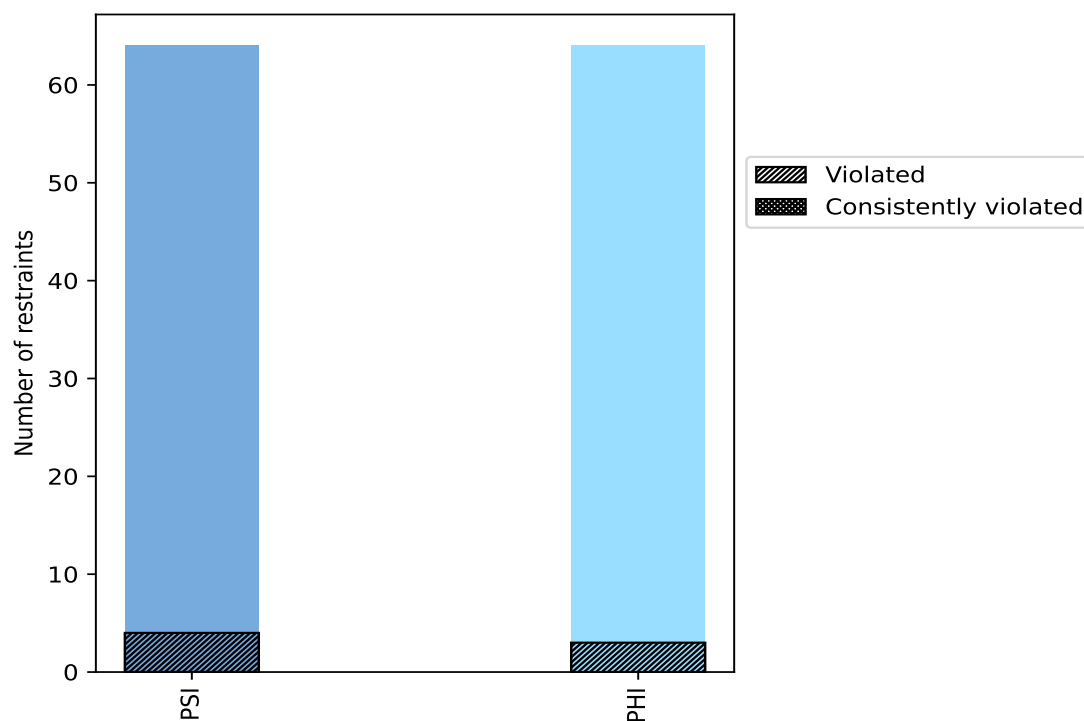
10.1 Summary of dihedral-angle violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	64	50.0	4	6.2	3.1	0	0.0	0.0
PHI	64	50.0	3	4.7	2.3	0	0.0	0.0
Total	128	100.0	7	5.5	5.5	0	0.0	0.0

