



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:53 AM UTC

PDB ID : 9VCD / pdb_00009vcd
BMRB ID : 52953
Title : N-terminal dimeric C2H2-domain of Drosophila melanogaster IMZF protein
Authors : Dukhalin, S.D.; Mariasina, S.S.; Polshakov, V.I.; Bocharov, E.V.; Balagurov, K.I.
Deposited on : 2025-06-05

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 : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

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 45%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:21-A:42, A:47-A:57, B:20-B:41, B:47-B:57 (66)	0.21	14

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

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

The models can be grouped into 6 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 7, 9, 11, 12, 14, 17, 19
2	6, 8, 10
3	4, 5
4	13, 18
5	3, 20
6	15, 16

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2064 atoms, of which 1008 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FI23536p1.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1031	334	504	89	100	4	
1	B	68	Total	C	H	N	O	S	0
			1031	334	504	89	100	4	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9W3J0
A	2	GLY	-	expression tag	UNP Q9W3J0
A	3	SER	-	expression tag	UNP Q9W3J0
A	4	PRO	-	expression tag	UNP Q9W3J0
A	5	GLU	-	expression tag	UNP Q9W3J0
A	6	PHE	-	expression tag	UNP Q9W3J0
B	1	SER	-	expression tag	UNP Q9W3J0
B	2	GLY	-	expression tag	UNP Q9W3J0
B	3	SER	-	expression tag	UNP Q9W3J0
B	4	PRO	-	expression tag	UNP Q9W3J0
B	5	GLU	-	expression tag	UNP Q9W3J0
B	6	PHE	-	expression tag	UNP Q9W3J0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

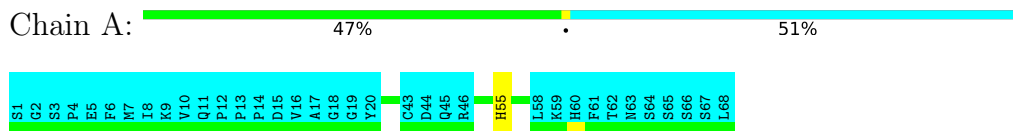
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

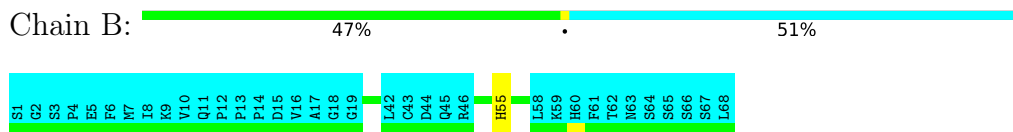
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: FI23536p1



- Molecule 1: FI23536p1

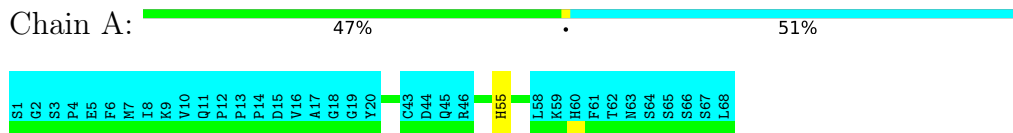


4.2 Scores per residue for each member of the ensemble

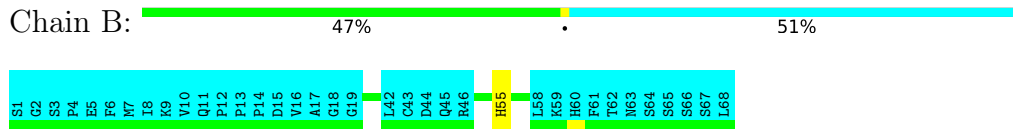
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: FI23536p1

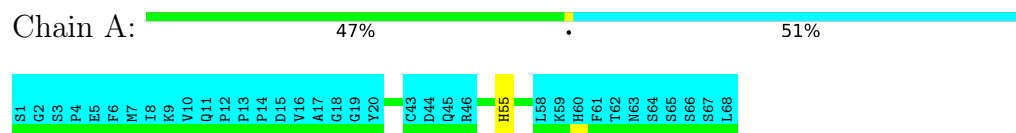


- Molecule 1: FI23536p1

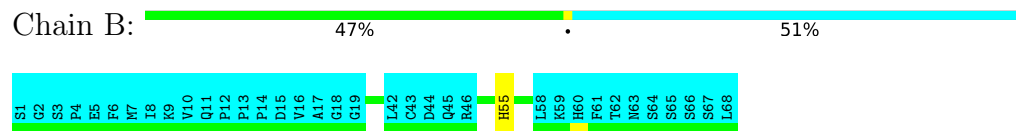


4.2.2 Score per residue for model 2

- Molecule 1: FI23536p1

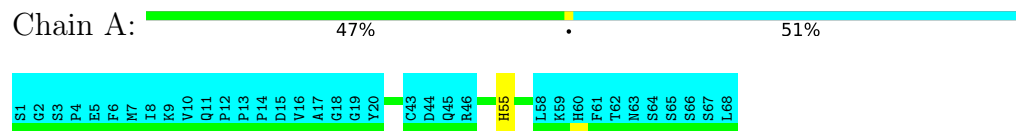


- Molecule 1: FI23536p1

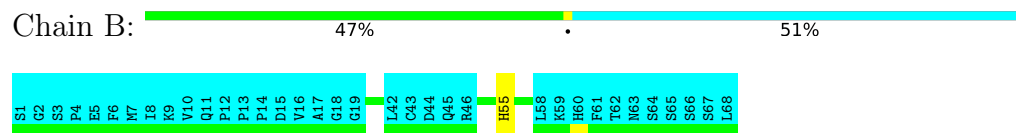


4.2.3 Score per residue for model 3

- Molecule 1: FI23536p1

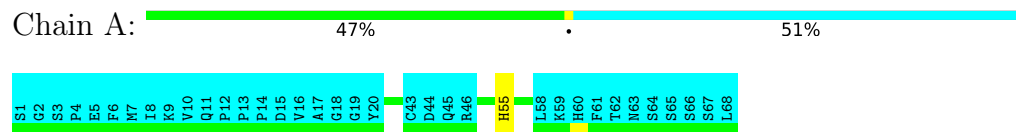


- Molecule 1: FI23536p1

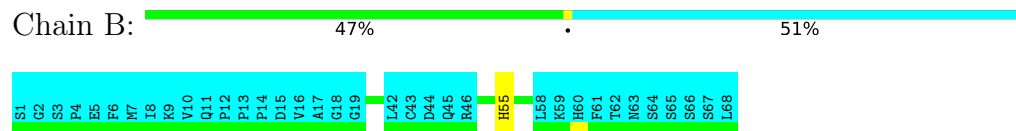


4.2.4 Score per residue for model 4

- Molecule 1: FI23536p1

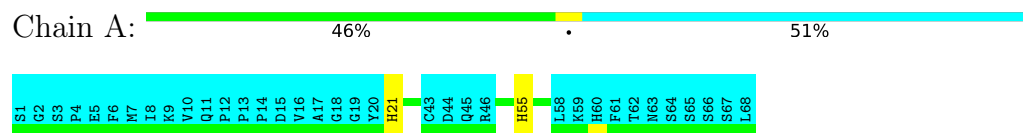


- Molecule 1: FI23536p1

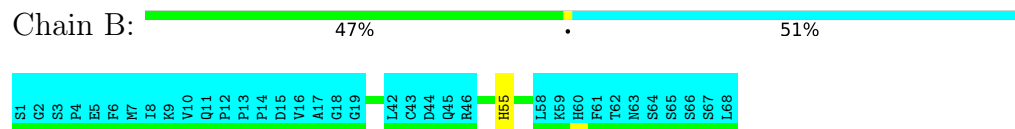


4.2.5 Score per residue for model 5

- Molecule 1: FI23536p1

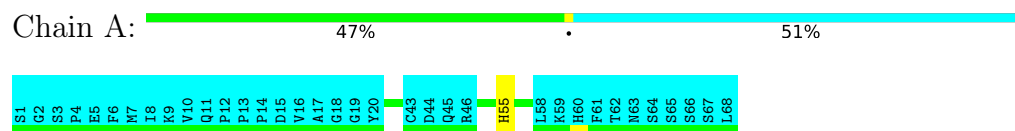


- Molecule 1: FI23536p1

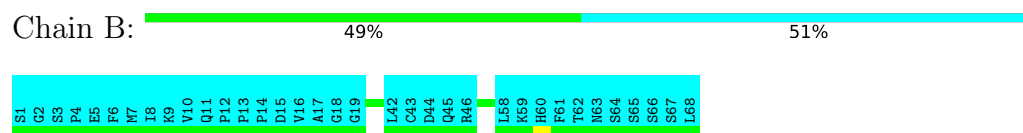


4.2.6 Score per residue for model 6

- Molecule 1: FI23536p1

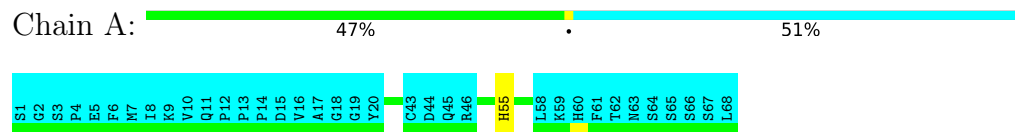


- Molecule 1: FI23536p1

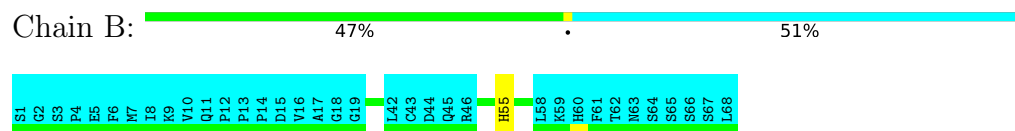


4.2.7 Score per residue for model 7

- Molecule 1: FI23536p1

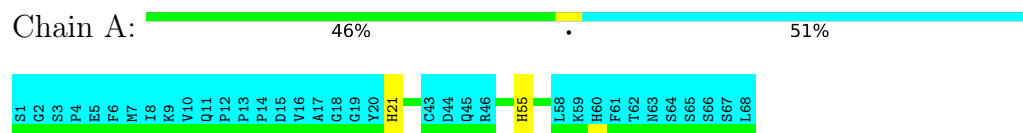


- Molecule 1: FI23536p1

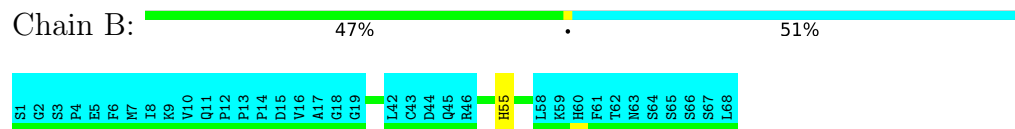


4.2.8 Score per residue for model 8

- Molecule 1: FI23536p1

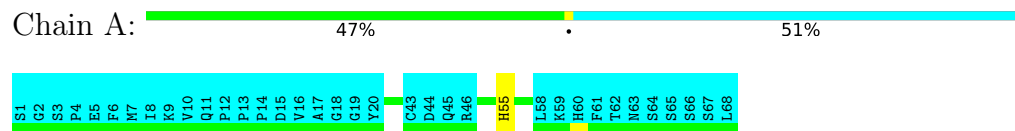


- Molecule 1: FI23536p1

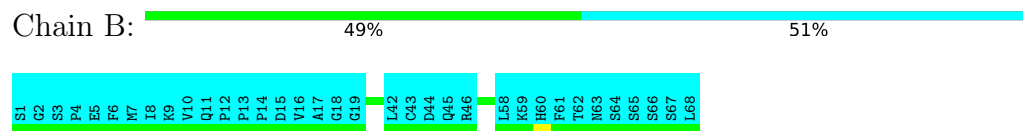


4.2.9 Score per residue for model 9

- Molecule 1: FI23536p1

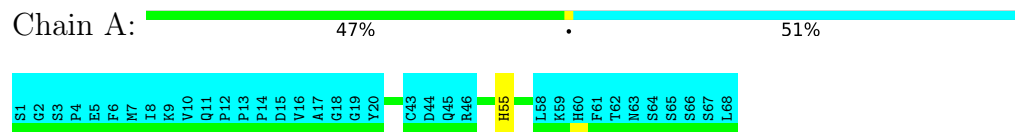


- Molecule 1: FI23536p1

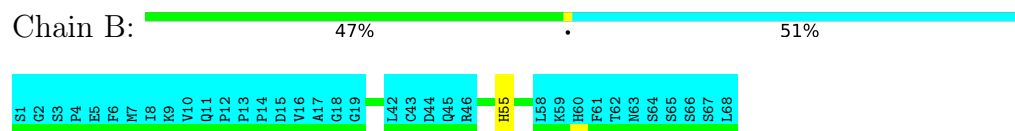


4.2.10 Score per residue for model 10

- Molecule 1: FI23536p1

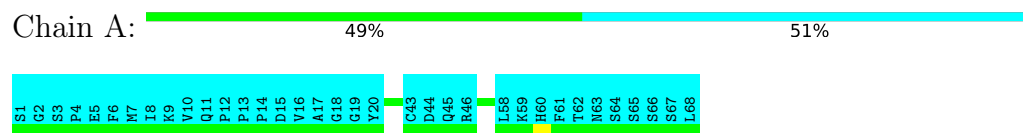


- Molecule 1: FI23536p1

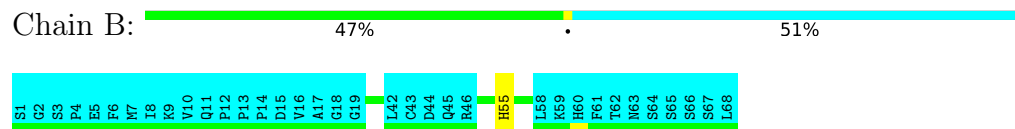


4.2.11 Score per residue for model 11

- Molecule 1: FI23536p1

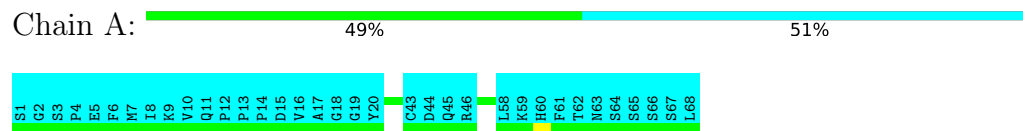


- Molecule 1: FI23536p1

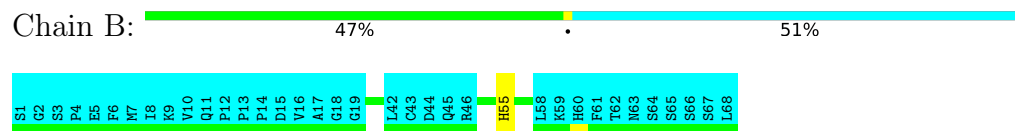


4.2.12 Score per residue for model 12

- Molecule 1: FI23536p1

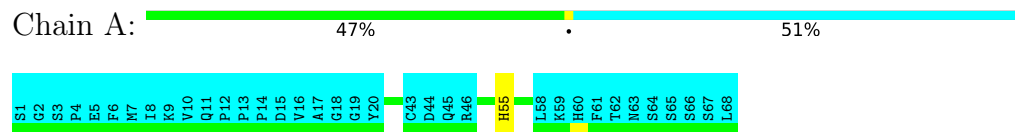


- Molecule 1: FI23536p1

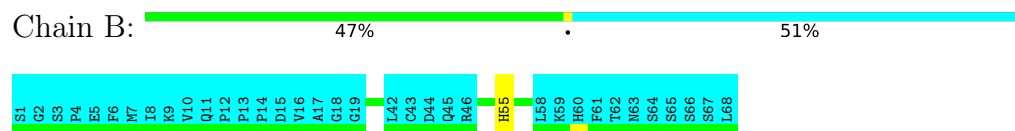


4.2.13 Score per residue for model 13

- Molecule 1: FI23536p1

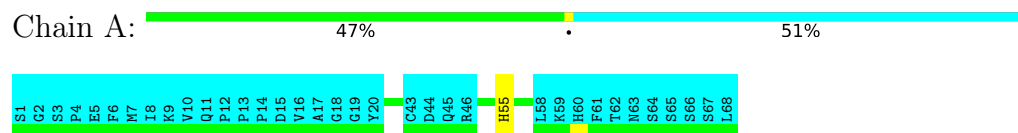


- Molecule 1: FI23536p1



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: FI23536p1

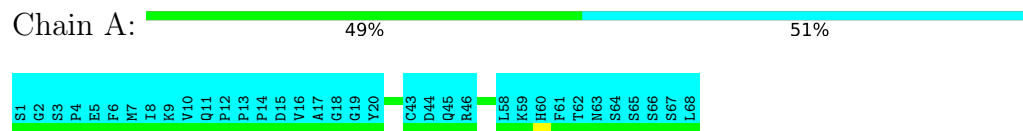


- Molecule 1: FI23536p1

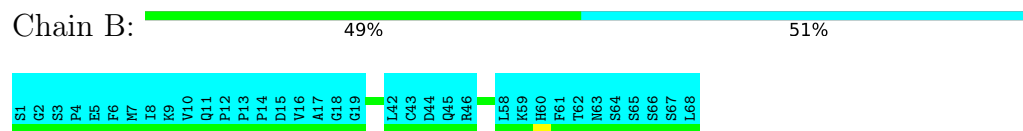


4.2.15 Score per residue for model 15

- Molecule 1: FI23536p1

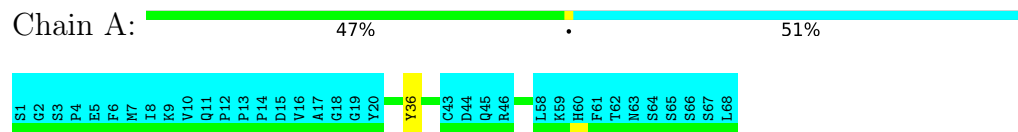


- Molecule 1: FI23536p1

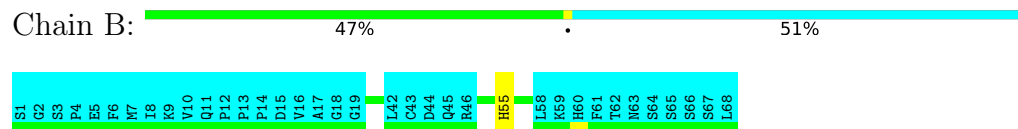


4.2.16 Score per residue for model 16

- Molecule 1: FI23536p1

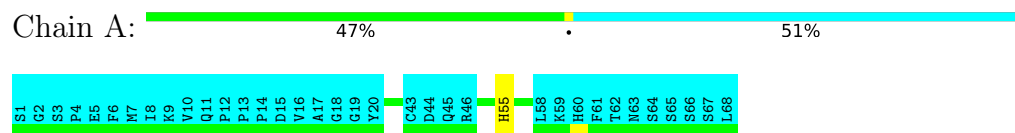


- Molecule 1: FI23536p1

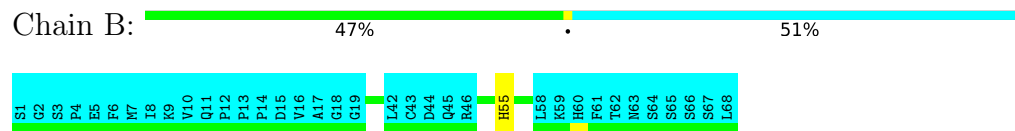


4.2.17 Score per residue for model 17

- Molecule 1: FI23536p1

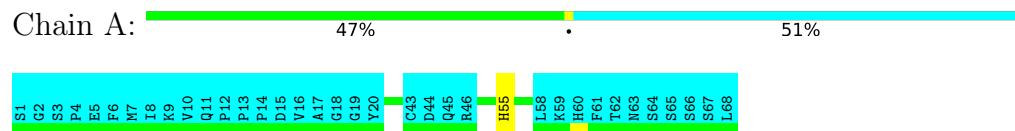


- Molecule 1: FI23536p1

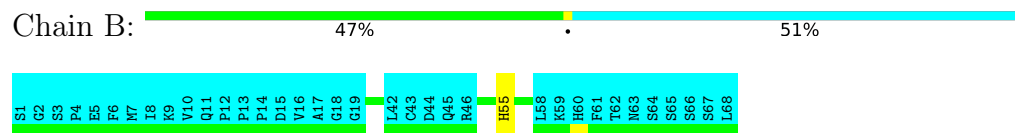


4.2.18 Score per residue for model 18

- Molecule 1: FI23536p1

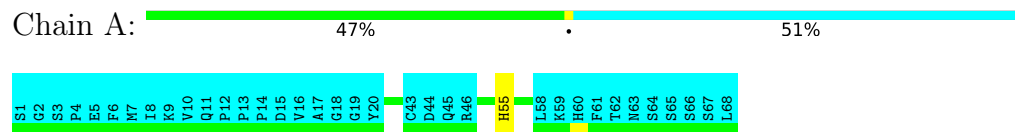


- Molecule 1: FI23536p1

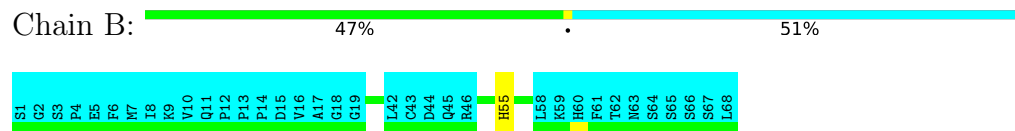


4.2.19 Score per residue for model 19

- Molecule 1: FI23536p1

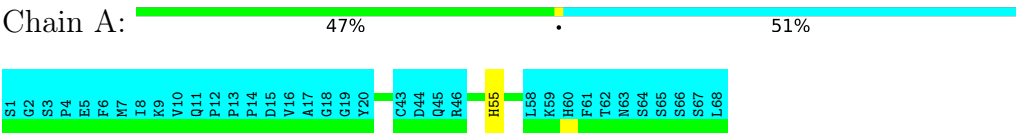


- Molecule 1: FI23536p1

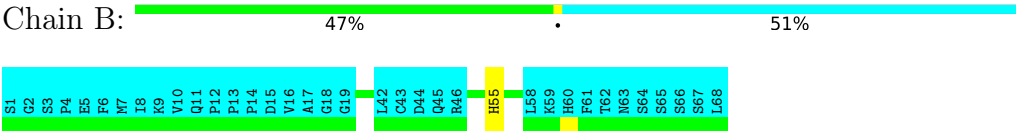


4.2.20 Score per residue for model 20

● Molecule 1: FI23536p1



● Molecule 1: FI23536p1



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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
CNS	structure calculation	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	701
Number of shifts mapped to atoms	701
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1300058657_cs_P1.str.V1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	701
Number of shifts mapped to atoms	701
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	60	-1.06 ± 0.15	Should be checked
$^{13}\text{C}_\beta$	56	-0.50 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	57	0.33 ± 0.16	None needed (< 0.5 ppm)
^{15}N	52	-0.86 ± 0.52	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 402 atoms were assigned a chemical shift out of a possible 895. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	161/322 (50%)	65/130 (50%)	66/132 (50%)	30/60 (50%)
Sidechain	200/458 (44%)	132/301 (44%)	67/143 (47%)	1/14 (7%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	41/115 (36%)	21/56 (38%)	20/53 (38%)	0/6 (0%)
Overall	402/895 (45%)	218/487 (45%)	153/328 (47%)	31/80 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 701 atoms were assigned a chemical shift out of a possible 1776. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	285/662 (43%)	116/268 (43%)	117/272 (43%)	52/122 (43%)
Sidechain	355/936 (38%)	230/612 (38%)	121/294 (41%)	4/30 (13%)
Aromatic	61/178 (34%)	31/88 (35%)	30/82 (37%)	0/8 (0%)
Overall	701/1776 (39%)	377/968 (39%)	268/648 (41%)	56/160 (35%)

7.1.4 Statistically unusual chemical shifts [i](#)

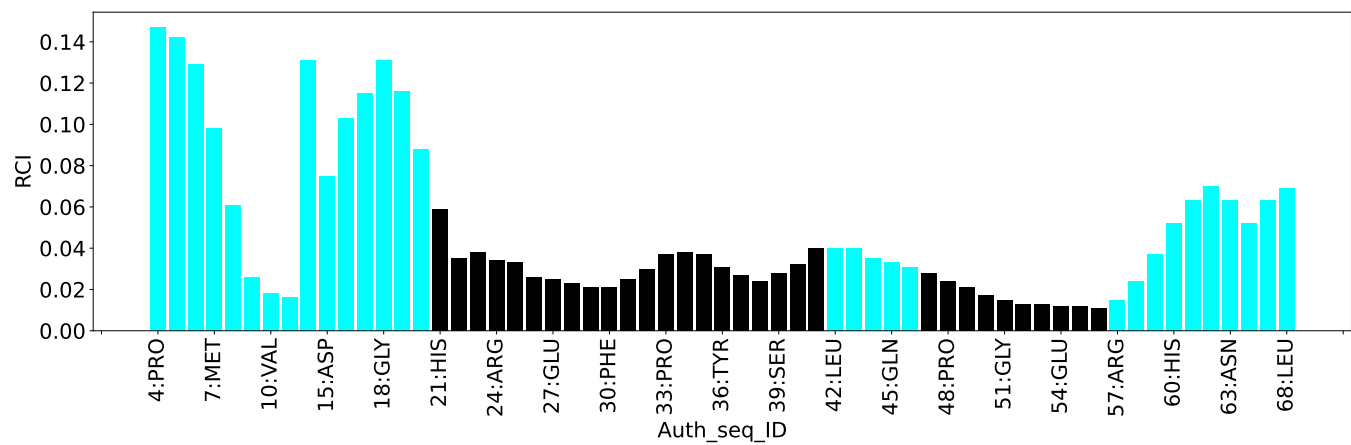
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	59	LYS	HB3	0.34	0.46 – 3.04	-5.5

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	1120
Intra-residue ($ i-j =0$)	478
Sequential ($ i-j =1$)	264
Medium range ($ i-j >1$ and $ i-j <5$)	84
Long range ($ i-j \geq 5$)	136
Inter-chain	78
Hydrogen bond restraints	72
Disulfide bond restraints	0
Total dihedral-angle restraints	350
Number of unmapped restraints	0
Number of restraints per residue	10.7
Number of long range restraints per residue ¹	1.2

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)	108.5	0.2
0.2-0.5 (Medium)	26.1	0.5
>0.5 (Large)	3.9	2.33

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)	55.6	9.77
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

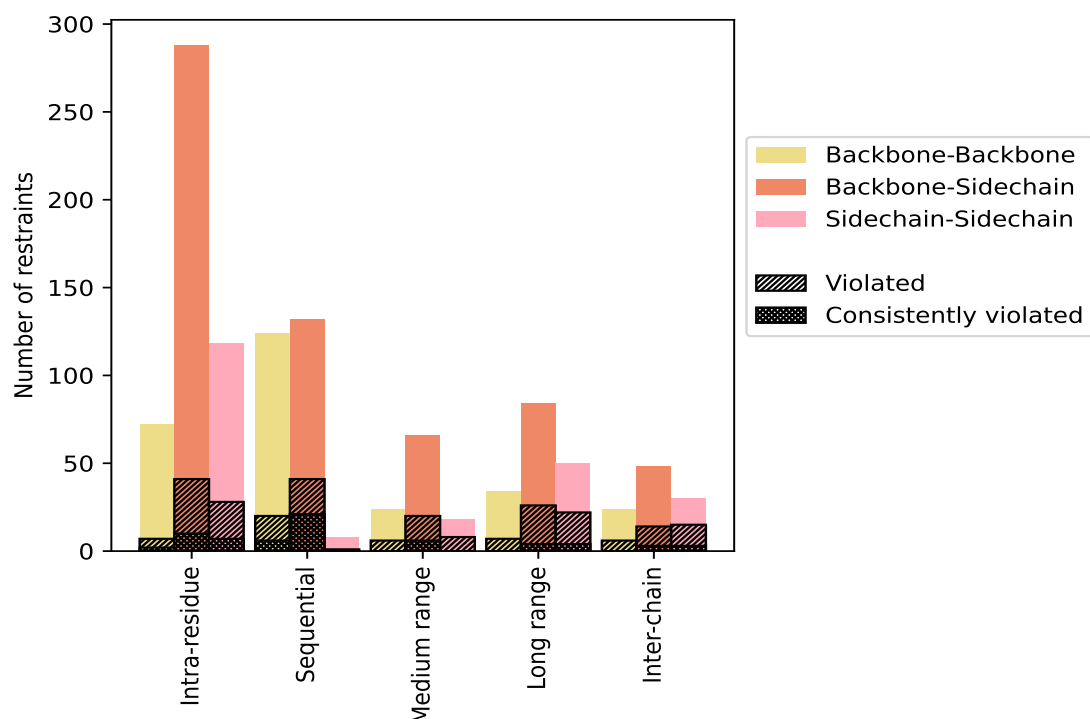
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	478	42.7	76	15.9	6.8	19	4.0	1.7
Backbone-Backbone	72	6.4	7	9.7	0.6	2	2.8	0.2
Backbone-Sidechain	288	25.7	41	14.2	3.7	10	3.5	0.9
Sidechain-Sidechain	118	10.5	28	23.7	2.5	7	5.9	0.6
Sequential ($i-j =1$)	264	23.6	62	23.5	5.5	27	10.2	2.4
Backbone-Backbone	124	11.1	20	16.1	1.8	6	4.8	0.5
Backbone-Sidechain	132	11.8	41	31.1	3.7	21	15.9	1.9
Sidechain-Sidechain	8	0.7	1	12.5	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	84	7.5	34	40.5	3.0	6	7.1	0.5
Backbone-Backbone	24	2.1	6	25.0	0.5	0	0.0	0.0
Backbone-Sidechain	42	3.8	20	47.6	1.8	6	14.3	0.5
Sidechain-Sidechain	18	1.6	8	44.4	0.7	0	0.0	0.0
Long range ($i-j \geq 5$)	136	12.1	55	40.4	4.9	8	5.9	0.7
Backbone-Backbone	34	3.0	7	20.6	0.6	0	0.0	0.0
Backbone-Sidechain	52	4.6	26	50.0	2.3	4	7.7	0.4
Sidechain-Sidechain	50	4.5	22	44.0	2.0	4	8.0	0.4
Inter-chain	78	7.0	30	38.5	2.7	6	7.7	0.5
Backbone-Backbone	24	2.1	6	25.0	0.5	0	0.0	0.0
Backbone-Sidechain	32	2.9	14	43.8	1.2	3	9.4	0.3
Sidechain-Sidechain	22	2.0	10	45.5	0.9	3	13.6	0.3
Hydrogen bond	72	6.4	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	1120	100.0	262	23.4	23.4	66	5.9	5.9
Backbone-Backbone	278	24.8	46	16.5	4.1	8	2.9	0.7
Backbone-Sidechain	618	55.2	142	23.0	12.7	44	7.1	3.9
Sidechain-Sidechain	224	20.0	74	33.0	6.6	14	6.2	1.2

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	32	42	18	25	23	140	0.2	2.33	0.2	0.17
2	42	45	16	27	22	152	0.21	2.17	0.24	0.16
3	36	42	20	30	20	148	0.22	2.29	0.26	0.17
4	40	45	12	29	18	144	0.24	2.14	0.26	0.18
5	38	43	16	30	19	146	0.21	2.16	0.25	0.17
6	33	40	17	31	24	145	0.17	0.67	0.08	0.16
7	36	42	17	28	20	143	0.19	2.29	0.2	0.16
8	34	40	16	33	24	147	0.17	0.66	0.08	0.16
9	37	41	14	28	21	141	0.2	2.32	0.2	0.17
10	34	42	16	29	26	147	0.18	0.65	0.1	0.16

Continued on next page...

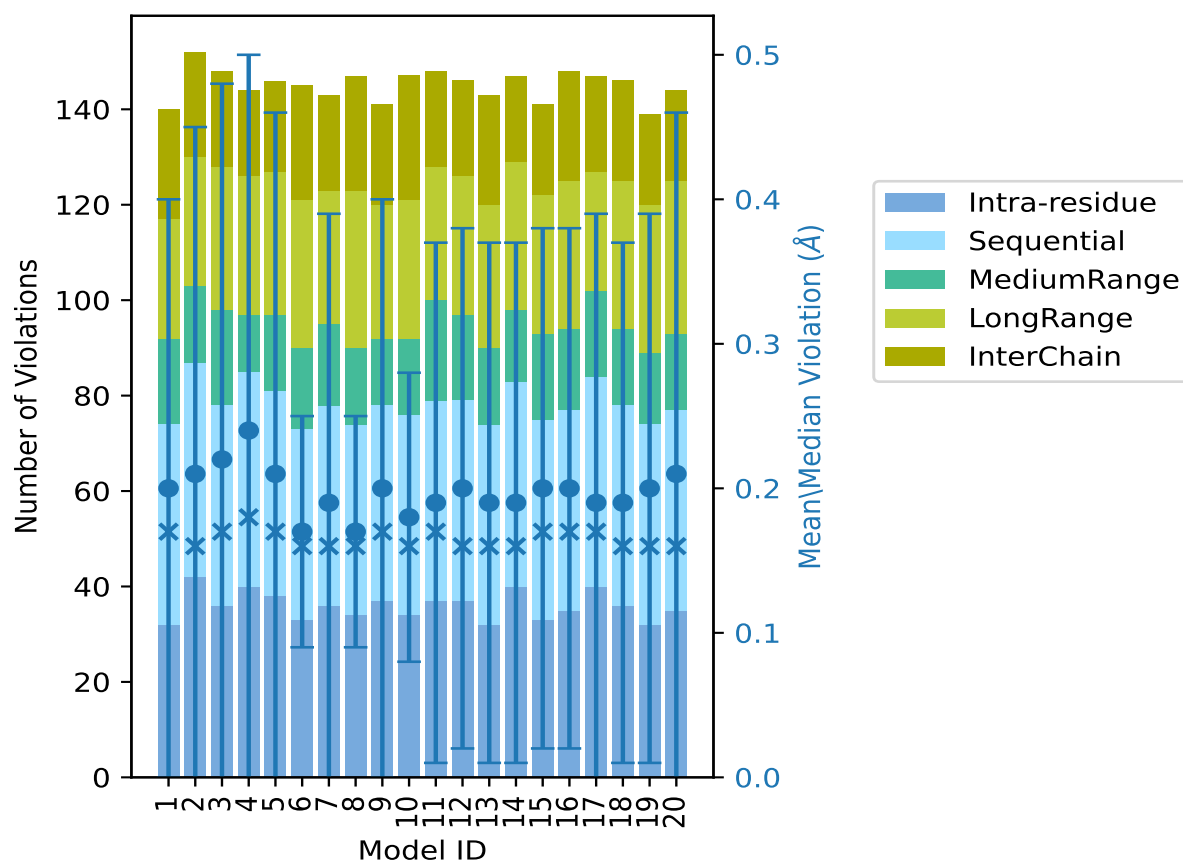
Continued from previous page...

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	37	42	21	28	20	148	0.19	2.16	0.18	0.17
12	37	42	18	29	20	146	0.2	2.15	0.18	0.16
13	32	42	16	30	23	143	0.19	2.17	0.18	0.16
14	40	43	15	31	18	147	0.19	2.15	0.18	0.16
15	33	42	18	29	19	141	0.2	2.14	0.18	0.17
16	35	42	17	31	23	148	0.2	2.15	0.18	0.17
17	40	44	18	25	20	147	0.19	2.33	0.2	0.17
18	36	42	16	31	21	146	0.19	2.16	0.18	0.16
19	32	42	15	31	19	139	0.2	2.16	0.19	0.16
20	35	42	16	32	19	144	0.21	2.31	0.25	0.16

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 ⓘ



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

9.3 Distance violation statistics for the ensemble

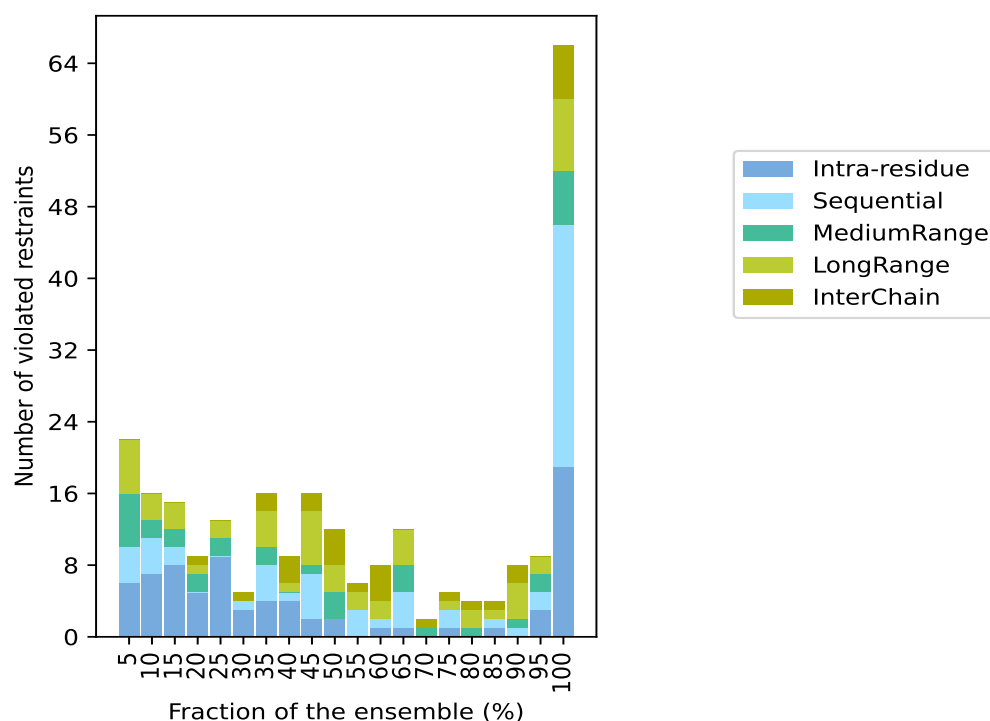
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 783(IR:402, SQ:202, MR:50, LR:81, IC:48) restraints are not 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	%
6	4	6	6	0	22	1	5.0
7	4	2	3	0	16	2	10.0
8	2	2	3	0	15	3	15.0
5	0	2	1	1	9	4	20.0
9	0	2	2	0	13	5	25.0
3	1	0	0	1	5	6	30.0
4	4	2	4	2	16	7	35.0
4	1	0	1	3	9	8	40.0
2	5	1	6	2	16	9	45.0
2	0	3	3	4	12	10	50.0
0	3	0	2	1	6	11	55.0
1	1	0	2	4	8	12	60.0
1	4	3	4	0	12	13	65.0
0	0	1	0	1	2	14	70.0
1	2	0	1	1	5	15	75.0
0	0	1	2	1	4	16	80.0
1	1	0	1	1	4	17	85.0
0	1	1	4	2	8	18	90.0
3	2	2	2	0	9	19	95.0
19	27	6	8	6	66	20	100.0