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

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



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

10.2 Dihedral-angle violation statistics for each model

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

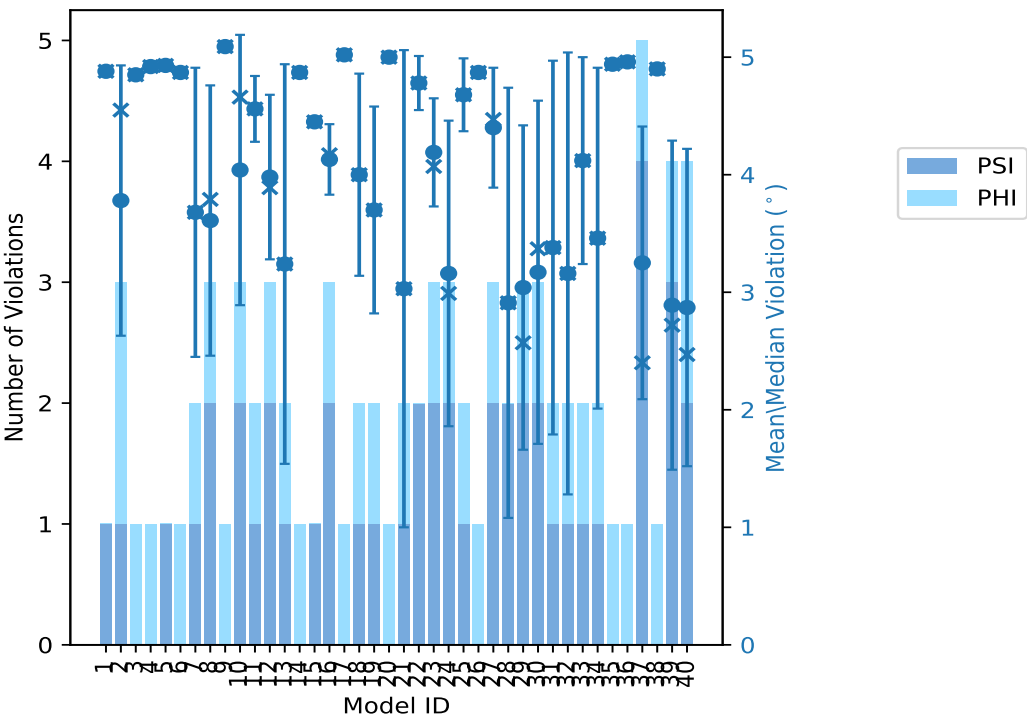
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	0	1	4.88	4.88	0.0	4.88
2	1	2	3	3.78	4.63	1.15	4.55
3	0	1	1	4.85	4.85	0.0	4.85
4	0	1	1	4.92	4.92	0.0	4.92
5	1	0	1	4.93	4.93	0.0	4.93
6	0	1	1	4.87	4.87	0.0	4.87
7	1	1	2	3.68	4.91	1.23	3.68
8	2	1	3	3.61	4.93	1.15	3.79
9	0	1	1	5.09	5.09	0.0	5.09
10	2	1	3	4.04	5.03	1.15	4.66
11	1	1	2	4.56	4.85	0.28	4.56
12	2	1	3	3.98	4.87	0.7	3.89
13	1	1	2	3.24	4.94	1.7	3.24
14	0	1	1	4.87	4.87	0.0	4.87
15	1	0	1	4.45	4.45	0.0	4.45
16	2	1	3	4.13	4.48	0.3	4.17
17	0	1	1	5.02	5.02	0.0	5.02
18	1	1	2	4.0	4.86	0.86	4.0
19	1	1	2	3.7	4.58	0.88	3.7
20	0	1	1	5.0	5.0	0.0	5.0
21	1	1	2	3.03	5.06	2.03	3.03
22	2	0	2	4.78	5.0	0.23	4.78
23	2	1	3	4.19	4.81	0.46	4.07
24	2	1	3	3.16	4.83	1.3	2.99
25	1	1	2	4.68	4.99	0.31	4.68
26	0	1	1	4.87	4.87	0.0	4.87
27	2	1	3	4.4	4.98	0.51	4.47
28	2	0	2	2.91	4.74	1.83	2.91
29	2	1	3	3.04	4.92	1.38	2.57
30	2	1	3	3.17	4.85	1.46	3.37
31	1	1	2	3.38	4.97	1.59	3.38
32	1	1	2	3.16	5.05	1.88	3.16
33	1	1	2	4.12	5.0	0.88	4.12
34	1	1	2	3.46	4.91	1.45	3.46
35	0	1	1	4.94	4.94	0.0	4.94
36	0	1	1	4.96	4.96	0.0	4.96
37	4	1	5	3.25	4.96	1.16	2.4
38	0	1	1	4.9	4.9	0.0	4.9

Continued on next page...

Continued from previous page...

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	3	1	4	2.89	5.0	1.4	2.72
40	2	2	4	2.87	4.95	1.35	2.47

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	1	2	1	2.5
0	1	1	2	5.0
0	0	0	3	7.5
0	0	0	4	10.0

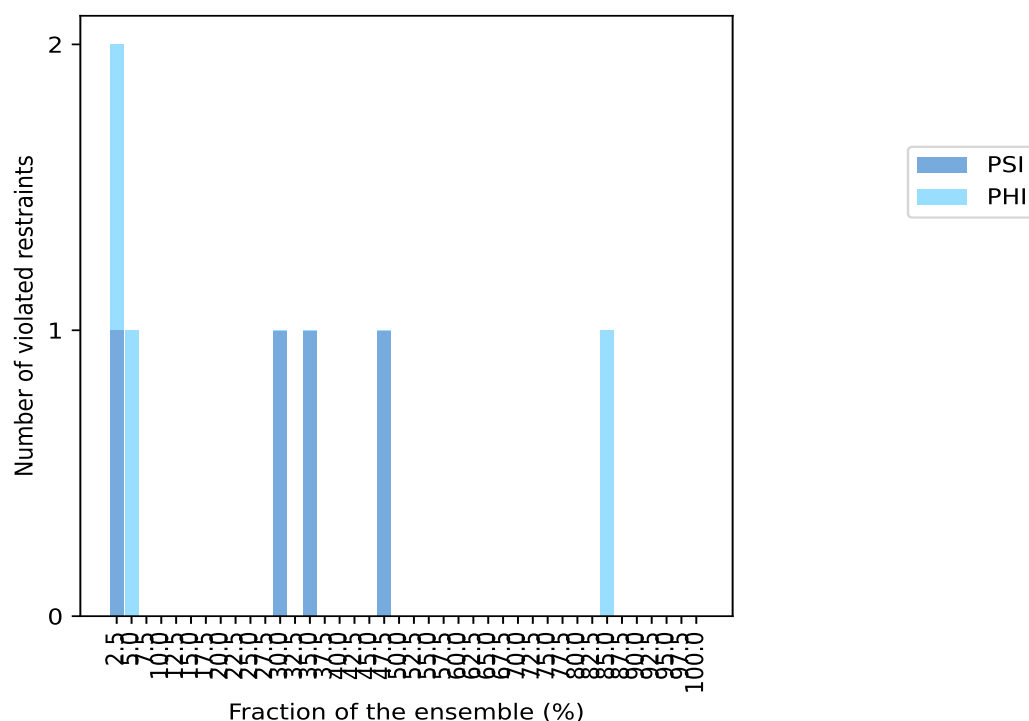
Continued on next page...

Continued from previous page...

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

¹ Number of models with violations

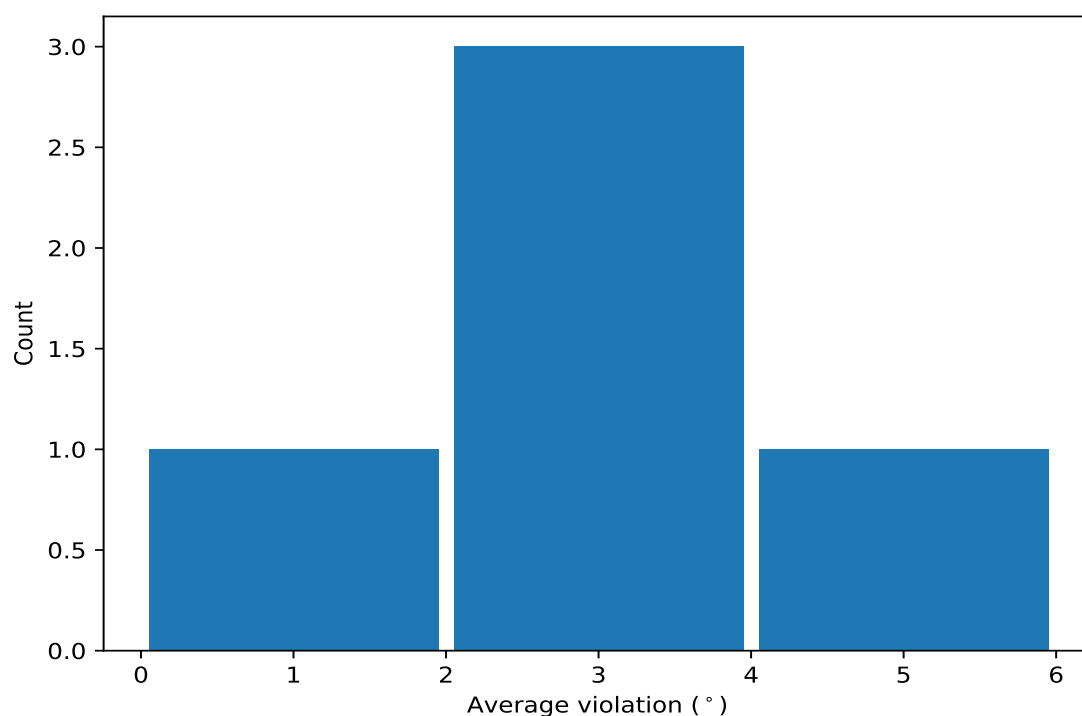
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