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

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

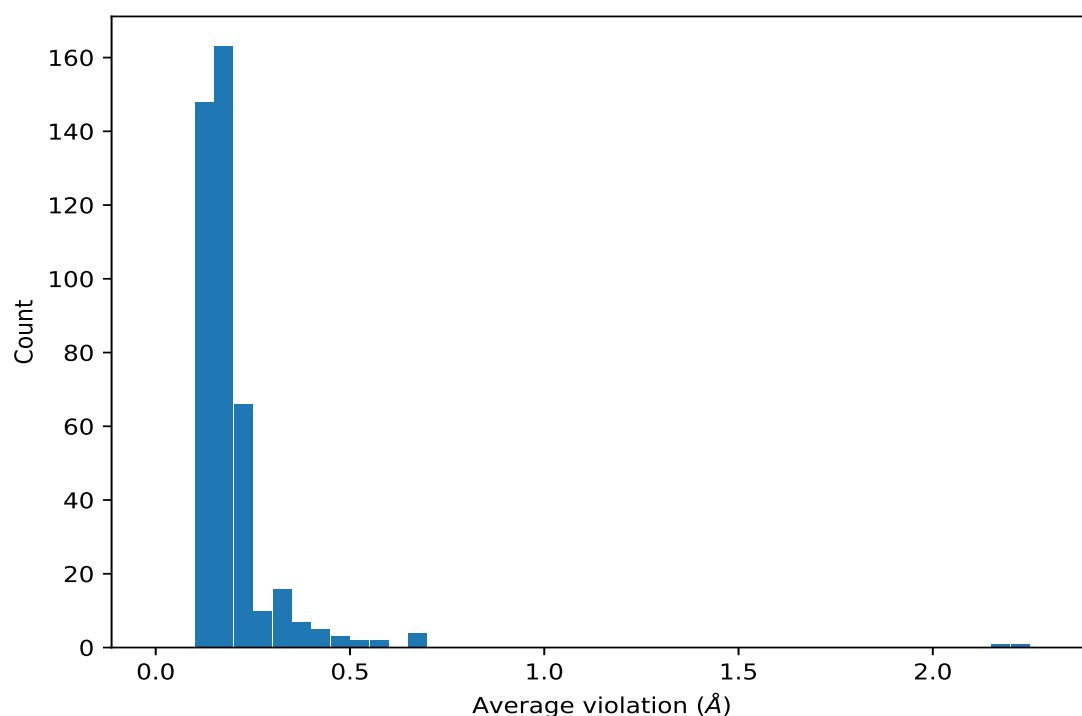
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	20	0.42	0.05	0.44
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	20	0.41	0.06	0.43
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	20	0.36	0.23	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	20	0.36	0.23	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	20	0.33	0.22	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	20	0.33	0.22	0.18
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	20	0.22	0.13	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	20	0.22	0.13	0.14
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	20	0.22	0.06	0.22
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	20	0.22	0.06	0.22
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	20	0.22	0.06	0.22
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	20	0.22	0.06	0.22
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	20	0.22	0.01	0.22
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	20	0.22	0.01	0.22
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	20	0.21	0.04	0.22
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	20	0.21	0.04	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	20	0.21	0.04	0.22
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	20	0.21	0.04	0.22
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	20	0.21	0.04	0.22
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	20	0.21	0.04	0.22
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	20	0.21	0.05	0.21
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	20	0.21	0.01	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	20	0.21	0.01	0.2
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	20	0.2	0.04	0.21
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	20	0.2	0.04	0.21
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	20	0.2	0.04	0.21
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	20	0.2	0.03	0.2
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	20	0.2	0.04	0.19
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	20	0.2	0.04	0.19
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	20	0.2	0.04	0.19
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	20	0.2	0.03	0.2
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	20	0.2	0.03	0.2
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	20	0.19	0.11	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	20	0.19	0.11	0.14
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	20	0.19	0.04	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	20	0.19	0.01	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	20	0.19	0.01	0.19
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	20	0.19	0.05	0.18
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	20	0.19	0.05	0.18
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	20	0.19	0.0	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	20	0.19	0.0	0.19
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	20	0.19	0.04	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	20	0.19	0.04	0.2
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	20	0.19	0.04	0.19
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	20	0.19	0.04	0.19
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	20	0.18	0.03	0.19
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	20	0.18	0.03	0.19
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	20	0.18	0.03	0.19
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	20	0.18	0.03	0.19
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	20	0.18	0.03	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	20	0.18	0.01	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	20	0.18	0.01	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	20	0.18	0.01	0.18
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	20	0.18	0.05	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	20	0.18	0.05	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	20	0.18	0.05	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	20	0.18	0.05	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	20	0.18	0.05	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	20	0.18	0.05	0.16
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	20	0.18	0.01	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	20	0.18	0.0	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	20	0.18	0.01	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	20	0.18	0.01	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	20	0.17	0.0	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	20	0.17	0.01	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	20	0.17	0.01	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	20	0.17	0.01	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	20	0.17	0.0	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	20	0.17	0.01	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	20	0.17	0.01	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	20	0.17	0.01	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	20	0.17	0.01	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	20	0.17	0.01	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	20	0.17	0.01	0.17
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	20	0.17	0.04	0.16
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	20	0.17	0.04	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	20	0.17	0.01	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	20	0.17	0.01	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	20	0.17	0.01	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	20	0.17	0.04	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	20	0.17	0.04	0.16
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	20	0.17	0.0	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	20	0.17	0.0	0.17
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	20	0.17	0.02	0.17
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	20	0.16	0.02	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	20	0.16	0.01	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	20	0.16	0.01	0.16
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	20	0.16	0.02	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	20	0.16	0.0	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	20	0.16	0.0	0.16
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	20	0.16	0.01	0.16
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	20	0.16	0.02	0.16
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	20	0.16	0.01	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	20	0.16	0.02	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	20	0.16	0.02	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	20	0.16	0.02	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	20	0.16	0.01	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	20	0.16	0.01	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	20	0.16	0.01	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	20	0.16	0.01	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	20	0.16	0.01	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	20	0.16	0.01	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	20	0.15	0.02	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	20	0.15	0.02	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	20	0.15	0.02	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	20	0.15	0.01	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	20	0.15	0.01	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	20	0.15	0.01	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	20	0.15	0.01	0.15
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	20	0.15	0.01	0.15
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	20	0.15	0.01	0.15
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	20	0.15	0.01	0.15
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	20	0.15	0.01	0.15
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	20	0.15	0.01	0.15
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	20	0.15	0.01	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	20	0.15	0.01	0.15
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	20	0.14	0.02	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	20	0.14	0.01	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	20	0.14	0.01	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	20	0.14	0.01	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	20	0.14	0.01	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	20	0.14	0.01	0.14
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	20	0.11	0.0	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	20	0.11	0.0	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	20	0.11	0.0	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	20	0.11	0.0	0.11
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	19	0.2	0.03	0.21
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	19	0.18	0.03	0.18
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	19	0.18	0.03	0.18
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	19	0.15	0.02	0.16
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	19	0.15	0.02	0.16
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	19	0.15	0.04	0.14
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	19	0.15	0.04	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	19	0.15	0.01	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	19	0.15	0.01	0.15
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	19	0.15	0.03	0.14
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	19	0.14	0.02	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	19	0.14	0.02	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	19	0.14	0.02	0.13
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	19	0.14	0.02	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	19	0.14	0.02	0.14
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	18	0.18	0.03	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	18	0.17	0.04	0.15
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	18	0.17	0.04	0.15
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	18	0.16	0.03	0.16
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	18	0.16	0.03	0.16
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	18	0.15	0.03	0.16
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	18	0.15	0.04	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	18	0.14	0.02	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	18	0.14	0.02	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	18	0.14	0.02	0.14
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	18	0.12	0.01	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	18	0.11	0.0	0.11
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	17	0.21	0.07	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	17	0.21	0.07	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	17	0.21	0.07	0.2
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	17	0.12	0.01	0.12
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	17	0.11	0.01	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	17	0.11	0.01	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	17	0.11	0.01	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	17	0.11	0.01	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	17	0.11	0.01	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	17	0.11	0.01	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	17	0.11	0.01	0.1
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	16	0.19	0.05	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	16	0.19	0.05	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	16	0.19	0.05	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	16	0.19	0.05	0.2
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	16	0.17	0.05	0.16
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	16	0.17	0.05	0.16
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	16	0.17	0.05	0.16
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	16	0.17	0.04	0.17
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	16	0.17	0.04	0.17
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	16	0.17	0.04	0.17
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	16	0.13	0.01	0.13
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	15	0.47	0.13	0.48
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	15	0.16	0.03	0.17
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	15	0.16	0.03	0.17
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	15	0.15	0.04	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	15	0.15	0.04	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	15	0.15	0.04	0.15
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	15	0.13	0.02	0.13
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	15	0.11	0.01	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	15	0.11	0.01	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	15	0.11	0.01	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	15	0.11	0.01	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	15	0.11	0.01	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	15	0.11	0.01	0.1
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	14	0.24	0.07	0.24
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	14	0.24	0.07	0.24
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	14	0.2	0.05	0.22
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	13	2.21	0.08	2.16
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	13	0.54	0.01	0.54
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	13	0.39	0.01	0.39
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	13	0.32	0.02	0.31
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	13	0.2	0.03	0.21
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	13	0.2	0.02	0.19
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	13	0.19	0.03	0.19
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	13	0.18	0.04	0.18
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	13	0.18	0.04	0.18
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	13	0.18	0.04	0.18
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	13	0.17	0.06	0.15
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	13	0.16	0.07	0.13
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	13	0.16	0.07	0.13
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	13	0.13	0.02	0.13
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	13	0.12	0.02	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	13	0.12	0.02	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	13	0.12	0.02	0.11
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	12	0.27	0.01	0.28
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	12	0.19	0.07	0.18
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	12	0.19	0.07	0.18
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	12	0.19	0.07	0.18
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	12	0.18	0.1	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	12	0.18	0.1	0.13
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	12	0.16	0.06	0.14
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	12	0.14	0.02	0.15
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	12	0.14	0.02	0.15
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	12	0.14	0.02	0.15
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	12	0.14	0.05	0.12
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	12	0.13	0.03	0.12
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	12	0.13	0.03	0.12
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	12	0.13	0.03	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	12	0.12	0.02	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	12	0.12	0.02	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	12	0.12	0.02	0.12
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	11	0.31	0.08	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	11	0.31	0.08	0.33
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	11	0.31	0.08	0.33
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	11	0.31	0.08	0.33
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	11	0.31	0.08	0.33
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	11	0.31	0.08	0.33
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	11	0.17	0.01	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	11	0.17	0.01	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	11	0.17	0.01	0.17
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	11	0.17	0.03	0.17
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	11	0.16	0.0	0.16
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	11	0.13	0.07	0.11
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	11	0.13	0.07	0.11
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	11	0.13	0.07	0.11
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	11	0.13	0.0	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	11	0.13	0.0	0.13
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	11	0.12	0.01	0.11
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	10	0.23	0.04	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	10	0.23	0.04	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	10	0.23	0.04	0.22
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	10	0.17	0.05	0.2
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	10	0.17	0.01	0.17
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	10	0.17	0.04	0.16
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	10	0.17	0.04	0.16
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	10	0.17	0.02	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	10	0.17	0.02	0.18
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	10	0.16	0.09	0.11
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	10	0.16	0.09	0.11
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	10	0.16	0.09	0.11
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	10	0.16	0.05	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	10	0.16	0.05	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	10	0.16	0.05	0.2
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	10	0.15	0.04	0.15
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	10	0.14	0.03	0.13
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	10	0.12	0.01	0.12
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	10	0.12	0.01	0.12
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	10	0.12	0.02	0.11
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	10	0.12	0.01	0.11
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	10	0.11	0.01	0.12
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	10	0.11	0.01	0.12
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	9	2.18	0.06	2.16
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	9	0.54	0.01	0.54
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	9	0.4	0.0	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	9	0.39	0.01	0.39
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	9	0.32	0.02	0.31
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	9	0.32	0.09	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	9	0.32	0.09	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	9	0.32	0.09	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	9	0.32	0.09	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	9	0.32	0.09	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	9	0.32	0.09	0.36
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	9	0.2	0.03	0.21
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	9	0.2	0.02	0.19
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	9	0.2	0.01	0.2
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	9	0.19	0.02	0.18
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	9	0.17	0.04	0.19
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	9	0.15	0.02	0.15
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	9	0.15	0.02	0.15
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	9	0.14	0.05	0.12
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	9	0.13	0.03	0.11
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	9	0.12	0.02	0.11
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	9	0.12	0.02	0.11
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	9	0.12	0.02	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	9	0.12	0.02	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	9	0.12	0.02	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	9	0.12	0.02	0.11
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	8	0.26	0.12	0.19
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	8	0.22	0.07	0.22
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	8	0.22	0.07	0.22
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	8	0.18	0.0	0.18
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	8	0.14	0.05	0.12
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	8	0.14	0.03	0.12
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	8	0.14	0.03	0.12
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	8	0.14	0.03	0.12
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	8	0.12	0.0	0.12
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	8	0.11	0.01	0.12
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	8	0.11	0.01	0.11
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	8	0.11	0.01	0.11
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	8	0.11	0.01	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	8	0.11	0.01	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	8	0.11	0.01	0.11
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	7	0.4	0.0	0.4
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	7	0.27	0.01	0.28
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	7	0.24	0.01	0.25
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	7	0.2	0.01	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	7	0.18	0.01	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	7	0.18	0.01	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	7	0.18	0.01	0.18
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	7	0.16	0.01	0.16
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	7	0.15	0.02	0.16
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	7	0.15	0.03	0.15
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	7	0.14	0.03	0.15
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	7	0.14	0.01	0.14
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	7	0.14	0.01	0.14
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	7	0.14	0.02	0.14
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	7	0.14	0.02	0.14
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	7	0.14	0.02	0.14
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	7	0.14	0.03	0.12
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	7	0.13	0.01	0.12
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	7	0.12	0.02	0.11
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	7	0.12	0.02	0.12
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	7	0.12	0.01	0.12
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	7	0.12	0.0	0.12
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	7	0.1	0.0	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	7	0.1	0.0	0.1
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	6	0.29	0.0	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	6	0.29	0.0	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	6	0.29	0.0	0.29
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	6	0.21	0.03	0.2
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	6	0.21	0.03	0.2
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	6	0.13	0.01	0.13
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	6	0.12	0.01	0.12
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	6	0.12	0.01	0.12
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	6	0.12	0.01	0.12
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	6	0.11	0.01	0.11
(1,431)	1:44:A:ASP:HB2	1:44:A:ASP:HA	5	0.38	0.0	0.38
(1,912)	1:44:B:ASP:HB2	1:44:B:ASP:HA	5	0.38	0.0	0.38
(1,343)	1:21:A:HIS:HD2	1:21:A:HIS:HB3	5	0.24	0.03	0.26
(1,824)	1:21:B:HIS:HD2	1:21:B:HIS:HB3	5	0.23	0.06	0.26
(1,566)	1:20:B:TYR:HE1	1:61:B:PHE:HA	5	0.21	0.06	0.21
(1,566)	1:20:B:TYR:HE2	1:61:B:PHE:HA	5	0.21	0.06	0.21
(1,825)	1:21:B:HIS:HD2	1:21:B:HIS:HB2	5	0.21	0.03	0.2
(1,118)	1:61:A:PHE:HB3	1:57:A:ARG:HA	5	0.2	0.04	0.19
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD21	5	0.2	0.01	0.2
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD22	5	0.2	0.01	0.2
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD23	5	0.2	0.01	0.2
(1,344)	1:21:A:HIS:HD2	1:21:A:HIS:HB2	5	0.2	0.03	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,848)	1:35:B:SER:H	1:35:B:SER:HB3	5	0.12	0.0	0.12
(1,108)	1:56:A:PHE:HE1	1:60:A:HIS:HD2	5	0.11	0.0	0.11
(1,108)	1:56:A:PHE:HE2	1:60:A:HIS:HD2	5	0.11	0.0	0.11
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG11	5	0.11	0.01	0.11
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG12	5	0.11	0.01	0.11
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG13	5	0.11	0.01	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG11	5	0.1	0.0	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG12	5	0.1	0.0	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG13	5	0.1	0.0	0.1
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG21	4	0.29	0.0	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG22	4	0.29	0.0	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG23	4	0.29	0.0	0.29
(1,154)	1:35:A:SER:HB3	1:31:A:SER:HB2	4	0.26	0.01	0.26
(1,645)	1:59:B:LYS:HD2	1:59:B:LYS:HA	4	0.17	0.03	0.17
(1,645)	1:59:B:LYS:HD3	1:59:B:LYS:HA	4	0.17	0.03	0.17
(1,244)	1:60:A:HIS:H	1:57:A:ARG:HA	4	0.16	0.04	0.18
(1,193)	1:55:A:HIS:HD2	1:55:A:HIS:HB2	4	0.15	0.04	0.14
(1,110)	1:56:A:PHE:HE1	1:25:A:CYS:HA	4	0.14	0.02	0.14
(1,110)	1:56:A:PHE:HE2	1:25:A:CYS:HA	4	0.14	0.02	0.14
(1,367)	1:35:A:SER:H	1:35:A:SER:HB3	4	0.12	0.0	0.12
(1,53)	1:25:A:CYS:H	1:28:B:VAL:HB	4	0.11	0.01	0.11
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG2	4	0.1	0.0	0.1
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG3	4	0.1	0.0	0.1
(1,374)	1:27:A:GLU:HG2	1:27:A:GLU:HA	3	0.65	0.0	0.65
(1,374)	1:27:A:GLU:HG3	1:27:A:GLU:HA	3	0.65	0.0	0.65
(1,405)	1:57:A:ARG:HD2	1:57:A:ARG:HG2	3	0.48	0.0	0.48
(1,886)	1:57:B:ARG:HD2	1:57:B:ARG:HG2	3	0.48	0.0	0.48
(1,382)	1:45:A:GLN:HA	1:45:A:GLN:HG3	3	0.37	0.37	0.11
(1,956)	1:63:B:ASN:HB2	1:63:B:ASN:HA	3	0.22	0.01	0.22
(1,470)	1:60:A:HIS:HB3	1:60:A:HIS:HD2	3	0.2	0.0	0.2
(1,725)	1:60:B:HIS:H	1:57:B:ARG:HA	3	0.13	0.02	0.12
(1,543)	1:58:A:LEU:H	1:57:A:ARG:HB2	3	0.13	0.01	0.12
(1,544)	1:58:A:LEU:H	1:58:A:LEU:HA	3	0.12	0.0	0.12
(1,589)	1:56:B:PHE:HE1	1:60:B:HIS:HD2	3	0.11	0.01	0.11
(1,589)	1:56:B:PHE:HE2	1:60:B:HIS:HD2	3	0.11	0.01	0.11
(1,453)	1:47:A:LEU:HD11	1:55:A:HIS:HB3	3	0.11	0.01	0.11
(1,453)	1:47:A:LEU:HD12	1:55:A:HIS:HB3	3	0.11	0.01	0.11
(1,453)	1:47:A:LEU:HD13	1:55:A:HIS:HB3	3	0.11	0.01	0.11
(1,476)	1:63:A:ASN:HA	1:63:A:ASN:HB3	3	0.11	0.01	0.1
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD11	3	0.11	0.0	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD12	3	0.11	0.0	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD13	3	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

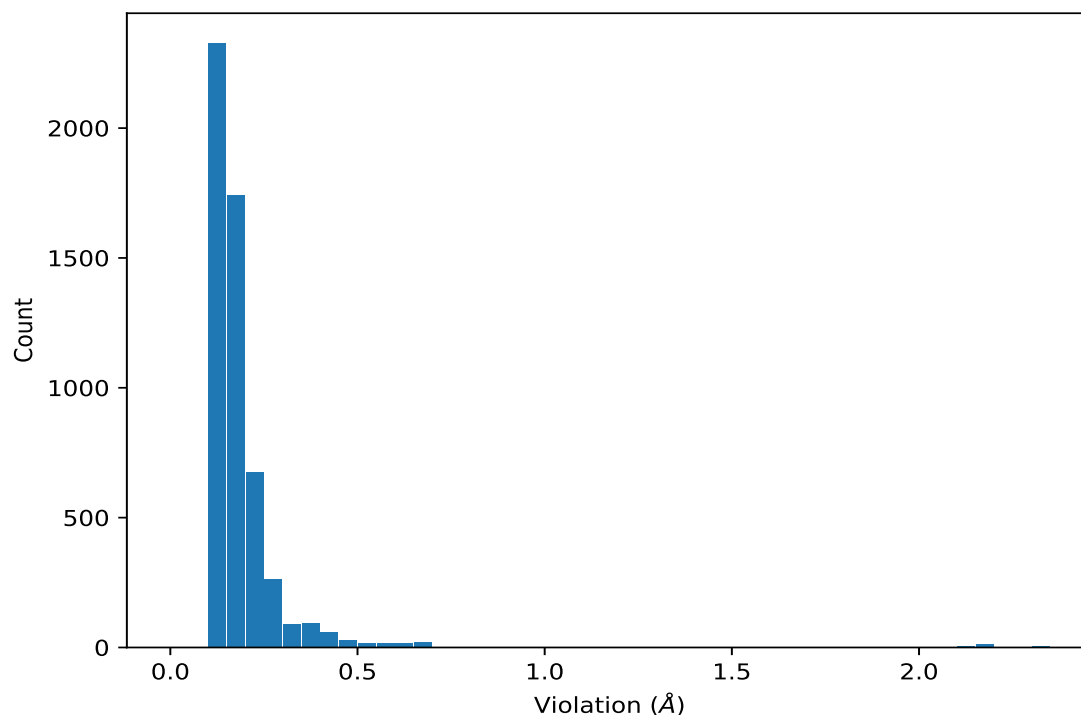
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,934)	1:47:B:LEU:HD11	1:55:B:HIS:HB3	3	0.11	0.0	0.11
(1,934)	1:47:B:LEU:HD12	1:55:B:HIS:HB3	3	0.11	0.0	0.11
(1,934)	1:47:B:LEU:HD13	1:55:B:HIS:HB3	3	0.11	0.0	0.11
(1,985)	1:36:B:TYR:H	1:35:B:SER:HB3	3	0.11	0.0	0.11
(1,855)	1:27:B:GLU:HG2	1:27:B:GLU:HA	2	0.66	0.01	0.66
(1,855)	1:27:B:GLU:HG3	1:27:B:GLU:HA	2	0.66	0.01	0.66
(1,253)	1:45:A:GLN:HE21	1:45:A:GLN:HG3	2	0.59	0.0	0.59
(1,734)	1:45:B:GLN:HE21	1:45:B:GLN:HG3	2	0.59	0.0	0.59
(1,478)	1:21:A:HIS:H	1:20:A:TYR:HA	2	0.41	0.09	0.41
(1,676)	1:32:B:ALA:HB1	1:30:B:PHE:HE1	2	0.24	0.08	0.24
(1,676)	1:32:B:ALA:HB1	1:30:B:PHE:HE2	2	0.24	0.08	0.24
(1,676)	1:32:B:ALA:HB2	1:30:B:PHE:HE1	2	0.24	0.08	0.24
(1,676)	1:32:B:ALA:HB2	1:30:B:PHE:HE2	2	0.24	0.08	0.24
(1,676)	1:32:B:ALA:HB3	1:30:B:PHE:HE1	2	0.24	0.08	0.24
(1,676)	1:32:B:ALA:HB3	1:30:B:PHE:HE2	2	0.24	0.08	0.24
(1,475)	1:63:A:ASN:HB2	1:63:A:ASN:HA	2	0.21	0.0	0.21
(1,951)	1:60:B:HIS:HB3	1:60:B:HIS:HD2	2	0.19	0.01	0.19
(1,959)	1:21:B:HIS:H	1:20:B:TYR:HA	2	0.15	0.05	0.15
(1,674)	1:55:B:HIS:HD2	1:55:B:HIS:HB2	2	0.14	0.02	0.14
(1,1024)	1:58:B:LEU:H	1:57:B:ARG:HB2	2	0.13	0.0	0.13
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD11	2	0.12	0.02	0.12
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD12	2	0.12	0.02	0.12
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD13	2	0.12	0.02	0.12
(1,591)	1:56:B:PHE:HE1	1:25:B:CYS:HA	2	0.12	0.02	0.12
(1,591)	1:56:B:PHE:HE2	1:25:B:CYS:HA	2	0.12	0.02	0.12
(1,1025)	1:58:B:LEU:H	1:58:B:LEU:HA	2	0.12	0.0	0.12
(1,504)	1:36:A:TYR:H	1:35:A:SER:HB3	2	0.11	0.01	0.11
(1,717)	1:28:B:VAL:HG11	1:36:B:TYR:HD1	2	0.11	0.0	0.11
(1,717)	1:28:B:VAL:HG11	1:36:B:TYR:HD2	2	0.11	0.0	0.11
(1,717)	1:28:B:VAL:HG12	1:36:B:TYR:HD1	2	0.11	0.0	0.11
(1,717)	1:28:B:VAL:HG12	1:36:B:TYR:HD2	2	0.11	0.0	0.11
(1,717)	1:28:B:VAL:HG13	1:36:B:TYR:HD1	2	0.11	0.0	0.11
(1,717)	1:28:B:VAL:HG13	1:36:B:TYR:HD2	2	0.11	0.0	0.11
(1,782)	1:43:B:CYS:H	1:40:B:CYS:HB2	2	0.11	0.01	0.11

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)
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	1	2.33
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	17	2.33
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	9	2.32
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	20	2.31
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	3	2.29
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	7	2.29
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	13	2.17
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	2	2.17
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	5	2.16
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	18	2.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	3	2.16
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	5	2.16
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	11	2.16
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	19	2.16
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	20	2.16
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	16	2.15
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	12	2.15
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	14	2.15
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	4	2.14
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	15	2.14
(1,655)	1:44:B:ASP:H	1:40:B:CYS:HB2	2	2.13
(1,174)	1:44:A:ASP:H	1:40:A:CYS:HB2	4	2.13
(1,382)	1:45:A:GLN:HA	1:45:A:GLN:HG3	4	0.9
(1,142)	1:45:A:GLN:HG2	1:46:A:ARG:H	4	0.86
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	6	0.67
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	6	0.67
(1,855)	1:27:B:GLU:HG2	1:27:B:GLU:HA	8	0.66
(1,855)	1:27:B:GLU:HG3	1:27:B:GLU:HA	8	0.66
(1,855)	1:27:B:GLU:HG2	1:27:B:GLU:HA	10	0.65
(1,855)	1:27:B:GLU:HG3	1:27:B:GLU:HA	10	0.65
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	4	0.65
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	4	0.65
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	16	0.65
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	16	0.65
(1,374)	1:27:A:GLU:HG2	1:27:A:GLU:HA	12	0.65
(1,374)	1:27:A:GLU:HG3	1:27:A:GLU:HA	12	0.65
(1,374)	1:27:A:GLU:HG2	1:27:A:GLU:HA	14	0.65
(1,374)	1:27:A:GLU:HG3	1:27:A:GLU:HA	14	0.65
(1,374)	1:27:A:GLU:HG2	1:27:A:GLU:HA	19	0.65
(1,374)	1:27:A:GLU:HG3	1:27:A:GLU:HA	19	0.65
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	4	0.65
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	4	0.65
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	7	0.65
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	7	0.65
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	18	0.65
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	18	0.65
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	1	0.64
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	1	0.64
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	9	0.64
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	9	0.64
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	5	0.64
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	5	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	10	0.64
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	10	0.64
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	15	0.64
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	15	0.64
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	2	0.63
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	2	0.63
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	3	0.63
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	3	0.63
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	19	0.63
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	19	0.63
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	3	0.63
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	3	0.63
(1,734)	1:45:B:GLN:HE21	1:45:B:GLN:HG3	2	0.59
(1,734)	1:45:B:GLN:HE21	1:45:B:GLN:HG3	4	0.59
(1,253)	1:45:A:GLN:HE21	1:45:A:GLN:HG3	9	0.59
(1,253)	1:45:A:GLN:HE21	1:45:A:GLN:HG3	17	0.59
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	10	0.58
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	12	0.58
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	19	0.58
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	7	0.57
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	14	0.57
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	17	0.56
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	3	0.56
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	4	0.56
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	6	0.55
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	2	0.55
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	5	0.55
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	7	0.55
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	14	0.55
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	5	0.54
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	15	0.54
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	18	0.54
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	3	0.54
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	9	0.54
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	11	0.54
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	12	0.54
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	19	0.54
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	4	0.53
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	13	0.53
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	16	0.53
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	2	0.53
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	17	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	20	0.53
(1,704)	1:43:B:CYS:H	1:44:B:ASP:H	20	0.52
(1,223)	1:43:A:CYS:H	1:44:A:ASP:H	1	0.52
(1,478)	1:21:A:HIS:H	1:20:A:TYR:HA	15	0.5
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	20	0.49
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	4	0.49
(1,886)	1:57:B:ARG:HD2	1:57:B:ARG:HG2	3	0.48
(1,886)	1:57:B:ARG:HD2	1:57:B:ARG:HG2	12	0.48
(1,886)	1:57:B:ARG:HD2	1:57:B:ARG:HG2	14	0.48
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	3	0.48
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	4	0.48
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	8	0.48
(1,405)	1:57:A:ARG:HD2	1:57:A:ARG:HG2	1	0.48
(1,405)	1:57:A:ARG:HD2	1:57:A:ARG:HG2	5	0.48
(1,405)	1:57:A:ARG:HD2	1:57:A:ARG:HG2	10	0.48
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	5	0.48
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	3	0.47
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	5	0.47
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	17	0.47
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	2	0.47
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	7	0.47
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	1	0.46
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	2	0.46
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	10	0.46
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	12	0.46
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	13	0.46
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	18	0.46
(1,433)	1:45:A:GLN:HG2	1:45:A:GLN:HA	4	0.46
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	19	0.46
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	1	0.45
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	19	0.45
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	10	0.45
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	10	0.45
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	17	0.45
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	3	0.44
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	6	0.44
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	14	0.44
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	6	0.43
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	8	0.43
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	9	0.43
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	14	0.43
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	8	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	8	0.43
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	7	0.43
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	7	0.43
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	7	0.43
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	7	0.43
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	7	0.43
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	7	0.43
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	13	0.42
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	13	0.42
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	16	0.42
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	16	0.42
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	15	0.42
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	7	0.41
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	7	0.41
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	17	0.41
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	17	0.41
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	11	0.41
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	1	0.41
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	1	0.41
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	9	0.41
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	9	0.41
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	20	0.41
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	20	0.41
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	10	0.41
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	18	0.41
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	3	0.4
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	20	0.4
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	4	0.4
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	4	0.4
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	16	0.4
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	16	0.4
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	6	0.4
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	6	0.4
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	6	0.4
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	2	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	5	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	8	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	10	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	11	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	14	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	16	0.4
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	19	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	20	0.4
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	1	0.4
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	7	0.4
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	9	0.4
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	17	0.4
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	2	0.4
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	4	0.4
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	5	0.4
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	6	0.4
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	8	0.4
(1,159)	1:21:A:HIS:HB2	1:21:A:HIS:HA	16	0.4
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	2	0.39
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	4	0.39
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	13	0.39
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	15	0.39
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	16	0.39
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	18	0.39
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	3	0.39
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	3	0.39
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	3	0.39
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	3	0.39
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	3	0.39
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	3	0.39
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	15	0.39
(1,640)	1:21:B:HIS:HB2	1:21:B:HIS:HA	9	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	2	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	3	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	5	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	11	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	12	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	14	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	19	0.39
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	20	0.39
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	4	0.39
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	4	0.39
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	4	0.39
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	4	0.39
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	4	0.39
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	4	0.39
(1,1007)	1:45:B:GLN:H	1:45:B:GLN:HA	5	0.38
(1,912)	1:44:B:ASP:HB2	1:44:B:ASP:HA	3	0.38
(1,912)	1:44:B:ASP:HB2	1:44:B:ASP:HA	4	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:44:B:ASP:HB2	1:44:B:ASP:HA	13	0.38
(1,912)	1:44:B:ASP:HB2	1:44:B:ASP:HA	16	0.38
(1,912)	1:44:B:ASP:HB2	1:44:B:ASP:HA	20	0.38
(1,431)	1:44:A:ASP:HB2	1:44:A:ASP:HA	1	0.38
(1,431)	1:44:A:ASP:HB2	1:44:A:ASP:HA	2	0.38
(1,431)	1:44:A:ASP:HB2	1:44:A:ASP:HA	7	0.38
(1,431)	1:44:A:ASP:HB2	1:44:A:ASP:HA	9	0.38
(1,431)	1:44:A:ASP:HB2	1:44:A:ASP:HA	20	0.38
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	5	0.38
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	5	0.38
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	5	0.38
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	5	0.38
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	5	0.38
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	5	0.38
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	4	0.37
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	4	0.37
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	4	0.37
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	4	0.37
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	4	0.37
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	4	0.37
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	19	0.37
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	19	0.37
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	19	0.37
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	19	0.37
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	19	0.37
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	19	0.37
(1,526)	1:45:A:GLN:H	1:45:A:GLN:HA	4	0.37
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	10	0.37
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	10	0.37
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	10	0.37
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	10	0.37
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	10	0.37
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	10	0.37
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	2	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	2	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	2	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	2	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	2	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	2	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	9	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	9	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	9	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	9	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	9	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	9	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	16	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	16	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	16	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	16	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	16	0.36
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	16	0.36
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	12	0.36
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	12	0.36
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	14	0.36
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	14	0.36
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	19	0.36
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	19	0.36
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	1	0.36
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	9	0.36
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	11	0.36
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	16	0.36
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	16	0.36
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	16	0.36
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	16	0.36
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	1	0.35
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	1	0.35
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	1	0.35
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	1	0.35
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	1	0.35
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	1	0.35
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	3	0.35
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	15	0.35
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	15	0.35
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	15	0.35
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	15	0.35
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	15	0.35
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	15	0.35
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	15	0.35
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	9	0.35
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	20	0.35
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	20	0.35
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	20	0.35
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	20	0.35
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	20	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	20	0.34
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	4	0.34
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	16	0.34
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	1	0.34
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	7	0.34
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	17	0.34
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	12	0.34
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	8	0.34
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	8	0.34
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	8	0.34
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	9	0.34
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	9	0.34
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	8	0.33
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	8	0.33
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	10	0.33
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	10	0.33
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	15	0.33
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	17	0.33
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	6	0.33
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	6	0.33
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	6	0.33
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	6	0.33
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	6	0.33
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	6	0.33
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	16	0.33
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	20	0.33
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	20	0.33
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	20	0.33
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	16	0.32
(1,676)	1:32:B:ALA:HB1	1:30:B:PHE:HE1	15	0.32
(1,676)	1:32:B:ALA:HB1	1:30:B:PHE:HE2	15	0.32
(1,676)	1:32:B:ALA:HB2	1:30:B:PHE:HE1	15	0.32
(1,676)	1:32:B:ALA:HB2	1:30:B:PHE:HE2	15	0.32
(1,676)	1:32:B:ALA:HB3	1:30:B:PHE:HE1	15	0.32
(1,676)	1:32:B:ALA:HB3	1:30:B:PHE:HE2	15	0.32
(1,562)	1:60:B:HIS:HD2	1:56:B:PHE:H	7	0.32
(1,478)	1:21:A:HIS:H	1:20:A:TYR:HA	16	0.32
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	3	0.32
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	3	0.32
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	3	0.32
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	3	0.32
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	3	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	3	0.32
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	18	0.32
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	18	0.32
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	18	0.32
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	18	0.32
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	18	0.32
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	18	0.32
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	3	0.32
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	4	0.32
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	8	0.32
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	13	0.32
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	16	0.32
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	16	0.32
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	16	0.32
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	16	0.32
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	4	0.31
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	13	0.31
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	15	0.31
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	18	0.31
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	2	0.31
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	5	0.31
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	20	0.31
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	13	0.31
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	13	0.31
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	13	0.31
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	1	0.31
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	1	0.31
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	19	0.31
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	19	0.31
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	2	0.3
(1,768)	1:44:B:ASP:H	1:45:B:GLN:H	5	0.3
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	17	0.3
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	11	0.3
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	12	0.3
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	14	0.3
(1,287)	1:44:A:ASP:H	1:45:A:GLN:H	19	0.3
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	13	0.3
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	13	0.3
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	13	0.3
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	19	0.29
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	19	0.29
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	19	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	12	0.29
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	12	0.29
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	12	0.29
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	12	0.29
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	12	0.29
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	12	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG21	1	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG22	1	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG23	1	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG21	3	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG22	3	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG23	3	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG21	8	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG22	8	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG23	8	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG21	11	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG22	11	0.29
(1,811)	1:62:B:THR:HA	1:62:B:THR:HG23	11	0.29
(1,343)	1:21:A:HIS:HD2	1:21:A:HIS:HB3	16	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	1	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	1	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	1	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	3	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	3	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	3	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	4	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	4	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	4	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	9	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	9	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	9	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	10	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	10	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	10	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG21	12	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG22	12	0.29
(1,330)	1:62:A:THR:HA	1:62:A:THR:HG23	12	0.29
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	4	0.29
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	16	0.29
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	16	0.29
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	16	0.29
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	3	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	3	0.29
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	3	0.29
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	3	0.29
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	10	0.28
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	10	0.28
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	10	0.28
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	3	0.28
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	3	0.28
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	3	0.28
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	3	0.28
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	3	0.28
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	3	0.28
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	3	0.28
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	13	0.28
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	16	0.28
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	20	0.28
(1,824)	1:21:B:HIS:HD2	1:21:B:HIS:HB3	6	0.28
(1,824)	1:21:B:HIS:HD2	1:21:B:HIS:HB3	11	0.28
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	4	0.28
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	15	0.28
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	15	0.28
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	15	0.28
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	17	0.28
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	17	0.28
(1,566)	1:20:B:TYR:HE1	1:61:B:PHE:HA	11	0.28
(1,566)	1:20:B:TYR:HE2	1:61:B:PHE:HA	11	0.28
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	16	0.28
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	16	0.28
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	16	0.28
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	16	0.28
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	16	0.28
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	16	0.28
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	1	0.28
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	2	0.28
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	7	0.28
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	9	0.28
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	20	0.28
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	1	0.28
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	9	0.28
(1,81)	1:60:A:HIS:HD2	1:56:A:PHE:H	16	0.28
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	15	0.28
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	15	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	15	0.28
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	15	0.28
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	18	0.28
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	18	0.28
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	18	0.28
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	18	0.28
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	2	0.27
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	4	0.27
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	12	0.27
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	12	0.27
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	12	0.27
(1,566)	1:20:B:TYR:HE1	1:61:B:PHE:HA	15	0.27
(1,566)	1:20:B:TYR:HE2	1:61:B:PHE:HA	15	0.27
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	5	0.27
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	11	0.27
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	12	0.27
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	14	0.27
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	19	0.27
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	8	0.27
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	8	0.27
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	8	0.27
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	6	0.27
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	6	0.27
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	6	0.27
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	6	0.27
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	12	0.27
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	12	0.27
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	12	0.27
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	20	0.27
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	20	0.27
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	20	0.27
(1,154)	1:35:A:SER:HB3	1:31:A:SER:HB2	10	0.27
(1,154)	1:35:A:SER:HB3	1:31:A:SER:HB2	14	0.27
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	11	0.27
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	19	0.27
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	18	0.27
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	18	0.27
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	4	0.27
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	7	0.27
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	7	0.27
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	12	0.26
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	12	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	12	0.26
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	17	0.26
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	17	0.26
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	17	0.26
(1,861)	1:44:B:ASP:H	1:44:B:ASP:HB2	5	0.26
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	2	0.26
(1,824)	1:21:B:HIS:HD2	1:21:B:HIS:HB3	14	0.26
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	8	0.26
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	8	0.26
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	8	0.26
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	10	0.26
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	10	0.26
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	10	0.26
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	9	0.26
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	9	0.26
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	9	0.26
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	17	0.26
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	2	0.26
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	2	0.26
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	2	0.26
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	3	0.26
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	15	0.26
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	2	0.26
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	2	0.26
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	13	0.26
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	16	0.26
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	18	0.26
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	3	0.26
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	3	0.26
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	3	0.26
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	3	0.26
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	3	0.26
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	3	0.26
(1,343)	1:21:A:HIS:HD2	1:21:A:HIS:HB3	8	0.26
(1,343)	1:21:A:HIS:HD2	1:21:A:HIS:HB3	12	0.26
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	6	0.26
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	6	0.26
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	6	0.26
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	8	0.26
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	8	0.26
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	11	0.26
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	11	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	11	0.26
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	17	0.26
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	17	0.26
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	12	0.26
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	17	0.26
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	15	0.26
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	15	0.26
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	19	0.26
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	19	0.26
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	12	0.26
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	12	0.26
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	12	0.26
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	12	0.26
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	14	0.26
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	14	0.26
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	5	0.26
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	5	0.26
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	15	0.26
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	15	0.26
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	8	0.25
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	20	0.25
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	20	0.25
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	20	0.25
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	20	0.25
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	20	0.25
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	20	0.25
(1,825)	1:21:B:HIS:HD2	1:21:B:HIS:HB2	3	0.25
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	7	0.25
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	7	0.25
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	7	0.25
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	11	0.25
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	11	0.25
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	11	0.25
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	4	0.25
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	9	0.25
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	8	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	5	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	5	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	10	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	10	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	11	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	11	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	12	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	12	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	14	0.25
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	14	0.25
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	10	0.25
(1,380)	1:44:A:ASP:H	1:44:A:ASP:HB2	4	0.25
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	6	0.25
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	6	0.25
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	6	0.25
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	16	0.25
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	16	0.25
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	16	0.25
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	10	0.25
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	11	0.25
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	2	0.25
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	2	0.25
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	2	0.25
(1,154)	1:35:A:SER:HB3	1:31:A:SER:HB2	2	0.25
(1,118)	1:61:A:PHE:HB3	1:57:A:ARG:HA	11	0.25
(1,118)	1:61:A:PHE:HB3	1:57:A:ARG:HA	12	0.25
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	7	0.25
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	7	0.25
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	1	0.25
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	1	0.25
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	1	0.25
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	1	0.25
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	11	0.25
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	11	0.25
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	11	0.25
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	11	0.25
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	14	0.25
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	14	0.25
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	14	0.25
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	14	0.25
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	11	0.25
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	11	0.25
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	11	0.25
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	11	0.25
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	18	0.25
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	18	0.25
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	20	0.24
(1,956)	1:63:B:ASN:HB2	1:63:B:ASN:HA	13	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	10	0.24
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	14	0.24
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	14	0.24
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	14	0.24
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	14	0.24
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	14	0.24
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	14	0.24
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	15	0.24
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	15	0.24
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	15	0.24
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	15	0.24
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	15	0.24
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	15	0.24
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	16	0.24
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	16	0.24
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	5	0.24
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	5	0.24
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	5	0.24
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	2	0.24
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	13	0.24
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	13	0.24
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	16	0.24
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	16	0.24
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	2	0.24
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	11	0.24
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	20	0.24
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	20	0.24
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	17	0.24
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	3	0.24
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	4	0.24
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	4	0.24
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	4	0.24
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	4	0.24
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	4	0.24
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	4	0.24
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	15	0.24
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	15	0.24
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	15	0.24
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	16	0.24
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	16	0.24
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	16	0.24
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	15	0.24
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	15	0.24
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	15	0.24
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	11	0.24
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	13	0.24
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	13	0.24
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	14	0.24
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	14	0.24
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	14	0.24
(1,154)	1:35:A:SER:HB3	1:31:A:SER:HB2	18	0.24
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	14	0.24
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	1	0.24
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	1	0.24
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	18	0.24
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	18	0.24
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	2	0.24
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	2	0.24
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	4	0.24
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	4	0.24
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	11	0.24
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	11	0.24
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	9	0.24
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	9	0.24
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	9	0.24
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	9	0.24
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	2	0.24
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	2	0.24
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	5	0.24
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	5	0.24
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	16	0.24
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	16	0.24
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	6	0.24
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	14	0.23
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	14	0.23
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	14	0.23
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	1	0.23
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	17	0.23
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	19	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	4	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	4	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	4	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	4	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	4	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	4	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	11	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	11	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	11	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	11	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	11	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	11	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	16	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	16	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	16	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	16	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	16	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	16	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	18	0.23
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	18	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	18	0.23
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	18	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	18	0.23
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	18	0.23
(1,825)	1:21:B:HIS:HD2	1:21:B:HIS:HB2	2	0.23
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	14	0.23
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	14	0.23
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	14	0.23
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	17	0.23
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	17	0.23
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	17	0.23
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	5	0.23
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	15	0.23
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	14	0.23
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	19	0.23
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	19	0.23
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	13	0.23
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	13	0.23
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	13	0.23
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	16	0.23
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	16	0.23
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	16	0.23
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	18	0.23
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	18	0.23
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	18	0.23
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	15	0.23
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	15	0.23
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	20	0.23
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	20	0.23
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	19	0.23
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	16	0.23
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	16	0.23
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	1	0.23
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	8	0.23
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	8	0.23
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	8	0.23
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	8	0.23
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	8	0.23
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	8	0.23
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	15	0.23
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	15	0.23
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	15	0.23
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	15	0.23
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	15	0.23
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	15	0.23
(1,344)	1:21:A:HIS:HD2	1:21:A:HIS:HB2	17	0.23
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	8	0.23
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	8	0.23
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	8	0.23
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	11	0.23
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	12	0.23
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	2	0.23
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	8	0.23
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	9	0.23
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	14	0.23
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	18	0.23
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	19	0.23
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	7	0.23
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	7	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	1	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	1	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	2	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	2	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	3	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	3	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	4	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	4	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	9	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	9	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	11	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	11	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	12	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	12	0.23
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	17	0.23
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	17	0.23
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	18	0.23
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	8	0.23
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	8	0.23
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	17	0.23
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	17	0.23
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	14	0.23
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	14	0.23
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	8	0.23
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	20	0.23
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	20	0.23
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	20	0.23
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	20	0.23
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	13	0.23
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	13	0.23
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	11	0.23
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	11	0.23
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	16	0.23
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	16	0.23
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	2	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	2	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	2	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	7	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	7	0.22
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	7	0.22
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	3	0.22
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	2	0.22
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	16	0.22
(1,956)	1:63:B:ASN:HB2	1:63:B:ASN:HA	2	0.22
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	6	0.22
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	7	0.22
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	12	0.22
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	5	0.22
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	5	0.22
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	5	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	5	0.22
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	5	0.22
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	5	0.22
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	17	0.22
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	17	0.22
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	17	0.22
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	17	0.22
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	17	0.22
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	17	0.22
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	2	0.22
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	17	0.22
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	17	0.22
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	13	0.22
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	18	0.22
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	1	0.22
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	1	0.22
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	1	0.22
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	9	0.22
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	18	0.22
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	15	0.22
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	15	0.22
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	4	0.22
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	4	0.22
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	4	0.22
(1,635)	1:35:B:SER:HB3	1:31:B:SER:HB2	17	0.22
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	2	0.22
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	2	0.22
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	4	0.22
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	4	0.22
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	5	0.22
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	5	0.22
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	18	0.22
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	18	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	1	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	1	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	3	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	3	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	8	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	8	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	17	0.22
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	17	0.22
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	10	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	7	0.22
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	8	0.22
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	20	0.22
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	20	0.22
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	20	0.22
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	20	0.22
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	20	0.22
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	20	0.22
(1,344)	1:21:A:HIS:HD2	1:21:A:HIS:HB2	5	0.22
(1,343)	1:21:A:HIS:HD2	1:21:A:HIS:HB3	5	0.22
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	13	0.22
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	13	0.22
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	11	0.22
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	11	0.22
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	2	0.22
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	19	0.22
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	20	0.22
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	6	0.22
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	6	0.22
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	16	0.22
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	13	0.22
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	13	0.22
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	1	0.22
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	1	0.22
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	1	0.22
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	3	0.22
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	3	0.22
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	3	0.22
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	4	0.22
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	4	0.22
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	4	0.22
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	5	0.22
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	5	0.22
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	5	0.22
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	19	0.22
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	19	0.22
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	19	0.22
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	5	0.22
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	5	0.22
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	7	0.22
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	7	0.22
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	14	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	14	0.22
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	19	0.22
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	19	0.22
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	20	0.22
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	20	0.22
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	1	0.22
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	1	0.22
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	15	0.22
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	15	0.22
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	2	0.22
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	20	0.22
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	13	0.22
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	13	0.22
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	6	0.22
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	6	0.22
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	16	0.22
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	6	0.22
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	6	0.22
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	6	0.22
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	6	0.22
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	19	0.22
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	19	0.22
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	19	0.22
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	19	0.22
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	19	0.22
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	19	0.22
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	3	0.21
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	5	0.21
(1,956)	1:63:B:ASN:HB2	1:63:B:ASN:HA	18	0.21
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	14	0.21
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	8	0.21
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	8	0.21
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	8	0.21
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	8	0.21
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	8	0.21
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	8	0.21
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	5	0.21
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	15	0.21
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	10	0.21
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	16	0.21
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	4	0.21
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	16	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	2	0.21
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	3	0.21
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	13	0.21
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	20	0.21
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	1	0.21
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	1	0.21
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	20	0.21
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	20	0.21
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	2	0.21
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	4	0.21
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	10	0.21
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD21	5	0.21
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD22	5	0.21
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD23	5	0.21
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD21	13	0.21
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD22	13	0.21
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD23	13	0.21
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	3	0.21
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	3	0.21
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	11	0.21
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	11	0.21
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	10	0.21
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	10	0.21
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	8	0.21
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	9	0.21
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	12	0.21
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	2	0.21
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	5	0.21
(1,566)	1:20:B:TYR:HE1	1:61:B:PHE:HA	18	0.21
(1,566)	1:20:B:TYR:HE2	1:61:B:PHE:HA	18	0.21
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	9	0.21
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	4	0.21
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	5	0.21
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	14	0.21
(1,475)	1:63:A:ASN:HB2	1:63:A:ASN:HA	2	0.21
(1,475)	1:63:A:ASN:HB2	1:63:A:ASN:HA	13	0.21
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	3	0.21
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	10	0.21
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	10	0.21
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	10	0.21
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	13	0.21
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	13	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	13	0.21
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	14	0.21
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	10	0.21
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	10	0.21
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	10	0.21
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	5	0.21