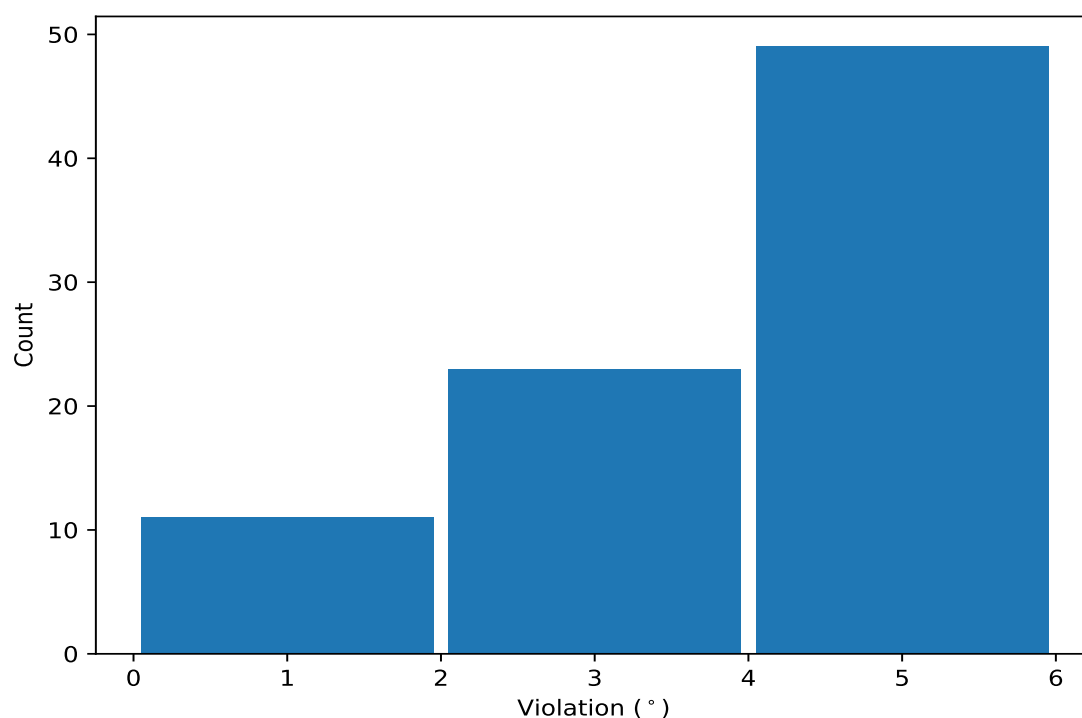
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	34	4.76	0.36	4.9
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	19	2.89	1.43	2.21
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	14	3.47	1.03	3.21
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	12	3.77	1.19	4.41
(1,125)	1:99:A:LYS:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	2	1.64	0.52	1.64

¹ Number of violated models, ²Standard 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 (°)
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	9	5.09
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	21	5.06
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	32	5.05
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	10	5.03
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	17	5.02
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	39	5.0
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	20	5.0
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	33	5.0
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	22	5.0
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	25	4.99
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	27	4.98
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	31	4.97
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	37	4.96
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	36	4.96
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	40	4.95
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	13	4.94
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	35	4.94
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	8	4.93
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	5	4.93
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	4	4.92
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	29	4.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	7	4.91
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	34	4.91
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	38	4.9
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	1	4.88
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	6	4.87
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	14	4.87
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	26	4.87
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	12	4.87
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	18	4.86
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	3	4.85
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	11	4.85
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	30	4.85
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	24	4.83
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	23	4.81
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	28	4.74
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	10	4.66
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	2	4.63
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	19	4.58
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	2	4.55
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	22	4.55
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	16	4.48
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	27	4.47
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	15	4.45
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	25	4.37
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	37	4.33
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	11	4.28
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	16	4.17
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	23	4.07
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	12	3.89
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	8	3.79
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	27	3.74
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	16	3.74
(1,105)	1:89:A:SER:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	23	3.7
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	30	3.37
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	33	3.25
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	40	3.19
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	12	3.17
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	18	3.14
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	39	3.04
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	24	2.99
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	19	2.83
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	29	2.57
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	7	2.46
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	10	2.42
(1,90)	1:81:A:LEU:N	1:81:A:LEU:CA	1:81:A:LEU:C	1:82:A:ARG:N	37	2.4
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	39	2.4
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	37	2.35
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	37	2.21
(1,125)	1:99:A:LYS:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	2	2.16
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	8	2.12
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	34	2.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	31	1.78
(1,120)	1:97:A:GLN:N	1:97:A:GLN:CA	1:97:A:GLN:C	1:98:A:TRP:N	40	1.75
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	24	1.67
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	29	1.63
(1,9)	1:34:A:GLN:C	1:35:A:VAL:N	1:35:A:VAL:CA	1:35:A:VAL:C	40	1.6
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	13	1.54
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	30	1.28
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	32	1.28
(1,125)	1:99:A:LYS:C	1:100:A:LYS:N	1:100:A:LYS:CA	1:100:A:LYS:C	39	1.13
(1,16)	1:38:A:LYS:N	1:38:A:LYS:CA	1:38:A:LYS:C	1:39:A:LEU:N	28	1.08
(1,32)	1:46:A:ASN:N	1:46:A:ASN:CA	1:46:A:ASN:C	1:47:A:PRO:N	21	1.0