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	17	0.21
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	4	0.21
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	4	0.21
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	8	0.21
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	8	0.21
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	17	0.21
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	17	0.21
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	7	0.21
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	7	0.21
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	7	0.21
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	14	0.21
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	14	0.21
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	14	0.21
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	9	0.21
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	9	0.21
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	9	0.21
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	11	0.21
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	11	0.21
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	11	0.21
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	16	0.21
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	16	0.21
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	1	0.21
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	1	0.21
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	1	0.21
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	17	0.21
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	17	0.21
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	17	0.21
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	6	0.21
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	6	0.21
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	8	0.21
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	8	0.21
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	13	0.21
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	13	0.21
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	2	0.21
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	10	0.21
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	10	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	5	0.21
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	7	0.21
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	13	0.21
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	16	0.21
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	3	0.21
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	3	0.21
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	11	0.21
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	11	0.21
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	1	0.21
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	1	0.21
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	12	0.21
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	12	0.21
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	2	0.21
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	2	0.21
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	2	0.21
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	2	0.21
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	3	0.21
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	3	0.21
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	3	0.21
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	3	0.21
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	13	0.21
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	13	0.21
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	13	0.21
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	13	0.21
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	4	0.21
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	4	0.21
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	4	0.21
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	4	0.21
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	3	0.21
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	3	0.21
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	10	0.21
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	10	0.21
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	1	0.21
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	1	0.21
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	3	0.21
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	3	0.21
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	4	0.21
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	4	0.21
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	15	0.21
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	15	0.21
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	20	0.21
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	20	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,959)	1:21:B:HIS:H	1:20:B:TYR:HA	4	0.2
(1,951)	1:60:B:HIS:HB3	1:60:B:HIS:HD2	15	0.2
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	9	0.2
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	4	0.2
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	16	0.2
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	18	0.2
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	4	0.2
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	1	0.2
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	8	0.2
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	12	0.2
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	17	0.2
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	19	0.2
(1,825)	1:21:B:HIS:HD2	1:21:B:HIS:HB2	14	0.2
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	3	0.2
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	12	0.2
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	12	0.2
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	12	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	1	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	1	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	1	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	11	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	11	0.2
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	11	0.2
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	6	0.2
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	6	0.2
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	6	0.2
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	10	0.2
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	10	0.2
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	10	0.2
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	8	0.2
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	11	0.2
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	8	0.2
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	8	0.2
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	11	0.2
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	11	0.2
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	3	0.2
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	13	0.2
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	16	0.2
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	17	0.2
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	11	0.2
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	12	0.2
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	18	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD21	18	0.2
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD22	18	0.2
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD23	18	0.2
(1,645)	1:59:B:LYS:HD2	1:59:B:LYS:HA	17	0.2
(1,645)	1:59:B:LYS:HD3	1:59:B:LYS:HA	17	0.2
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	8	0.2
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	8	0.2
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	8	0.2
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	20	0.2
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	20	0.2
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	20	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	1	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	1	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	6	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	6	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	7	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	7	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	8	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	8	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	9	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	9	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	10	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	10	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	12	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	12	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	14	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	14	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	17	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	17	0.2
(1,614)	1:52:B:TYR:HB2	1:53:B:PRO:HA	19	0.2
(1,614)	1:52:B:TYR:HB3	1:53:B:PRO:HA	19	0.2
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	5	0.2
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	13	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	4	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	4	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	6	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	6	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	12	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	12	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	14	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	14	0.2
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	16	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	16	0.2
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	1	0.2
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	14	0.2
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	6	0.2
(1,559)	1:62:A:THR:H	1:62:A:THR:HG21	17	0.2
(1,559)	1:62:A:THR:H	1:62:A:THR:HG22	17	0.2
(1,559)	1:62:A:THR:H	1:62:A:THR:HG23	17	0.2
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	2	0.2
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	12	0.2
(1,470)	1:60:A:HIS:HB3	1:60:A:HIS:HD2	11	0.2
(1,470)	1:60:A:HIS:HB3	1:60:A:HIS:HD2	12	0.2
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	6	0.2
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	13	0.2
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	15	0.2
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	16	0.2
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	2	0.2
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	11	0.2
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	12	0.2
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	14	0.2
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	20	0.2
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	8	0.2
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	14	0.2
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	14	0.2
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	14	0.2
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	14	0.2
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	14	0.2
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	14	0.2
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	1	0.2
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	10	0.2
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	8	0.2
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	8	0.2
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	15	0.2
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	15	0.2
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	16	0.2
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	16	0.2
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	3	0.2
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	5	0.2
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	15	0.2
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	15	0.2
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	15	0.2
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	9	0.2
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	9	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:60:A:HIS:H	1:57:A:ARG:HA	11	0.2
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	12	0.2
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	12	0.2
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	15	0.2
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	15	0.2
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	5	0.2
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	5	0.2
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	5	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	1	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	2	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	3	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	4	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	5	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	8	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	9	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	13	0.2
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	20	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	2	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	2	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	2	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	17	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	17	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	17	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	20	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	20	0.2
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	20	0.2
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	9	0.2
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	9	0.2
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	9	0.2
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	6	0.2
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	6	0.2
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	6	0.2
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	16	0.2
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	16	0.2
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	16	0.2
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	15	0.2
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	15	0.2
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	16	0.2
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	16	0.2
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	4	0.2
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	16	0.2
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	16	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	6	0.2
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	13	0.2
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	13	0.2
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	5	0.2
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	5	0.2
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	12	0.2
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	12	0.2
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	7	0.2
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	7	0.2
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	2	0.2
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	2	0.2
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	2	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	6	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	6	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	6	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	6	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	9	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	9	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	9	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	9	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	15	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	15	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	15	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	15	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	20	0.2
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	20	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	20	0.2
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	20	0.2
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	3	0.2
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	3	0.2
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	7	0.2
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	7	0.2
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	9	0.2
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	9	0.2
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	12	0.2
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	12	0.2
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	20	0.2
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	20	0.2
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	10	0.2
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	10	0.2
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	11	0.2
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	11	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	6	0.19
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	6	0.19
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	6	0.19
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	13	0.19
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	15	0.19
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	4	0.19
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	13	0.19
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	15	0.19
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	18	0.19
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	7	0.19
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	7	0.19
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	7	0.19
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	7	0.19
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	7	0.19
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	7	0.19
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	9	0.19
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	9	0.19
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	9	0.19
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	9	0.19
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	9	0.19
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	9	0.19
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	10	0.19
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	10	0.19
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	10	0.19
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	10	0.19
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	10	0.19
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	10	0.19
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	1	0.19
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	1	0.19
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	1	0.19
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	10	0.19
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	10	0.19
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	10	0.19
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	12	0.19
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	12	0.19
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	12	0.19
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	16	0.19
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	16	0.19
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	16	0.19
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	17	0.19
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	17	0.19
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	17	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,856)	1:43:B:CYS:H	1:42:B:LEU:HB3	13	0.19
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	1	0.19
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	2	0.19
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	3	0.19
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	19	0.19
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	3	0.19
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	7	0.19
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	14	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	1	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	2	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	3	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	4	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	5	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	6	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	7	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	8	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	9	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	10	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	11	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	12	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	13	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	14	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	15	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	16	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	17	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	18	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	19	0.19
(1,807)	1:29:B:LEU:HA	1:29:B:LEU:HB3	20	0.19
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	6	0.19
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	11	0.19
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	11	0.19
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	13	0.19
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	13	0.19
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	14	0.19
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	14	0.19
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	9	0.19
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	9	0.19
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	9	0.19
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	19	0.19
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	19	0.19
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	19	0.19
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	3	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	3	0.19
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	3	0.19
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	20	0.19
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	20	0.19
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	20	0.19
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	8	0.19
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	8	0.19
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	8	0.19
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	9	0.19
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	9	0.19
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	5	0.19
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	6	0.19
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	13	0.19
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	13	0.19
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	9	0.19
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	9	0.19
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	9	0.19
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	5	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	1	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	5	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	6	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	7	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	8	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	10	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	12	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	14	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	18	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	19	0.19
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	20	0.19
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	19	0.19
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	19	0.19
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	19	0.19
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	5	0.19
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	6	0.19
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	6	0.19
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	6	0.19
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD21	20	0.19
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD22	20	0.19
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD23	20	0.19
(1,645)	1:59:B:LYS:HD2	1:59:B:LYS:HA	7	0.19
(1,645)	1:59:B:LYS:HD3	1:59:B:LYS:HA	7	0.19
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	3	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	3	0.19
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	3	0.19
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	12	0.19
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	12	0.19
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	12	0.19
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	2	0.19
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	2	0.19
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	2	0.19
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	4	0.19
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	4	0.19
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	4	0.19
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	6	0.19
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	6	0.19
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	6	0.19
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	9	0.19
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	9	0.19
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	9	0.19
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	16	0.19
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	16	0.19
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	16	0.19
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	18	0.19
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	5	0.19
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	5	0.19
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	19	0.19
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	19	0.19
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	11	0.19
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	17	0.19
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	6	0.19
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	1	0.19
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	4	0.19
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	9	0.19
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	20	0.19
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	18	0.19
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	18	0.19
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	2	0.19
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	4	0.19
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	11	0.19
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	20	0.19
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	17	0.19
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	19	0.19
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	20	0.19
(1,470)	1:60:A:HIS:HB3	1:60:A:HIS:HD2	18	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	7	0.19
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	7	0.19
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	7	0.19
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	7	0.19
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	7	0.19
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	7	0.19
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	16	0.19
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	16	0.19
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	16	0.19
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	5	0.19
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	19	0.19
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	4	0.19
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	5	0.19
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	7	0.19
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	10	0.19
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	3	0.19
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	10	0.19
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	17	0.19
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	18	0.19
(1,344)	1:21:A:HIS:HD2	1:21:A:HIS:HB2	12	0.19
(1,343)	1:21:A:HIS:HD2	1:21:A:HIS:HB3	17	0.19
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	19	0.19
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	19	0.19
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	19	0.19
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	19	0.19
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	19	0.19
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	19	0.19
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	5	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	1	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	2	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	3	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	4	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	5	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	6	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	7	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	8	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	9	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	10	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	11	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	12	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	13	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	14	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	15	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	16	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	17	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	18	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	19	0.19
(1,326)	1:29:A:LEU:HA	1:29:A:LEU:HB3	20	0.19
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	11	0.19
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	11	0.19
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	6	0.19
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	6	0.19
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	10	0.19
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	10	0.19
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	18	0.19
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	18	0.19
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	18	0.19
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	1	0.19
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	1	0.19
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	3	0.19
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	3	0.19
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	13	0.19
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	13	0.19
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	12	0.19
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	12	0.19
(1,244)	1:60:A:HIS:H	1:57:A:ARG:HA	12	0.19
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	9	0.19
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	1	0.19
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	1	0.19
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	6	0.19
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	6	0.19
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	11	0.19
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	11	0.19
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	20	0.19
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	20	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	4	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	4	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	4	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	12	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	12	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	12	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	18	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	18	0.19
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	18	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	3	0.19
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	4	0.19
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	9	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	7	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	10	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	14	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	15	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	16	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	17	0.19
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	19	0.19
(1,193)	1:55:A:HIS:HD2	1:55:A:HIS:HB2	11	0.19
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	13	0.19
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	13	0.19
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	13	0.19
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	15	0.19
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	15	0.19
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	15	0.19
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	2	0.19
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	6	0.19
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	17	0.19
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	12	0.19
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	12	0.19
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	12	0.19
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	17	0.19
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	17	0.19
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	17	0.19
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	10	0.19
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	10	0.19
(1,133)	1:52:A:TYR:HB2	1:53:A:PRO:HA	18	0.19
(1,133)	1:52:A:TYR:HB3	1:53:A:PRO:HA	18	0.19
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	19	0.19
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	3	0.19
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	3	0.19
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	8	0.19
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	8	0.19
(1,118)	1:61:A:PHE:HB3	1:57:A:ARG:HA	18	0.19
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	4	0.19
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	15	0.19
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	16	0.19
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	6	0.19
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	9	0.19
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	9	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	18	0.19
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	18	0.19
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	4	0.19
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	4	0.19
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	12	0.19
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	12	0.19
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	7	0.19
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	7	0.19
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	9	0.19
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	9	0.19
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	17	0.19
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	17	0.19
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	6	0.19
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	12	0.19
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	12	0.19
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	12	0.19
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	17	0.19
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	17	0.19
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	17	0.19
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	17	0.19
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	5	0.19
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	5	0.19
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	5	0.19
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	5	0.19
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	18	0.19
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	18	0.19
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	6	0.19
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	6	0.19
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	13	0.19
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	13	0.19
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	8	0.19
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	8	0.19
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	12	0.19
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	12	0.19
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	13	0.19
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	13	0.19
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	19	0.19
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	19	0.19
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	10	0.19
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	17	0.19
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	11	0.18
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	5	0.18
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	16	0.18
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	19	0.18
(1,951)	1:60:B:HIS:HB3	1:60:B:HIS:HD2	11	0.18
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	1	0.18
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	10	0.18
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	15	0.18
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	19	0.18
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	13	0.18
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	13	0.18
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	13	0.18
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	13	0.18
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	13	0.18
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	13	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	6	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	6	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	6	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	7	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	7	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	7	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	8	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	8	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	8	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	9	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	9	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	9	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	11	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	11	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	11	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	13	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	13	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	13	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	14	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	14	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	14	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	18	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	18	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	18	0.18
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	19	0.18
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	19	0.18
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	19	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	3	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	4	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	5	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	13	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	15	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	16	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	18	0.18
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	20	0.18
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	9	0.18
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	12	0.18
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	16	0.18
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	9	0.18
(1,825)	1:21:B:HIS:HD2	1:21:B:HIS:HB2	6	0.18
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	6	0.18
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	9	0.18
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	14	0.18
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	19	0.18
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	9	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	5	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	5	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	6	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	6	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	7	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	7	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	15	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	15	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	18	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	18	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	20	0.18
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	20	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	1	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	1	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	9	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	9	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	11	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	11	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	19	0.18
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	19	0.18
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	2	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	2	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	2	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	3	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	3	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	4	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	4	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	5	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	5	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	8	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	8	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	18	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	18	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	20	0.18
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	20	0.18
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	11	0.18
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	11	0.18
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	11	0.18
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	19	0.18
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	19	0.18
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	19	0.18
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	4	0.18
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	4	0.18
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	16	0.18
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	16	0.18
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	15	0.18
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	15	0.18
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	7	0.18
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	10	0.18
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	5	0.18
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	5	0.18
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	7	0.18
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	7	0.18
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	9	0.18
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	9	0.18
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	14	0.18
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	14	0.18
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	15	0.18
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	15	0.18
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	15	0.18
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	20	0.18
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	20	0.18
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	20	0.18
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	9	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	1	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	1	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	7	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	7	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	7	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	9	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	9	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	9	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	17	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	17	0.18
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	17	0.18
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD21	15	0.18
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD22	15	0.18
(1,659)	1:27:B:GLU:H	1:41:B:LEU:HD23	15	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	3	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	5	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	6	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	7	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	9	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	18	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	19	0.18
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	20	0.18
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	7	0.18
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	7	0.18
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	7	0.18
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	10	0.18
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	10	0.18
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	10	0.18
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	17	0.18
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	17	0.18
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	17	0.18
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	1	0.18
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	1	0.18
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	1	0.18
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	12	0.18
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	12	0.18
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	12	0.18
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	16	0.18
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	7	0.18
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	7	0.18
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	13	0.18
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	13	0.18
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	8	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	14	0.18
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	2	0.18
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	11	0.18
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	1	0.18
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	1	0.18
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	7	0.18
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	11	0.18
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	2	0.18
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	4	0.18
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	8	0.18
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	13	0.18
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	13	0.18
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	13	0.18
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	13	0.18
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	13	0.18
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	13	0.18
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	13	0.18
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	17	0.18
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	17	0.18
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	17	0.18
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	17	0.18
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	17	0.18
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	17	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	1	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	1	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	1	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	6	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	6	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	6	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	8	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	8	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	8	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	10	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	10	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	10	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	13	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	13	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	13	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	15	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	15	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	15	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	17	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	17	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	17	0.18
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	18	0.18
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	18	0.18
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	18	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	1	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	2	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	3	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	4	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	5	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	7	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	9	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	11	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	12	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	14	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	17	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	19	0.18
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	20	0.18
(1,375)	1:43:A:CYS:H	1:42:A:LEU:HB3	4	0.18
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	3	0.18
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	6	0.18
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	8	0.18
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	15	0.18
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	18	0.18
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	6	0.18
(1,344)	1:21:A:HIS:HD2	1:21:A:HIS:HB2	8	0.18
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	6	0.18
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	18	0.18
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	18	0.18
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	15	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	1	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	1	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	2	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	2	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	9	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	9	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	13	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	13	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	16	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	16	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	17	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	17	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	20	0.18
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	20	0.18
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	1	0.18
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	9	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	2	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	2	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	3	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	3	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	4	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	4	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	5	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	5	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	7	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	7	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	9	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	9	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	11	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	11	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	12	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	12	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	14	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	14	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	17	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	17	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	19	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	19	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	20	0.18
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	20	0.18
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	3	0.18
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	3	0.18
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	3	0.18
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	4	0.18
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	4	0.18
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	8	0.18
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	8	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	3	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	3	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	4	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	4	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	5	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	5	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	11	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	11	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	14	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	14	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	20	0.18
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	20	0.18
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	1	0.18
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	6	0.18
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	11	0.18
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	12	0.18
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	12	0.18
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	19	0.18
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	19	0.18
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	19	0.18
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	6	0.18
(1,193)	1:55:A:HIS:HD2	1:55:A:HIS:HB2	12	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	8	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	8	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	8	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	18	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	18	0.18
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	18	0.18
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	5	0.18
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	1	0.18
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	1	0.18
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	1	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	1	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	3	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	5	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	6	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	8	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	9	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	10	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	13	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	14	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	15	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	16	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	17	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	19	0.18
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	20	0.18
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	9	0.18
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	9	0.18
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	20	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	20	0.18
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	16	0.18
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	16	0.18
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	16	0.18
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	11	0.18
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	11	0.18
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	11	0.18
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	6	0.18
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	9	0.18
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	17	0.18
(1,118)	1:61:A:PHE:HB3	1:57:A:ARG:HA	17	0.18
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	4	0.18
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	8	0.18
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	4	0.18
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	4	0.18
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	10	0.18
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	10	0.18
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	17	0.18
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	5	0.18
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	5	0.18
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	5	0.18
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	5	0.18
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	18	0.18
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	18	0.18
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	18	0.18
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	18	0.18
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	14	0.18
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	14	0.18
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	7	0.18
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	7	0.18
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	16	0.18
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	16	0.18
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	17	0.18
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	17	0.18
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	14	0.18
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	4	0.18
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	4	0.18
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	4	0.18
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	18	0.17
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	4	0.17
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	4	0.17
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	4	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG21	15	0.17
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG22	15	0.17
(1,1040)	1:62:B:THR:H	1:62:B:THR:HG23	15	0.17
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	4	0.17
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	16	0.17
(1,1011)	1:47:B:LEU:H	1:39:B:SER:HA	18	0.17
(1,999)	1:41:B:LEU:H	1:40:B:CYS:HB2	20	0.17
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	3	0.17
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	15	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	1	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	2	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	3	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	4	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	5	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	6	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	7	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	8	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	9	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	10	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	11	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	12	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	13	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	14	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	15	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	16	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	17	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	18	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	19	0.17
(1,980)	1:34:B:ALA:H	1:34:B:ALA:HA	20	0.17
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	1	0.17
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	7	0.17
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	11	0.17
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	12	0.17
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	18	0.17
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	20	0.17
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	6	0.17
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	8	0.17
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	11	0.17
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	16	0.17
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	20	0.17
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	8	0.17
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	8	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	1	0.17
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	1	0.17
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	1	0.17
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	1	0.17
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	1	0.17
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	1	0.17
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	6	0.17
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	6	0.17
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	6	0.17
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	6	0.17
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	6	0.17
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	6	0.17
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	19	0.17
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	19	0.17
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	19	0.17
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	19	0.17
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	19	0.17
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	19	0.17
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	2	0.17
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	2	0.17
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	2	0.17
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	3	0.17
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	3	0.17
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	3	0.17
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	4	0.17
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	4	0.17
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	4	0.17
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	5	0.17
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	5	0.17
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	5	0.17
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	15	0.17
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	15	0.17
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	15	0.17
(1,926)	1:49:B:LEU:HD11	1:49:B:LEU:HB3	20	0.17
(1,926)	1:49:B:LEU:HD12	1:49:B:LEU:HB3	20	0.17
(1,926)	1:49:B:LEU:HD13	1:49:B:LEU:HB3	20	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	1	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	6	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	7	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	8	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	9	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	10	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	11	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	12	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	14	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	17	0.17
(1,858)	1:42:B:LEU:HA	1:42:B:LEU:HB2	19	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	7	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	8	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	10	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	11	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	13	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	14	0.17
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	17	0.17
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	11	0.17
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	14	0.17
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	15	0.17
(1,825)	1:21:B:HIS:HD2	1:21:B:HIS:HB2	11	0.17
(1,824)	1:21:B:HIS:HD2	1:21:B:HIS:HB3	2	0.17
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	7	0.17
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	8	0.17
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	11	0.17
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	12	0.17
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	4	0.17
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	7	0.17
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	11	0.17
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	19	0.17
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	12	0.17
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	12	0.17
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	14	0.17
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	14	0.17
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	17	0.17
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	17	0.17
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	7	0.17
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	7	0.17
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	16	0.17
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	16	0.17
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	16	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	1	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	1	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	7	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	7	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	9	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	10	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	10	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	12	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	12	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	13	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	13	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	14	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	14	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	15	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	15	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	16	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	16	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	17	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	17	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	19	0.17
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	19	0.17
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	4	0.17
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	4	0.17
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	4	0.17
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	15	0.17
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	15	0.17
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	15	0.17
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	12	0.17
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	12	0.17
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	12	0.17
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	17	0.17
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	17	0.17
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	17	0.17
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	5	0.17
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	5	0.17
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	4	0.17
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	4	0.17
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	5	0.17
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	15	0.17
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	16	0.17
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	19	0.17
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	14	0.17
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	14	0.17
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	14	0.17
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	11	0.17
(1,678)	1:56:B:PHE:H	1:55:B:HIS:HB2	15	0.17
(1,676)	1:32:B:ALA:HB1	1:30:B:PHE:HE1	16	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:32:B:ALA:HB1	1:30:B:PHE:HE2	16	0.17
(1,676)	1:32:B:ALA:HB2	1:30:B:PHE:HE1	16	0.17
(1,676)	1:32:B:ALA:HB2	1:30:B:PHE:HE2	16	0.17
(1,676)	1:32:B:ALA:HB3	1:30:B:PHE:HE1	16	0.17
(1,676)	1:32:B:ALA:HB3	1:30:B:PHE:HE2	16	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	10	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	10	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	10	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	11	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	11	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	11	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	12	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	12	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	12	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	14	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	14	0.17
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	14	0.17
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	9	0.17
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	20	0.17
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	20	0.17
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	20	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	1	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	2	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	4	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	8	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	10	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	11	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	12	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	13	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	14	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	15	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	16	0.17
(1,658)	1:30:B:PHE:H	1:29:B:LEU:HB3	17	0.17
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	11	0.17
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	11	0.17
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	11	0.17
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	14	0.17
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	14	0.17
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	14	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	3	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	3	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	3	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	8	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	8	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	8	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	11	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	11	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	11	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	14	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	14	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	14	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	15	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	15	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	15	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	17	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	17	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	17	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	18	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	18	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	18	0.17
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	19	0.17
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	19	0.17
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	19	0.17
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	3	0.17
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	3	0.17
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	3	0.17
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	3	0.17
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	6	0.17
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	10	0.17
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	20	0.17
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	9	0.17
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	9	0.17
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	7	0.17
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	10	0.17
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	15	0.17
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	17	0.17
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	8	0.17
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	8	0.17
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	5	0.17
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	1	0.17
(1,518)	1:41:A:LEU:H	1:40:A:CYS:HB2	9	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	1	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	2	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	3	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	4	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	5	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	6	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	7	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	8	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	9	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	10	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	11	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	12	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	13	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	14	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	15	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	16	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	17	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	18	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	19	0.17
(1,499)	1:34:A:ALA:H	1:34:A:ALA:HA	20	0.17
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	13	0.17
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	20	0.17
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	7	0.17
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	14	0.17
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	19	0.17
(1,457)	1:57:A:ARG:HD2	1:57:A:ARG:HG3	20	0.17
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	11	0.17
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	11	0.17
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	11	0.17
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	11	0.17
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	11	0.17
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	11	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	2	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	2	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	2	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	3	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	3	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	3	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	4	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	4	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	4	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	5	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	5	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	5	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	7	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	7	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	7	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	9	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	9	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	9	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	11	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	11	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	11	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	19	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	19	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	19	0.17
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	20	0.17
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	20	0.17
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	20	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	6	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	8	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	10	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	13	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	15	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	16	0.17
(1,377)	1:42:A:LEU:HA	1:42:A:LEU:HB2	18	0.17
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	2	0.17
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	13	0.17
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	14	0.17
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	7	0.17
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	14	0.17
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	15	0.17
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD21	12	0.17
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD22	12	0.17
(1,339)	1:27:A:GLU:HG2	1:41:A:LEU:HD23	12	0.17
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD21	12	0.17
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD22	12	0.17
(1,339)	1:27:A:GLU:HG3	1:41:A:LEU:HD23	12	0.17
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	5	0.17
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	10	0.17
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	15	0.17
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	16	0.17
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	15	0.17
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	6	0.17
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	10	0.17
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	8	0.17
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	8	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	17	0.17
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	17	0.17
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	17	0.17
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	17	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	1	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	1	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	6	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	6	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	8	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	8	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	10	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	10	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	15	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	15	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	16	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	16	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	18	0.17
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	18	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	5	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	5	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	5	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	12	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	12	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	12	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	14	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	14	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	14	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	20	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	20	0.17
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	20	0.17
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	2	0.17
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	3	0.17
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	4	0.17
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	1	0.17
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	3	0.17
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	6	0.17
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	13	0.17
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	20	0.17
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	3	0.17
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	3	0.17
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	9	0.17
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	10	0.17
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	10	0.17
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	18	0.17
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	18	0.17
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	16	0.17
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	11	0.17
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	12	0.17
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	10	0.17
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	10	0.17
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	10	0.17
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	16	0.17
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	16	0.17
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	16	0.17
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	13	0.17
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	19	0.17
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	9	0.17
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	9	0.17
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	9	0.17
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	2	0.17
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	4	0.17
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	7	0.17
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	11	0.17
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	18	0.17
(1,164)	1:59:A:LYS:HD2	1:59:A:LYS:HA	1	0.17
(1,164)	1:59:A:LYS:HD3	1:59:A:LYS:HA	1	0.17
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	7	0.17
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	7	0.17
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	7	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	1	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	1	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	1	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	2	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	2	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	2	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	3	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	3	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	3	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	4	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	4	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	4	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	5	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	5	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	5	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	9	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	9	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	9	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	10	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	10	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	10	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	14	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	14	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	14	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	17	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	17	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	17	0.17
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	19	0.17
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	19	0.17
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	19	0.17
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	1	0.17
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	17	0.17
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	9	0.17
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	9	0.17
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	9	0.17
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	1	0.17
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	3	0.17
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	5	0.17
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	14	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	2	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	2	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	7	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	7	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	13	0.17
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	13	0.17
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	10	0.17
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	13	0.17
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	5	0.17
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	5	0.17
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	12	0.17
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	12	0.17
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	20	0.17
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	20	0.17
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	15	0.17
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	15	0.17
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	16	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	16	0.17
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	10	0.17
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	1	0.17
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	12	0.17
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	15	0.17
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	16	0.17
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	16	0.17
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	16	0.17
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	16	0.17
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	16	0.17
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	16	0.17
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	3	0.17
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	3	0.17
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	3	0.17
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	3	0.17
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	3	0.17
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	3	0.17
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	6	0.17
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	6	0.17
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	6	0.17
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	6	0.17
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	6	0.17
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	6	0.17
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	18	0.17
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	18	0.17
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	18	0.17
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	18	0.17
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	18	0.17
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	18	0.17
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	15	0.17
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	15	0.17
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	15	0.17
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	13	0.17
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	13	0.17
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	5	0.17
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	5	0.17
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	9	0.17
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	9	0.17
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	7	0.17
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	7	0.17
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	7	0.17
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	2	0.16
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	4	0.16
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	19	0.16
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	5	0.16
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	6	0.16
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	8	0.16
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	11	0.16
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	11	0.16
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	16	0.16
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	16	0.16
(1,938)	1:57:B:ARG:HD2	1:57:B:ARG:HG3	13	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	1	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	1	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	6	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	6	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	10	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	10	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	12	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	12	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	13	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	13	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	17	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	17	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	18	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	18	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	19	0.16
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	19	0.16
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	14	0.16
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	14	0.16
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	14	0.16
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	5	0.16
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	15	0.16
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	18	0.16
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	20	0.16
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	6	0.16
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	13	0.16
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	18	0.16
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	1	0.16
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	2	0.16
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	5	0.16
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	10	0.16
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	2	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	5	0.16
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	13	0.16
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	19	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	1	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	1	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	2	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	2	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	3	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	3	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	4	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	4	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	5	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	5	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	6	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	6	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	7	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	7	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	8	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	8	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	9	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	9	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	10	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	10	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	11	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	11	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	12	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	12	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	13	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	13	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	14	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	14	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	15	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	15	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	16	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	16	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	17	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	17	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	18	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	18	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	19	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	19	0.16
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG2	20	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:54:B:GLU:H	1:54:B:GLU:HG3	20	0.16
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	15	0.16
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	15	0.16
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	15	0.16
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	20	0.16
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	20	0.16
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	20	0.16
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	6	0.16
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	6	0.16
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG2	11	0.16
(1,760)	1:37:B:GLU:H	1:37:B:GLU:HG3	11	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	2	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	2	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	2	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	6	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	6	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	6	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	9	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	9	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	9	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	12	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	12	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	12	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	14	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	14	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	14	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	19	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	19	0.16
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	19	0.16
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	16	0.16
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	16	0.16
(1,725)	1:60:B:HIS:H	1:57:B:ARG:HA	11	0.16
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	13	0.16
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	16	0.16
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	18	0.16
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	1	0.16
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	2	0.16
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	2	0.16
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	4	0.16
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	4	0.16
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	10	0.16
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	10	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	12	0.16
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	12	0.16
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	1	0.16
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	1	0.16
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	1	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	1	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	6	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	7	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	8	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	10	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	12	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	14	0.16
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	17	0.16
(1,674)	1:55:B:HIS:HD2	1:55:B:HIS:HB2	15	0.16
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	6	0.16
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	6	0.16
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	6	0.16
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD11	8	0.16
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD12	8	0.16
(1,670)	1:56:B:PHE:H	1:47:B:LEU:HD13	8	0.16
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	7	0.16
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	7	0.16
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	7	0.16
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	10	0.16
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	10	0.16
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	10	0.16
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	6	0.16
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	6	0.16
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	6	0.16
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	5	0.16
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	5	0.16
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	5	0.16
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	7	0.16
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	7	0.16
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	7	0.16
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	10	0.16
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	10	0.16
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	10	0.16
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	13	0.16
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	13	0.16
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	13	0.16
(1,641)	1:38:B:VAL:HG11	1:37:B:GLU:HA	20	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,641)	1:38:B:VAL:HG12	1:37:B:GLU:HA	20	0.16
(1,641)	1:38:B:VAL:HG13	1:37:B:GLU:HA	20	0.16
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	16	0.16
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	3	0.16
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	20	0.16
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	20	0.16
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	20	0.16
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	20	0.16
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	1	0.16
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	2	0.16
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	4	0.16
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	8	0.16
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	19	0.16
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	18	0.16
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	18	0.16
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	4	0.16
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	18	0.16
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	3	0.16
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	3	0.16
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	6	0.16
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	6	0.16
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	19	0.16
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	19	0.16
(1,566)	1:20:B:TYR:HE1	1:61:B:PHE:HA	5	0.16
(1,566)	1:20:B:TYR:HE2	1:61:B:PHE:HA	5	0.16
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	19	0.16
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	4	0.16
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	5	0.16
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	9	0.16
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	12	0.16
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	13	0.16
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	18	0.16
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	3	0.16
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	4	0.16
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	11	0.16
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	17	0.16
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	16	0.16
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	1	0.16
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	1	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	1	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	1	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	3	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	3	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	7	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	7	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	8	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	8	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	10	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	10	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	13	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	13	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	17	0.16
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	17	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	1	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	1	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	1	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	1	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	1	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	1	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	5	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	5	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	5	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	5	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	5	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	5	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	18	0.16
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	18	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	18	0.16
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	18	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	18	0.16
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	18	0.16
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	12	0.16
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	12	0.16
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	12	0.16
(1,445)	1:49:A:LEU:HD11	1:49:A:LEU:HB3	14	0.16
(1,445)	1:49:A:LEU:HD12	1:49:A:LEU:HB3	14	0.16
(1,445)	1:49:A:LEU:HD13	1:49:A:LEU:HB3	14	0.16
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	16	0.16
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	16	0.16
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	16	0.16
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	16	0.16
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	17	0.16
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	19	0.16
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	20	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	13	0.16
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	19	0.16
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	20	0.16
(1,344)	1:21:A:HIS:HD2	1:21:A:HIS:HB2	16	0.16
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	3	0.16
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	8	0.16
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	13	0.16
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	14	0.16
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	3	0.16
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	17	0.16
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	18	0.16
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	18	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	1	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	1	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	2	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	2	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	3	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	3	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	4	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	4	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	5	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	5	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	6	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	6	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	7	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	7	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	8	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	8	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	9	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	9	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	10	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	10	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	12	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	12	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	13	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	13	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	14	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	14	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	15	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	15	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	16	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	16	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	17	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	17	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	18	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	18	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	19	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	19	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG2	20	0.16
(1,315)	1:54:A:GLU:H	1:54:A:GLU:HG3	20	0.16
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG2	13	0.16
(1,279)	1:37:A:GLU:H	1:37:A:GLU:HG3	13	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	2	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	2	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	2	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	9	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	9	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	9	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	11	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	11	0.16
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	11	0.16
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	18	0.16
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	18	0.16
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	18	0.16
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	2	0.16
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	2	0.16
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	16	0.16
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	16	0.16
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	18	0.16
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	18	0.16
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	19	0.16
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	19	0.16
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	19	0.16
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	19	0.16
(1,244)	1:60:A:HIS:H	1:57:A:ARG:HA	18	0.16
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	7	0.16
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	16	0.16
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	7	0.16
(1,241)	1:30:A:PHE:HZ	1:32:A:ALA:HA	15	0.16
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	5	0.16
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	5	0.16
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	19	0.16
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	19	0.16
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	15	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	15	0.16
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	15	0.16
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	1	0.16
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	6	0.16
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	8	0.16
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	10	0.16
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	13	0.16
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	15	0.16
(1,197)	1:56:A:PHE:H	1:55:A:HIS:HB2	18	0.16
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD11	6	0.16
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD12	6	0.16
(1,189)	1:56:A:PHE:H	1:47:A:LEU:HD13	6	0.16
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	18	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	7	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	7	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	7	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	8	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	8	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	8	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	17	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	17	0.16
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	17	0.16
(1,177)	1:30:A:PHE:H	1:29:A:LEU:HB3	12	0.16
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	15	0.16
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	15	0.16
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	15	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	7	0.16
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	7	0.16
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	7	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	8	0.16
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	8	0.16
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	8	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	13	0.16
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	13	0.16
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	13	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	15	0.16
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	15	0.16
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	15	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	18	0.16
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	18	0.16
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	18	0.16
(1,160)	1:38:A:VAL:HG11	1:37:A:GLU:HA	20	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:38:A:VAL:HG12	1:37:A:GLU:HA	20	0.16
(1,160)	1:38:A:VAL:HG13	1:37:A:GLU:HA	20	0.16
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	1	0.16
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	1	0.16
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	1	0.16
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	7	0.16
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	11	0.16
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	15	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	4	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	4	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	9	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	9	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	14	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	14	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	20	0.16
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	20	0.16
(1,110)	1:56:A:PHE:HE1	1:25:A:CYS:HA	3	0.16
(1,110)	1:56:A:PHE:HE2	1:25:A:CYS:HA	3	0.16
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	8	0.16
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	3	0.16
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	10	0.16
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	18	0.16
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	6	0.16
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	6	0.16
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	20	0.16
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	20	0.16
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	2	0.16
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	2	0.16
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	11	0.16
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	11	0.16
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	5	0.16
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	5	0.16
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	8	0.16
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	9	0.16
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	11	0.16
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	6	0.16
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	6	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	1	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	1	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	1	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	1	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	1	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	2	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	2	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	2	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	2	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	2	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	2	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	3	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	3	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	3	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	3	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	3	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	3	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	4	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	4	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	4	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	4	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	4	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	4	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	6	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	6	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	6	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	6	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	6	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	6	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	8	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	8	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	8	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	8	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	8	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	8	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	9	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	9	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	9	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	9	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	9	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	9	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	10	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	10	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	10	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	10	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	10	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	10	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	14	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	14	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	14	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	14	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	14	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	14	0.16
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	17	0.16
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	17	0.16
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	17	0.16
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	17	0.16
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	17	0.16
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	17	0.16
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	4	0.16
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	4	0.16
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	4	0.16
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	4	0.16
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	4	0.16
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	4	0.16
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	5	0.16
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	5	0.16
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	5	0.16
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	5	0.16
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	5	0.16
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	5	0.16
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	12	0.16
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	12	0.16
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	12	0.16
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	12	0.16
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	12	0.16
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	12	0.16
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	7	0.16
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	7	0.16
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	7	0.16
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	1	0.16
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	1	0.16
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	1	0.16
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	1	0.16
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	17	0.16
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	17	0.16
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	17	0.16
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	17	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	6	0.16
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	6	0.16
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	4	0.16
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	4	0.16
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	8	0.16
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	8	0.16
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	14	0.16
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	14	0.16
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	18	0.16
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	18	0.16
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	10	0.16
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	10	0.16
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	10	0.16
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	13	0.16
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	13	0.16
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	13	0.16
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	18	0.16
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	18	0.16
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	18	0.16
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	11	0.16
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	11	0.16
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	11	0.16
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	11	0.15
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	18	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	5	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	6	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	7	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	8	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	9	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	12	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	13	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	14	0.15
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	17	0.15
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	9	0.15
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	13	0.15
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	14	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	3	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	5	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	7	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	9	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	14	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	17	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	19	0.15
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	20	0.15
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	6	0.15
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	6	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	1	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	1	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	6	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	6	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	10	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	10	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	14	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	14	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	17	0.15
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	17	0.15
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	5	0.15
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	5	0.15
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	13	0.15
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	13	0.15
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	20	0.15
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	20	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	2	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	2	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	4	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	4	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	5	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	5	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	7	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	7	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	9	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	9	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	11	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	11	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	14	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	14	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	20	0.15
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	20	0.15
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	11	0.15
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD1	2	0.15
(1,927)	1:49:B:LEU:HD21	1:36:B:TYR:HD2	2	0.15
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD1	2	0.15
(1,927)	1:49:B:LEU:HD22	1:36:B:TYR:HD2	2	0.15
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD1	2	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,927)	1:49:B:LEU:HD23	1:36:B:TYR:HD2	2	0.15
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	11	0.15
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	11	0.15
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	11	0.15
(1,850)	1:27:B:GLU:H	1:26:B:GLY:HA3	6	0.15
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	5	0.15
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	10	0.15
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	10	0.15
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	10	0.15
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	10	0.15
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	10	0.15
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	10	0.15
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	3	0.15
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	13	0.15
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	17	0.15
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	20	0.15
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	6	0.15
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	18	0.15
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	1	0.15
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	20	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	1	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	1	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	1	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	5	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	5	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	5	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	7	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	7	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	7	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	8	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	8	0.15
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	8	0.15
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	7	0.15
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	7	0.15
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	7	0.15
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	14	0.15
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	14	0.15
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	14	0.15
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	2	0.15
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	2	0.15
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	18	0.15
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	18	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	20	0.15
(1,722)	1:30:B:PHE:HZ	1:32:B:ALA:HA	12	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	5	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	5	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	5	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	16	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	16	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	16	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	19	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	19	0.15
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	19	0.15
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	9	0.15
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	11	0.15
(1,702)	1:42:B:LEU:H	1:43:B:CYS:H	19	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	8	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	8	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	8	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	14	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	14	0.15
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	14	0.15
(1,645)	1:59:B:LYS:HD2	1:59:B:LYS:HA	4	0.15
(1,645)	1:59:B:LYS:HD3	1:59:B:LYS:HA	4	0.15
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	19	0.15
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	19	0.15
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	19	0.15
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	11	0.15
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	12	0.15
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	9	0.15
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	20	0.15
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	20	0.15
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	1	0.15
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	6	0.15
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	17	0.15
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	3	0.15
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	19	0.15
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	9	0.15
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	9	0.15
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	3	0.15
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	12	0.15
(1,530)	1:47:A:LEU:H	1:39:A:SER:HA	14	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	2	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	6	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	10	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	11	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	15	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	16	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	19	0.15
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	20	0.15
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	8	0.15
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	9	0.15
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	15	0.15
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	18	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	3	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	5	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	6	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	9	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	10	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	13	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	14	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	15	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	18	0.15
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	19	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	8	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	8	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	9	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	9	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	13	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	13	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	15	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	15	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	16	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	16	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	20	0.15
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	20	0.15
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	3	0.15
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	3	0.15
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	5	0.15
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	5	0.15
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	14	0.15
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	14	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	2	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	2	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	6	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	6	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	12	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	12	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	16	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	16	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	19	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	19	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	20	0.15
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	20	0.15
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	6	0.15
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	6	0.15
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	6	0.15
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	6	0.15
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	6	0.15
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	6	0.15
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	15	0.15
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	15	0.15
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	18	0.15
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	18	0.15
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	11	0.15
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	12	0.15
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	5	0.15
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	12	0.15
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	7	0.15
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	11	0.15
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	12	0.15
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	19	0.15
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	20	0.15
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	11	0.15
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	12	0.15
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	18	0.15
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	19	0.15
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	19	0.15
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	12	0.15
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	12	0.15
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	12	0.15
(1,294)	1:45:A:GLN:H	1:40:A:CYS:HB2	7	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	6	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	6	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	6	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	8	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	8	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	10	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	10	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	10	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	13	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	13	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	13	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	16	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	16	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	16	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	18	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	18	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	18	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	19	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	19	0.15
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	19	0.15
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	10	0.15
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	10	0.15
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	14	0.15
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	19	0.15
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	2	0.15
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	2	0.15
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	2	0.15
(1,227)	1:62:A:THR:H	1:61:A:PHE:HA	2	0.15
(1,221)	1:42:A:LEU:H	1:43:A:CYS:H	18	0.15
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	14	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	10	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	10	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	10	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	13	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	13	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	13	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	19	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	19	0.15
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	19	0.15
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	10	0.15
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	10	0.15
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	10	0.15
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	18	0.15
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	18	0.15
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	18	0.15
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	15	0.15
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	7	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	9	0.15
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	12	0.15
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	18	0.15
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	20	0.15
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	18	0.15
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	18	0.15
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	19	0.15
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	19	0.15
(1,110)	1:56:A:PHE:HE1	1:25:A:CYS:HA	6	0.15
(1,110)	1:56:A:PHE:HE2	1:25:A:CYS:HA	6	0.15
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	3	0.15
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	11	0.15
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	4	0.15
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	4	0.15
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	15	0.15
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	15	0.15
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	2	0.15
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	2	0.15
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	3	0.15
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	3	0.15
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	16	0.15
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	16	0.15
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	5	0.15
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	9	0.15
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	15	0.15
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	6	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	7	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	7	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	7	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	7	0.15
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	7	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	7	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	11	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	11	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	11	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	11	0.15
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	11	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	11	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	12	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	12	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	12	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	12	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	12	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	12	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	13	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	13	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	13	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	13	0.15
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	13	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	13	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	15	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	15	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	15	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	15	0.15
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	15	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	15	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	19	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	19	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	19	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	19	0.15
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	19	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	19	0.15
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	20	0.15
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	20	0.15
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	20	0.15
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	20	0.15
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	20	0.15
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	20	0.15
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	2	0.15
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	2	0.15
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	2	0.15
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	2	0.15
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	2	0.15
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	2	0.15
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	10	0.15
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	10	0.15
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	10	0.15
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	10	0.15
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	10	0.15
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	10	0.15
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	14	0.15
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	14	0.15
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	14	0.15
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	14	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	14	0.15
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	14	0.15
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	15	0.15
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	15	0.15
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	15	0.15
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	15	0.15
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	15	0.15
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	15	0.15
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	8	0.15
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	8	0.15
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	8	0.15
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	4	0.15
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	4	0.15
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	4	0.15
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	4	0.15
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	7	0.15
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	7	0.15
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	7	0.15
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	7	0.15
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	8	0.15
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	8	0.15
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	9	0.15
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	9	0.15
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	1	0.15
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	1	0.15
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	2	0.15
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	2	0.15
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	5	0.15
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	5	0.15
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	1	0.15
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	1	0.15
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	1	0.15
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	17	0.15
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	17	0.15
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	17	0.15
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	19	0.15
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	19	0.15
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	19	0.15
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	15	0.14
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	16	0.14
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	10	0.14
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	11	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	18	0.14
(1,984)	1:35:B:SER:H	1:36:B:TYR:H	20	0.14
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	2	0.14
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	3	0.14
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	4	0.14
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	17	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	1	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	2	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	4	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	6	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	8	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	10	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	11	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	12	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	13	0.14
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	18	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	2	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	2	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	3	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	3	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	4	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	4	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	7	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	7	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	8	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	8	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	11	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	11	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	12	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	12	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	13	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	13	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	18	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	18	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	19	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	19	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	20	0.14
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	20	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	1	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	1	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	2	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	3	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	3	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	6	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	6	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	8	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	8	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	9	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	9	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	10	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	10	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	11	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	11	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	12	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	12	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	14	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	14	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	15	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	15	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	18	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	18	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG2	19	0.14
(1,944)	1:59:B:LYS:HB3	1:59:B:LYS:HG3	19	0.14
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	3	0.14
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	3	0.14
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	15	0.14
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	15	0.14
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG2	16	0.14
(1,933)	1:54:B:GLU:HB3	1:54:B:GLU:HG3	16	0.14
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	8	0.14
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	8	0.14
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	9	0.14
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	9	0.14
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	12	0.14
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	12	0.14
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	14	0.14
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	14	0.14
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	17	0.14
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	17	0.14
(1,824)	1:21:B:HIS:HD2	1:21:B:HIS:HB3	3	0.14
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	4	0.14
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	16	0.14
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	18	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	15	0.14
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	16	0.14
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	17	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	3	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	3	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	4	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	4	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	13	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	13	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	18	0.14
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	18	0.14
(1,775)	1:45:B:GLN:H	1:40:B:CYS:HB2	3	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	10	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	10	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	10	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	11	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	11	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	11	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	16	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	16	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	16	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	17	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	17	0.14
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	17	0.14
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	1	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	1	0.14
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	6	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	6	0.14
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	7	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	7	0.14
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	10	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	10	0.14
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	12	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	12	0.14
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	19	0.14
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	19	0.14
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	5	0.14
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	5	0.14
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	13	0.14
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	13	0.14
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	6	0.14
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	6	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	17	0.14
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	17	0.14
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	10	0.14
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	10	0.14
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	4	0.14
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	4	0.14
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	4	0.14
(1,708)	1:62:B:THR:H	1:61:B:PHE:HA	16	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	1	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	1	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	1	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	12	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	12	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	12	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	13	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	13	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	13	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	19	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	19	0.14
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	19	0.14
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	1	0.14
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	1	0.14
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	1	0.14
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	1	0.14
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	18	0.14
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	20	0.14
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	6	0.14
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	6	0.14
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	6	0.14
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	12	0.14
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	14	0.14
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	7	0.14
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	17	0.14
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	16	0.14
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	12	0.14
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	2	0.14
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	2	0.14
(1,566)	1:20:B:TYR:HE1	1:61:B:PHE:HA	9	0.14
(1,566)	1:20:B:TYR:HE2	1:61:B:PHE:HA	9	0.14
(1,543)	1:58:A:LEU:H	1:57:A:ARG:HB2	18	0.14
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	1	0.14
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	3	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	7	0.14
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	8	0.14
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	14	0.14
(1,503)	1:35:A:SER:H	1:36:A:TYR:H	17	0.14
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	1	0.14
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	2	0.14
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	5	0.14
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	16	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	1	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	2	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	7	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	8	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	11	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	17	0.14
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	20	0.14
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	13	0.14
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	13	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	2	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	2	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	5	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	5	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	6	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	6	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	7	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	7	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	10	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	10	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	11	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	11	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	17	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	17	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	18	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	18	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	19	0.14
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	19	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	2	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	2	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	4	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	4	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	6	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	6	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	7	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	7	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	10	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	10	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	11	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	11	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	12	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	12	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	15	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	15	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	17	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	17	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	18	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	18	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG2	19	0.14
(1,463)	1:59:A:LYS:HB3	1:59:A:LYS:HG3	19	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	4	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	4	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	9	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	9	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	14	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	14	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	15	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	15	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	18	0.14
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	18	0.14
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	18	0.14
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	10	0.14
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	10	0.14
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	10	0.14
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	10	0.14
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	10	0.14
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	10	0.14
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	6	0.14
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	6	0.14
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	8	0.14
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	8	0.14
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	13	0.14
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	13	0.14
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	16	0.14
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	16	0.14
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	11	0.14
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	11	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	11	0.14
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	1	0.14
(1,369)	1:27:A:GLU:H	1:26:A:GLY:HA3	9	0.14
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	2	0.14
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	9	0.14
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	16	0.14
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	1	0.14
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	2	0.14
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	4	0.14
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	9	0.14
(1,334)	1:48:A:PRO:HD2	1:47:A:LEU:HA	17	0.14
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	16	0.14
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	14	0.14
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	14	0.14
(1,321)	1:50:A:ASP:H	1:49:A:LEU:HG	15	0.14
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	1	0.14
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	1	0.14
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	17	0.14
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	17	0.14
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	1	0.14
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	1	0.14
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	1	0.14
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	9	0.14
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	9	0.14
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	9	0.14
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	4	0.14
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	4	0.14
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	4	0.14
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	7	0.14
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	7	0.14
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	7	0.14
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	3	0.14
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	3	0.14
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	3	0.14
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	5	0.14
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	5	0.14
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	5	0.14
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	5	0.14
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	5	0.14
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	20	0.14
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	20	0.14
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	18	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	2	0.14
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	2	0.14
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	11	0.14
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	11	0.14
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	11	0.14
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD11	18	0.14
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD12	18	0.14
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD13	18	0.14
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	6	0.14
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	6	0.14
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	6	0.14
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	8	0.14
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	8	0.14
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	8	0.14
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	16	0.14
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	10	0.14
(1,118)	1:61:A:PHE:HB3	1:57:A:ARG:HA	10	0.14
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	8	0.14
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	13	0.14
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	16	0.14
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	12	0.14
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	15	0.14
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	15	0.14
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	19	0.14
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	19	0.14
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	1	0.14
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	1	0.14
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	6	0.14
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	6	0.14
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	19	0.14
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	19	0.14
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	5	0.14
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	12	0.14
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	19	0.14
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	7	0.14
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	3	0.14
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	18	0.14
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	15	0.14
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	20	0.14
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	10	0.14
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	7	0.14
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	12	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	14	0.14
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	5	0.14
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	5	0.14
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	5	0.14
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	5	0.14
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	5	0.14
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	5	0.14
(1,44)	1:29:A:LEU:HD11	1:25:B:CYS:H	18	0.14
(1,44)	1:29:A:LEU:HD12	1:25:B:CYS:H	18	0.14
(1,44)	1:29:A:LEU:HD13	1:25:B:CYS:H	18	0.14
(1,44)	1:29:A:LEU:HD21	1:25:B:CYS:H	18	0.14
(1,44)	1:29:A:LEU:HD22	1:25:B:CYS:H	18	0.14
(1,44)	1:29:A:LEU:HD23	1:25:B:CYS:H	18	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	7	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	7	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	7	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	7	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	7	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	7	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	9	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	9	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	9	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	9	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	9	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	9	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	11	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	11	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	11	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	11	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	11	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	11	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	13	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	13	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	13	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	13	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	13	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	13	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	16	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	16	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	16	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	16	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	16	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	16	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	17	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	17	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	17	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	17	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	17	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	17	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	19	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	19	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	19	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	19	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	19	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	19	0.14
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	20	0.14
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	20	0.14
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	20	0.14
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	20	0.14
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	20	0.14
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	20	0.14
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	2	0.14
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	2	0.14
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	2	0.14
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	2	0.14
(1,22)	1:30:B:PHE:HD1	1:23:A:LEU:HG	17	0.14
(1,22)	1:30:B:PHE:HD2	1:23:A:LEU:HG	17	0.14
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	6	0.14
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	6	0.14
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	5	0.14
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	5	0.14
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	5	0.14
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	5	0.14
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	10	0.14
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	10	0.14
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	10	0.14
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	9	0.13
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	6	0.13
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	19	0.13
(1,1024)	1:58:B:LEU:H	1:57:B:ARG:HB2	11	0.13
(1,1024)	1:58:B:LEU:H	1:57:B:ARG:HB2	15	0.13
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	10	0.13
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	15	0.13
(1,972)	1:30:B:PHE:H	1:29:B:LEU:HB2	16	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	5	0.13
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	5	0.13
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	7	0.13
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	7	0.13
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	14	0.13
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	14	0.13
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	7	0.13
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	5	0.13
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	5	0.13
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	9	0.13
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	9	0.13
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG2	15	0.13
(1,946)	1:59:B:LYS:HE3	1:59:B:LYS:HG3	15	0.13
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	3	0.13
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	1	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	1	0.13
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	6	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	6	0.13
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	7	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	7	0.13
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	10	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	10	0.13
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	11	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	11	0.13
(1,913)	1:45:B:GLN:HB2	1:46:B:ARG:H	19	0.13
(1,913)	1:45:B:GLN:HB3	1:46:B:ARG:H	19	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	5	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	5	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	5	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	7	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	7	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	7	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	12	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	12	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	12	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	17	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	17	0.13
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	17	0.13
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	2	0.13
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	2	0.13
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	2	0.13
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	2	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	2	0.13
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	2	0.13
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD21	8	0.13
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD22	8	0.13
(1,820)	1:27:B:GLU:HG2	1:41:B:LEU:HD23	8	0.13
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD21	8	0.13
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD22	8	0.13
(1,820)	1:27:B:GLU:HG3	1:41:B:LEU:HD23	8	0.13
(1,815)	1:48:B:PRO:HD2	1:47:B:LEU:HA	15	0.13
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	8	0.13
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	8	0.13
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	16	0.13
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	16	0.13
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	13	0.13
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	13	0.13
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	13	0.13
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	8	0.13
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	8	0.13
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	17	0.13
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	17	0.13
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	3	0.13
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	3	0.13
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	6	0.13
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	6	0.13
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	7	0.13
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	7	0.13
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	7	0.13
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	12	0.13
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	12	0.13
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	12	0.13
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	1	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	3	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	3	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	3	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	5	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	5	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	5	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	9	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	9	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	9	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	15	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	15	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	15	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	17	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	17	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	17	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	18	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	18	0.13
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	18	0.13
(1,645)	1:59:B:LYS:HD2	1:59:B:LYS:HA	16	0.13
(1,645)	1:59:B:LYS:HD3	1:59:B:LYS:HA	16	0.13
(1,643)	1:42:B:LEU:HD21	1:25:B:CYS:HA	9	0.13
(1,643)	1:42:B:LEU:HD22	1:25:B:CYS:HA	9	0.13
(1,643)	1:42:B:LEU:HD23	1:25:B:CYS:HA	9	0.13
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	6	0.13
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	10	0.13
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	7	0.13
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	11	0.13
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	15	0.13
(1,605)	1:46:B:ARG:HG2	1:39:B:SER:HA	8	0.13
(1,605)	1:46:B:ARG:HG3	1:39:B:SER:HA	8	0.13
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	3	0.13
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	7	0.13
(1,591)	1:56:B:PHE:HE1	1:25:B:CYS:HA	16	0.13
(1,591)	1:56:B:PHE:HE2	1:25:B:CYS:HA	16	0.13
(1,589)	1:56:B:PHE:HE1	1:60:B:HIS:HD2	2	0.13
(1,589)	1:56:B:PHE:HE2	1:60:B:HIS:HD2	2	0.13
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	3	0.13
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	5	0.13
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	7	0.13
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	7	0.13
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	13	0.13
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	13	0.13
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	15	0.13
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	15	0.13
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	1	0.13
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	16	0.13
(1,544)	1:58:A:LEU:H	1:58:A:LEU:HA	11	0.13
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	7	0.13
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	10	0.13
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	14	0.13
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	19	0.13
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	4	0.13
(1,491)	1:30:A:PHE:H	1:29:A:LEU:HB2	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	9	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	9	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	11	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	11	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	16	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	16	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	20	0.13
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	20	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	3	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	3	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	4	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	4	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	12	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	12	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG2	14	0.13
(1,465)	1:59:A:LYS:HE3	1:59:A:LYS:HG3	14	0.13
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG2	5	0.13
(1,452)	1:54:A:GLU:HB3	1:54:A:GLU:HG3	5	0.13
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	17	0.13
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	9	0.13
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	9	0.13
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	9	0.13
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	9	0.13
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	9	0.13
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	9	0.13
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	12	0.13
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	12	0.13
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	12	0.13
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	12	0.13
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	12	0.13
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	12	0.13
(1,432)	1:45:A:GLN:HB2	1:46:A:ARG:H	10	0.13
(1,432)	1:45:A:GLN:HB3	1:46:A:ARG:H	10	0.13
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	8	0.13
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	8	0.13
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	8	0.13
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	1	0.13
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	4	0.13
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	6	0.13
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	8	0.13
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	9	0.13
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	12	0.13
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB2	19	0.13
(1,322)	1:28:A:VAL:H	1:27:A:GLU:HB3	19	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	2	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	2	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	5	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	5	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	11	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	11	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	12	0.13
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	12	0.13
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	19	0.13
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	19	0.13
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	19	0.13
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	20	0.13
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	20	0.13
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	20	0.13
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	17	0.13
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	17	0.13
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	17	0.13
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	19	0.13
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	19	0.13
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	19	0.13
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	14	0.13
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	14	0.13
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	15	0.13
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	15	0.13
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	17	0.13
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	17	0.13
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	2	0.13
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	2	0.13
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	5	0.13
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	20	0.13
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	16	0.13
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	16	0.13
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	1	0.13
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	1	0.13
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	8	0.13
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	8	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	10	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	10	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	10	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	13	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	13	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	13	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	16	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	16	0.13
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	16	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	4	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	4	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	4	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	6	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	6	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	6	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	11	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	11	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	11	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	12	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	12	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	12	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	14	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	14	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	14	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	15	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	15	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	15	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	20	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	20	0.13
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	20	0.13
(1,162)	1:42:A:LEU:HD21	1:25:A:CYS:HA	13	0.13
(1,162)	1:42:A:LEU:HD22	1:25:A:CYS:HA	13	0.13
(1,162)	1:42:A:LEU:HD23	1:25:A:CYS:HA	13	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	1	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	3	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	5	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	6	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	7	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	8	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	9	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	11	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	12	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	13	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	17	0.13
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	19	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	8	0.13
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	13	0.13
(1,127)	1:59:A:LYS:H	1:58:A:LEU:HB3	16	0.13
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	6	0.13
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	6	0.13
(1,110)	1:56:A:PHE:HE1	1:25:A:CYS:HA	16	0.13
(1,110)	1:56:A:PHE:HE2	1:25:A:CYS:HA	16	0.13
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	5	0.13
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	10	0.13
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	10	0.13
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	14	0.13
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	14	0.13
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	16	0.13
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	16	0.13
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	14	0.13
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	14	0.13
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	9	0.13
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	9	0.13
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	3	0.13
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	3	0.13
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	18	0.13
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	18	0.13
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	10	0.13
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	14	0.13
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	20	0.13
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	7	0.13
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	10	0.13
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	3	0.13
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	13	0.13
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	1	0.13
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	7	0.13
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	12	0.13
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	20	0.13
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	10	0.13
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	14	0.13
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	11	0.13
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	2	0.13
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	19	0.13
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	10	0.13
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	10	0.13
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	10	0.13
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	15	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	15	0.13
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	15	0.13
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	20	0.13
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	20	0.13
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	20	0.13
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	1	0.13
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	1	0.13
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	1	0.13
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	1	0.13
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	1	0.13
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	1	0.13
(1,43)	1:29:B:LEU:HD11	1:25:A:CYS:H	8	0.13
(1,43)	1:29:B:LEU:HD12	1:25:A:CYS:H	8	0.13
(1,43)	1:29:B:LEU:HD13	1:25:A:CYS:H	8	0.13
(1,43)	1:29:B:LEU:HD21	1:25:A:CYS:H	8	0.13
(1,43)	1:29:B:LEU:HD22	1:25:A:CYS:H	8	0.13
(1,43)	1:29:B:LEU:HD23	1:25:A:CYS:H	8	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	6	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	6	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	6	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	15	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	15	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	15	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	17	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	17	0.13
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	17	0.13
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	17	0.13
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	17	0.13
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	17	0.13
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	8	0.13
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	8	0.13
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	8	0.13
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	8	0.13
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	14	0.13
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	14	0.13
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	14	0.13
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	14	0.13
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	4	0.13
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	5	0.13
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	5	0.13
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	5	0.13
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	6	0.13
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	6	0.13
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	6	0.13
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	14	0.13
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	14	0.13
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	14	0.13
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	2	0.13
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	2	0.13
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	2	0.13
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	8	0.13
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	8	0.13
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	8	0.13
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	14	0.13
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	14	0.13
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	14	0.13
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	14	0.12
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	7	0.12
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	9	0.12
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	14	0.12
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	17	0.12
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	15	0.12
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	16	0.12
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	8	0.12
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	13	0.12
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	10	0.12
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	12	0.12
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	17	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	4	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	5	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	7	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	9	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	16	0.12
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	17	0.12
(1,1025)	1:58:B:LEU:H	1:58:B:LEU:HA	11	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	12	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	12	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	13	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	13	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	15	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	15	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	17	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	17	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	20	0.12
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	20	0.12
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	2	0.12
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	4	0.12
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	9	0.12
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	17	0.12
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	18	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	8	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	8	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	8	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	9	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	9	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	9	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	19	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	19	0.12
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	19	0.12
(1,848)	1:35:B:SER:H	1:35:B:SER:HB3	2	0.12
(1,848)	1:35:B:SER:H	1:35:B:SER:HB3	9	0.12
(1,848)	1:35:B:SER:H	1:35:B:SER:HB3	14	0.12
(1,848)	1:35:B:SER:H	1:35:B:SER:HB3	17	0.12
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	20	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	6	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	6	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	6	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	6	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	6	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	6	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	7	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	7	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	7	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	7	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	7	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	7	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	12	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	12	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	12	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	12	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	12	0.12
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	12	0.12
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	9	0.12
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	20	0.12
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	8	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	8	0.12
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB2	10	0.12
(1,803)	1:28:B:VAL:H	1:27:B:GLU:HB3	10	0.12
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	10	0.12
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	10	0.12
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	3	0.12
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	3	0.12
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	3	0.12
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	13	0.12
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	13	0.12
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	13	0.12
(1,782)	1:43:B:CYS:H	1:40:B:CYS:HB2	6	0.12
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	18	0.12
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	18	0.12
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	18	0.12
(1,730)	1:42:B:LEU:HD11	1:56:B:PHE:HZ	16	0.12
(1,730)	1:42:B:LEU:HD12	1:56:B:PHE:HZ	16	0.12
(1,730)	1:42:B:LEU:HD13	1:56:B:PHE:HZ	16	0.12
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	11	0.12
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	11	0.12
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	13	0.12
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	13	0.12
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	14	0.12
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	14	0.12
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	18	0.12
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	18	0.12
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	20	0.12
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	20	0.12
(1,725)	1:60:B:HIS:H	1:57:B:ARG:HA	15	0.12
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	9	0.12
(1,724)	1:61:B:PHE:H	1:57:B:ARG:HA	11	0.12
(1,721)	1:30:B:PHE:HE1	1:32:B:ALA:HA	3	0.12
(1,721)	1:30:B:PHE:HE2	1:32:B:ALA:HA	3	0.12
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	1	0.12
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	1	0.12
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	5	0.12
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	5	0.12
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	7	0.12
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	7	0.12
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	11	0.12
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	11	0.12
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	12	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	12	0.12
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	13	0.12
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	13	0.12
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	13	0.12
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	16	0.12
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	16	0.12
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	16	0.12
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	8	0.12
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	13	0.12
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	19	0.12
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	8	0.12
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	10	0.12
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	12	0.12
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	1	0.12
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	8	0.12
(1,575)	1:37:B:GLU:HA	1:48:B:PRO:HA	15	0.12
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	7	0.12
(1,574)	1:49:B:LEU:HA	1:38:B:VAL:HB	14	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	2	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	3	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	4	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	6	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	8	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	9	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	13	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	14	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	15	0.12
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	20	0.12
(1,544)	1:58:A:LEU:H	1:58:A:LEU:HA	12	0.12
(1,544)	1:58:A:LEU:H	1:58:A:LEU:HA	18	0.12
(1,543)	1:58:A:LEU:H	1:57:A:ARG:HB2	11	0.12
(1,543)	1:58:A:LEU:H	1:57:A:ARG:HB2	12	0.12
(1,504)	1:36:A:TYR:H	1:35:A:SER:HB3	18	0.12
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	6	0.12
(1,497)	1:32:A:ALA:H	1:31:A:SER:HB3	12	0.12
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	1	0.12
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	1	0.12
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	2	0.12
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	2	0.12
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	8	0.12
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	8	0.12
(1,476)	1:63:A:ASN:HA	1:63:A:ASN:HB3	17	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	4	0.12
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	4	0.12
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	14	0.12
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	14	0.12
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	3	0.12
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	6	0.12
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	9	0.12
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	17	0.12
(1,453)	1:47:A:LEU:HD11	1:55:A:HIS:HB3	18	0.12
(1,453)	1:47:A:LEU:HD12	1:55:A:HIS:HB3	18	0.12
(1,453)	1:47:A:LEU:HD13	1:55:A:HIS:HB3	18	0.12
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	14	0.12
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	14	0.12
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	14	0.12
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	14	0.12
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	14	0.12
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	14	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	4	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	4	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	4	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	18	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	18	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	18	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	20	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	20	0.12
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	20	0.12
(1,367)	1:35:A:SER:H	1:35:A:SER:HB3	2	0.12
(1,367)	1:35:A:SER:H	1:35:A:SER:HB3	10	0.12
(1,367)	1:35:A:SER:H	1:35:A:SER:HB3	14	0.12
(1,367)	1:35:A:SER:H	1:35:A:SER:HB3	18	0.12
(1,361)	1:24:A:ARG:H	1:23:A:LEU:HB3	11	0.12
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	18	0.12
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	19	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	3	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	3	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	3	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	3	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	3	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	3	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	10	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	10	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	10	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	10	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	10	0.12
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	10	0.12
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	7	0.12
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	14	0.12
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	20	0.12
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	7	0.12
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	7	0.12
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	20	0.12
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	20	0.12
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	3	0.12
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	3	0.12
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	3	0.12
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	14	0.12
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	14	0.12
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	14	0.12
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG11	1	0.12
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG12	1	0.12
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG13	1	0.12
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG11	17	0.12
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG12	17	0.12
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG13	17	0.12
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD11	1	0.12
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD12	1	0.12
(1,261)	1:50:A:ASP:H	1:49:A:LEU:HD13	1	0.12
(1,259)	1:50:A:ASP:H	1:48:A:PRO:HB2	15	0.12
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	20	0.12
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	20	0.12
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	20	0.12
(1,248)	1:56:A:PHE:HE1	1:61:A:PHE:HB3	7	0.12
(1,248)	1:56:A:PHE:HE2	1:61:A:PHE:HB3	7	0.12
(1,245)	1:52:A:TYR:HE1	1:40:A:CYS:HA	18	0.12
(1,245)	1:52:A:TYR:HE2	1:40:A:CYS:HA	18	0.12
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	15	0.12
(1,240)	1:30:A:PHE:HE1	1:32:A:ALA:HA	14	0.12
(1,240)	1:30:A:PHE:HE2	1:32:A:ALA:HA	14	0.12
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	6	0.12
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	6	0.12
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	7	0.12
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	7	0.12
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	11	0.12
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	11	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	3	0.12
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	3	0.12
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	3	0.12
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	4	0.12
(1,182)	1:19:A:GLY:H	1:20:A:TYR:H	20	0.12
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	2	0.12
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	2	0.12
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	2	0.12
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	16	0.12
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	16	0.12
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	16	0.12
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	20	0.12
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	7	0.12
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	7	0.12
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	7	0.12
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	5	0.12
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	5	0.12
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	10	0.12
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	15	0.12
(1,110)	1:56:A:PHE:HE1	1:25:A:CYS:HA	19	0.12
(1,110)	1:56:A:PHE:HE2	1:25:A:CYS:HA	19	0.12
(1,108)	1:56:A:PHE:HE1	1:60:A:HIS:HD2	3	0.12
(1,108)	1:56:A:PHE:HE2	1:60:A:HIS:HD2	3	0.12
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	2	0.12
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	14	0.12
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	8	0.12
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	8	0.12
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	5	0.12
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	5	0.12
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	8	0.12
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	8	0.12
(1,78)	1:36:B:TYR:HE1	1:56:A:PHE:H	10	0.12
(1,78)	1:36:B:TYR:HE2	1:56:A:PHE:H	10	0.12
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	8	0.12
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	8	0.12
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	13	0.12
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	13	0.12
(1,77)	1:36:A:TYR:HE1	1:56:B:PHE:H	20	0.12
(1,77)	1:36:A:TYR:HE2	1:56:B:PHE:H	20	0.12
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	1	0.12
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	13	0.12
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	16	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	17	0.12
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	4	0.12
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	13	0.12
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	11	0.12
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	1	0.12
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	2	0.12
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	12	0.12
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	3	0.12
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	9	0.12
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	18	0.12
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	1	0.12
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	3	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	2	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	5	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	8	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	11	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	12	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	16	0.12
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	17	0.12
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	14	0.12
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	16	0.12
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	20	0.12
(1,53)	1:25:A:CYS:H	1:28:B:VAL:HB	3	0.12
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	16	0.12
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	16	0.12
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	16	0.12
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	18	0.12
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	18	0.12
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	18	0.12
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	13	0.12
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	13	0.12
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	13	0.12
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	8	0.12
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	8	0.12
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	8	0.12
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	8	0.12
(1,24)	1:30:B:PHE:HE1	1:61:A:PHE:HZ	16	0.12
(1,24)	1:30:B:PHE:HE2	1:61:A:PHE:HZ	16	0.12
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	19	0.12
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	1	0.12
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	1	0.12
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	4	0.12
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	4	0.12
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	4	0.12
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	11	0.12
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	11	0.12
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	11	0.12
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	20	0.12
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	20	0.12
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	20	0.12
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	2	0.12
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	2	0.12
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	2	0.12
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	4	0.12
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	4	0.12
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	4	0.12
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	1	0.11
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	6	0.11
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	7	0.11
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	8	0.11
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	10	0.11
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	12	0.11
(2,6)	1:40:B:CYS:SG	2:101:B:ZN:ZN	19	0.11
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	1	0.11
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	6	0.11
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	8	0.11
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	10	0.11
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	12	0.11
(2,5)	1:43:B:CYS:SG	2:101:B:ZN:ZN	19	0.11
(2,3)	1:55:A:HIS:NE2	2:101:A:ZN:ZN	18	0.11
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	10	0.11
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	13	0.11
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	6	0.11
(2,1)	1:43:A:CYS:SG	2:101:A:ZN:ZN	10	0.11
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	14	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	1	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	2	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	3	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	6	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	8	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	10	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	12	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	13	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	14	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	18	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	19	0.11
(1,1029)	1:60:B:HIS:H	1:59:B:LYS:HA	20	0.11
(1,1025)	1:58:B:LEU:H	1:58:B:LEU:HA	15	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	1	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	2	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	3	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	5	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	6	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	7	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	8	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	9	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	10	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	11	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	12	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	13	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	16	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	17	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	18	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	19	0.11
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	20	0.11
(1,998)	1:41:B:LEU:H	1:26:B:GLY:HA3	6	0.11
(1,985)	1:36:B:TYR:H	1:35:B:SER:HB3	9	0.11
(1,985)	1:36:B:TYR:H	1:35:B:SER:HB3	15	0.11
(1,978)	1:32:B:ALA:H	1:31:B:SER:HB3	16	0.11
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG2	18	0.11
(1,969)	1:28:B:VAL:H	1:27:B:GLU:HG3	18	0.11
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	8	0.11
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	17	0.11
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	2	0.11
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	2	0.11
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	5	0.11
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	5	0.11
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	9	0.11
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	9	0.11
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	5	0.11
(1,937)	1:57:B:ARG:HD3	1:57:B:ARG:HG2	7	0.11
(1,934)	1:47:B:LEU:HD11	1:55:B:HIS:HB3	9	0.11
(1,934)	1:47:B:LEU:HD12	1:55:B:HIS:HB3	9	0.11
(1,934)	1:47:B:LEU:HD13	1:55:B:HIS:HB3	9	0.11
(1,934)	1:47:B:LEU:HD11	1:55:B:HIS:HB3	11	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:47:B:LEU:HD12	1:55:B:HIS:HB3	11	0.11
(1,934)	1:47:B:LEU:HD13	1:55:B:HIS:HB3	11	0.11
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	18	0.11
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	18	0.11
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	18	0.11
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG2	1	0.11
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG3	1	0.11
(1,848)	1:35:B:SER:H	1:35:B:SER:HB3	4	0.11
(1,842)	1:24:B:ARG:H	1:23:B:LEU:HB3	4	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	1	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	2	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	3	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	4	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	5	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	6	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	7	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	8	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	9	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	10	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	11	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	12	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	13	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	14	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	15	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	16	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	17	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	18	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	19	0.11
(1,831)	1:22:B:ASN:HA	1:22:B:ASN:HB2	20	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	4	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	4	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	4	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	4	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	4	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	4	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	5	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	5	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	5	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	5	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	5	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	5	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	19	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	19	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	19	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	19	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	19	0.11
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	19	0.11
(1,809)	1:57:B:ARG:HG2	1:57:B:ARG:HA	10	0.11
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	10	0.11
(1,806)	1:41:B:LEU:HB2	1:25:B:CYS:HA	14	0.11
(1,802)	1:50:B:ASP:H	1:49:B:LEU:HG	3	0.11
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG2	20	0.11
(1,800)	1:47:B:LEU:H	1:46:B:ARG:HG3	20	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG11	13	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG12	13	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG13	13	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG11	15	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG12	15	0.11
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG13	15	0.11
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD11	13	0.11
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD12	13	0.11
(1,742)	1:50:B:ASP:H	1:49:B:LEU:HD13	13	0.11
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	3	0.11
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	3	0.11
(1,725)	1:60:B:HIS:H	1:57:B:ARG:HA	16	0.11
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	8	0.11
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	8	0.11
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	18	0.11
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	18	0.11
(1,720)	1:30:B:PHE:HE1	1:34:B:ALA:HA	19	0.11
(1,720)	1:30:B:PHE:HE2	1:34:B:ALA:HA	19	0.11
(1,717)	1:28:B:VAL:HG11	1:36:B:TYR:HD1	6	0.11
(1,717)	1:28:B:VAL:HG11	1:36:B:TYR:HD2	6	0.11
(1,717)	1:28:B:VAL:HG12	1:36:B:TYR:HD1	6	0.11
(1,717)	1:28:B:VAL:HG12	1:36:B:TYR:HD2	6	0.11
(1,717)	1:28:B:VAL:HG13	1:36:B:TYR:HD1	6	0.11
(1,717)	1:28:B:VAL:HG13	1:36:B:TYR:HD2	6	0.11
(1,717)	1:28:B:VAL:HG11	1:36:B:TYR:HD1	8	0.11
(1,717)	1:28:B:VAL:HG11	1:36:B:TYR:HD2	8	0.11
(1,717)	1:28:B:VAL:HG12	1:36:B:TYR:HD1	8	0.11
(1,717)	1:28:B:VAL:HG12	1:36:B:TYR:HD2	8	0.11
(1,717)	1:28:B:VAL:HG13	1:36:B:TYR:HD1	8	0.11
(1,717)	1:28:B:VAL:HG13	1:36:B:TYR:HD2	8	0.11
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	8	0.11
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	8	0.11
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD11	10	0.11
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD12	10	0.11
(1,714)	1:39:B:SER:HB3	1:29:B:LEU:HD13	10	0.11
(1,674)	1:55:B:HIS:HD2	1:55:B:HIS:HB2	11	0.11
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	2	0.11
(1,663)	1:19:B:GLY:H	1:20:B:TYR:H	7	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD11	11	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD12	11	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD13	11	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD11	14	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD12	14	0.11
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD13	14	0.11
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	5	0.11
(1,634)	1:35:B:SER:HB2	1:31:B:SER:HB2	7	0.11
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	6	0.11
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	13	0.11
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	14	0.11
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	10	0.11
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	10	0.11
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	10	0.11
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	12	0.11
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	12	0.11
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	12	0.11
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	13	0.11
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	13	0.11
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	13	0.11
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	16	0.11
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	16	0.11
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	16	0.11
(1,608)	1:59:B:LYS:H	1:58:B:LEU:HB3	17	0.11
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	15	0.11
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	15	0.11
(1,599)	1:61:B:PHE:HB3	1:57:B:ARG:HA	19	0.11
(1,597)	1:38:B:VAL:HG21	1:52:B:TYR:HE1	4	0.11
(1,597)	1:38:B:VAL:HG21	1:52:B:TYR:HE2	4	0.11
(1,597)	1:38:B:VAL:HG22	1:52:B:TYR:HE1	4	0.11
(1,597)	1:38:B:VAL:HG22	1:52:B:TYR:HE2	4	0.11
(1,597)	1:38:B:VAL:HG23	1:52:B:TYR:HE1	4	0.11
(1,597)	1:38:B:VAL:HG23	1:52:B:TYR:HE2	4	0.11
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	10	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	19	0.11
(1,589)	1:56:B:PHE:HE1	1:60:B:HIS:HD2	5	0.11
(1,589)	1:56:B:PHE:HE2	1:60:B:HIS:HD2	5	0.11
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD1	4	0.11
(1,571)	1:34:B:ALA:HA	1:36:B:TYR:HD2	4	0.11
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	5	0.11
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	7	0.11
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	10	0.11
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	17	0.11
(1,548)	1:60:A:HIS:H	1:59:A:LYS:HA	19	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	1	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	2	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	5	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	6	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	7	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	8	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	9	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	10	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	11	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	13	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	14	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	15	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	16	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	17	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	18	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	19	0.11
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	20	0.11
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG2	17	0.11
(1,488)	1:28:A:VAL:H	1:27:A:GLU:HG3	17	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	3	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	3	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	5	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	5	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	6	0.11
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	6	0.11
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	11	0.11
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	15	0.11
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	16	0.11
(1,456)	1:57:A:ARG:HD3	1:57:A:ARG:HG2	18	0.11
(1,453)	1:47:A:LEU:HD11	1:55:A:HIS:HB3	15	0.11
(1,453)	1:47:A:LEU:HD12	1:55:A:HIS:HB3	15	0.11
(1,453)	1:47:A:LEU:HD13	1:55:A:HIS:HB3	15	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	2	0.11
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	2	0.11
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	2	0.11
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	2	0.11
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	2	0.11
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	2	0.11
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD1	19	0.11
(1,446)	1:49:A:LEU:HD21	1:36:A:TYR:HD2	19	0.11
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD1	19	0.11
(1,446)	1:49:A:LEU:HD22	1:36:A:TYR:HD2	19	0.11
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD1	19	0.11
(1,446)	1:49:A:LEU:HD23	1:36:A:TYR:HD2	19	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	2	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	2	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	2	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	10	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	10	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	10	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	12	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	12	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	12	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	13	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	13	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	13	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	14	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	14	0.11
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	14	0.11
(1,382)	1:45:A:GLN:HA	1:45:A:GLN:HG3	15	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	1	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	2	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	3	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	4	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	5	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	6	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	7	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	8	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	9	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	10	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	11	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	12	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	13	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	14	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	15	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	16	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	17	0.11
(1,350)	1:22:A:ASN:HA	1:22:A:ASN:HB2	20	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	1	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	1	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	1	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	1	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	1	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	1	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	9	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	9	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	9	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	9	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	9	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	9	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	11	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	11	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	11	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	11	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	11	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	11	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	14	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	14	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	14	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	14	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	14	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	14	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	16	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	16	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	16	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	16	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	16	0.11
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	16	0.11
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	4	0.11
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	13	0.11
(1,328)	1:57:A:ARG:HG2	1:57:A:ARG:HA	19	0.11
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	7	0.11
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	16	0.11
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	3	0.11
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	3	0.11
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG11	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG12	9	0.11
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG13	9	0.11
(1,301)	1:43:A:CYS:H	1:40:A:CYS:HB2	13	0.11
(1,249)	1:42:A:LEU:HD11	1:56:A:PHE:HZ	4	0.11
(1,249)	1:42:A:LEU:HD12	1:56:A:PHE:HZ	4	0.11
(1,249)	1:42:A:LEU:HD13	1:56:A:PHE:HZ	4	0.11
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE1	7	0.11
(1,246)	1:40:A:CYS:HB3	1:52:A:TYR:HE2	7	0.11
(1,244)	1:60:A:HIS:H	1:57:A:ARG:HA	1	0.11
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	17	0.11
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	10	0.11
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	10	0.11
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	17	0.11
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	17	0.11
(1,236)	1:28:A:VAL:HG11	1:36:A:TYR:HD1	6	0.11
(1,236)	1:28:A:VAL:HG11	1:36:A:TYR:HD2	6	0.11
(1,236)	1:28:A:VAL:HG12	1:36:A:TYR:HD1	6	0.11
(1,236)	1:28:A:VAL:HG12	1:36:A:TYR:HD2	6	0.11
(1,236)	1:28:A:VAL:HG13	1:36:A:TYR:HD1	6	0.11
(1,236)	1:28:A:VAL:HG13	1:36:A:TYR:HD2	6	0.11
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD11	8	0.11
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD12	8	0.11
(1,233)	1:39:A:SER:HB3	1:29:A:LEU:HD13	8	0.11
(1,193)	1:55:A:HIS:HD2	1:55:A:HIS:HB2	18	0.11
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	5	0.11
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	5	0.11
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	5	0.11
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD11	18	0.11
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD12	18	0.11
(1,179)	1:27:A:GLU:H	1:41:A:LEU:HD13	18	0.11
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	8	0.11
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	8	0.11
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	8	0.11
(1,153)	1:35:A:SER:HB2	1:31:A:SER:HB2	4	0.11
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	4	0.11
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	10	0.11
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	20	0.11
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	2	0.11
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	2	0.11
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	2	0.11
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	3	0.11
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	3	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	3	0.11
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	16	0.11
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	16	0.11
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	16	0.11
(1,144)	1:42:A:LEU:HD11	1:25:A:CYS:HA	20	0.11
(1,144)	1:42:A:LEU:HD12	1:25:A:CYS:HA	20	0.11
(1,144)	1:42:A:LEU:HD13	1:25:A:CYS:HA	20	0.11
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	11	0.11
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	11	0.11
(1,108)	1:56:A:PHE:HE1	1:60:A:HIS:HD2	14	0.11
(1,108)	1:56:A:PHE:HE2	1:60:A:HIS:HD2	14	0.11
(1,108)	1:56:A:PHE:HE1	1:60:A:HIS:HD2	15	0.11
(1,108)	1:56:A:PHE:HE2	1:60:A:HIS:HD2	15	0.11
(1,108)	1:56:A:PHE:HE1	1:60:A:HIS:HD2	16	0.11
(1,108)	1:56:A:PHE:HE2	1:60:A:HIS:HD2	16	0.11
(1,108)	1:56:A:PHE:HE1	1:60:A:HIS:HD2	17	0.11
(1,108)	1:56:A:PHE:HE2	1:60:A:HIS:HD2	17	0.11
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	7	0.11
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	17	0.11
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	19	0.11
(1,94)	1:37:A:GLU:HA	1:48:A:PRO:HA	20	0.11
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	2	0.11
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	2	0.11
(1,85)	1:20:A:TYR:HE1	1:61:A:PHE:HA	13	0.11
(1,85)	1:20:A:TYR:HE2	1:61:A:PHE:HA	13	0.11
(1,82)	1:52:A:TYR:HE1	1:56:A:PHE:H	12	0.11
(1,82)	1:52:A:TYR:HE2	1:56:A:PHE:H	12	0.11
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	2	0.11
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	2	0.11
(1,75)	1:22:A:ASN:H	1:32:B:ALA:H	18	0.11
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	2	0.11
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	7	0.11
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	11	0.11
(1,71)	1:32:A:ALA:H	1:20:B:TYR:HB3	17	0.11
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	11	0.11
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	12	0.11
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	13	0.11
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	1	0.11
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	3	0.11
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	13	0.11
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	18	0.11
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	19	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	20	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	1	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	2	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	3	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	5	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	9	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	12	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	13	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	15	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	17	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	18	0.11
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	19	0.11
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	3	0.11
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	6	0.11
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	7	0.11
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	10	0.11
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	17	0.11
(1,53)	1:25:A:CYS:H	1:28:B:VAL:HB	20	0.11
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	1	0.11
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	1	0.11
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	1	0.11
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	11	0.11
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	11	0.11
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	11	0.11
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	14	0.11
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	14	0.11
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	14	0.11
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	1	0.11
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	1	0.11
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	1	0.11
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	6	0.11
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	6	0.11
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	6	0.11
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	17	0.11
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	17	0.11
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	17	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	1	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	1	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	1	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	8	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	8	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	10	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	10	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	10	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	19	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	19	0.11
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	19	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	9	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	9	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	9	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	18	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	18	0.11
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	18	0.11
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	10	0.11
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	10	0.11
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	10	0.11
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	10	0.11
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD1	13	0.11
(1,34)	1:36:B:TYR:HE1	1:56:A:PHE:HD2	13	0.11
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD1	13	0.11
(1,34)	1:36:B:TYR:HE2	1:56:A:PHE:HD2	13	0.11
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD1	10	0.11
(1,33)	1:36:A:TYR:HE1	1:56:B:PHE:HD2	10	0.11
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD1	10	0.11
(1,33)	1:36:A:TYR:HE2	1:56:B:PHE:HD2	10	0.11
(1,23)	1:30:A:PHE:HE1	1:61:B:PHE:HZ	3	0.11
(1,23)	1:30:A:PHE:HE2	1:61:B:PHE:HZ	3	0.11
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	8	0.11
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	9	0.11
(1,20)	1:21:B:HIS:HA	1:31:A:SER:HA	16	0.11
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	2	0.11
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	2	0.11
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	2	0.11
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	9	0.11
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	9	0.11
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	9	0.11
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	16	0.11
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	16	0.11
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	16	0.11
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	4	0.11
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	4	0.11
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	4	0.11
(1,11)	1:29:A:LEU:HD21	1:24:B:ARG:HA	18	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:29:A:LEU:HD22	1:24:B:ARG:HA	18	0.11
(1,11)	1:29:A:LEU:HD23	1:24:B:ARG:HA	18	0.11
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	9	0.11
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	9	0.11
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	9	0.11
(1,3)	1:49:A:LEU:HD11	1:50:B:ASP:HA	12	0.11
(1,3)	1:49:A:LEU:HD12	1:50:B:ASP:HA	12	0.11
(1,3)	1:49:A:LEU:HD13	1:50:B:ASP:HA	12	0.11
(2,2)	1:40:A:CYS:SG	2:101:A:ZN:ZN	8	0.1
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	2	0.1
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	6	0.1
(1,1039)	1:62:B:THR:H	1:62:B:THR:HB	7	0.1
(1,1032)	1:60:B:HIS:H	1:60:B:HIS:HB2	4	0.1
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	4	0.1
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	14	0.1
(1,1019)	1:52:B:TYR:H	1:51:B:GLY:HA2	15	0.1
(1,985)	1:36:B:TYR:H	1:35:B:SER:HB3	17	0.1
(1,959)	1:21:B:HIS:H	1:20:B:TYR:HA	7	0.1
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	6	0.1
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	10	0.1
(1,957)	1:63:B:ASN:HA	1:63:B:ASN:HB3	14	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	3	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	3	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	15	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	15	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	18	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	18	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG2	20	0.1
(1,945)	1:59:B:LYS:HE2	1:59:B:LYS:HG3	20	0.1
(1,934)	1:47:B:LEU:HD11	1:55:B:HIS:HB3	19	0.1
(1,934)	1:47:B:LEU:HD12	1:55:B:HIS:HB3	19	0.1
(1,934)	1:47:B:LEU:HD13	1:55:B:HIS:HB3	19	0.1
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	2	0.1
(1,932)	1:52:B:TYR:HA	1:55:B:HIS:HB2	20	0.1
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	4	0.1
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	4	0.1
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	4	0.1
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD11	20	0.1
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD12	20	0.1
(1,909)	1:25:B:CYS:HB2	1:42:B:LEU:HD13	20	0.1
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG2	7	0.1
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG3	7	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG2	14	0.1
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG3	14	0.1
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG2	19	0.1
(1,899)	1:37:B:GLU:HB3	1:37:B:GLU:HG3	19	0.1
(1,852)	1:37:B:GLU:HG2	1:37:B:GLU:HB2	18	0.1
(1,852)	1:37:B:GLU:HG3	1:37:B:GLU:HB2	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	3	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	3	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	3	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	3	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	3	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	3	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	9	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	9	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	9	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	9	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	9	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	9	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	10	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	10	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	10	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	10	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	10	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	10	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	11	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	11	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	11	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	11	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	11	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	11	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	13	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	13	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	13	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	13	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	13	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	13	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	14	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	14	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	14	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	14	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	14	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	14	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	15	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	15	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	15	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	15	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	15	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	15	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	16	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	16	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	16	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	16	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	16	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	16	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	18	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD11	20	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD12	20	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD13	20	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD21	20	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD22	20	0.1
(1,829)	1:23:B:LEU:HA	1:23:B:LEU:HD23	20	0.1
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD21	2	0.1
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD22	2	0.1
(1,793)	1:26:B:GLY:H	1:41:B:LEU:HD23	2	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG11	5	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG12	5	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG13	5	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG11	18	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG12	18	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG13	18	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG11	20	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG12	20	0.1
(1,786)	1:38:B:VAL:H	1:38:B:VAL:HG13	20	0.1
(1,782)	1:43:B:CYS:H	1:40:B:CYS:HB2	7	0.1
(1,729)	1:56:B:PHE:HE1	1:61:B:PHE:HB3	2	0.1
(1,729)	1:56:B:PHE:HE2	1:61:B:PHE:HB3	2	0.1
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE1	20	0.1
(1,727)	1:40:B:CYS:HB3	1:52:B:TYR:HE2	20	0.1
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD11	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD12	2	0.1
(1,660)	1:27:B:GLU:H	1:41:B:LEU:HD13	2	0.1
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD11	7	0.1
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD12	7	0.1
(1,651)	1:55:B:HIS:H	1:47:B:LEU:HD13	7	0.1
(1,627)	1:39:B:SER:HA	1:46:B:ARG:HA	12	0.1
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	8	0.1
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	8	0.1
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	8	0.1
(1,625)	1:42:B:LEU:HD11	1:25:B:CYS:HA	17	0.1
(1,625)	1:42:B:LEU:HD12	1:25:B:CYS:HA	17	0.1
(1,625)	1:42:B:LEU:HD13	1:25:B:CYS:HA	17	0.1
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD1	11	0.1
(1,602)	1:61:B:PHE:HB3	1:56:B:PHE:HD2	11	0.1
(1,594)	1:55:B:HIS:H	1:52:B:TYR:HA	11	0.1
(1,593)	1:55:B:HIS:HD2	1:56:B:PHE:HA	14	0.1
(1,592)	1:56:B:PHE:H	1:53:B:PRO:HA	8	0.1
(1,591)	1:56:B:PHE:HE1	1:25:B:CYS:HA	20	0.1
(1,591)	1:56:B:PHE:HE2	1:25:B:CYS:HA	20	0.1
(1,589)	1:56:B:PHE:HE1	1:60:B:HIS:HD2	3	0.1
(1,589)	1:56:B:PHE:HE2	1:60:B:HIS:HD2	3	0.1
(1,558)	1:62:A:THR:H	1:62:A:THR:HB	17	0.1
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	3	0.1
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	4	0.1
(1,538)	1:52:A:TYR:H	1:51:A:GLY:HA2	12	0.1
(1,504)	1:36:A:TYR:H	1:35:A:SER:HB3	2	0.1
(1,494)	1:31:A:SER:H	1:31:A:SER:HA	14	0.1
(1,476)	1:63:A:ASN:HA	1:63:A:ASN:HB3	5	0.1
(1,476)	1:63:A:ASN:HA	1:63:A:ASN:HB3	8	0.1
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	7	0.1
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	7	0.1
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	12	0.1
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	12	0.1
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG2	17	0.1
(1,464)	1:59:A:LYS:HE2	1:59:A:LYS:HG3	17	0.1
(1,453)	1:47:A:LEU:HD11	1:55:A:HIS:HB3	13	0.1
(1,453)	1:47:A:LEU:HD12	1:55:A:HIS:HB3	13	0.1
(1,453)	1:47:A:LEU:HD13	1:55:A:HIS:HB3	13	0.1
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	1	0.1
(1,451)	1:52:A:TYR:HA	1:55:A:HIS:HB2	3	0.1
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	5	0.1
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	5	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	5	0.1
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD11	6	0.1
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD12	6	0.1
(1,428)	1:25:A:CYS:HB2	1:42:A:LEU:HD13	6	0.1
(1,408)	1:33:A:PRO:HG2	1:34:A:ALA:HB1	4	0.1
(1,408)	1:33:A:PRO:HG2	1:34:A:ALA:HB2	4	0.1
(1,408)	1:33:A:PRO:HG2	1:34:A:ALA:HB3	4	0.1
(1,382)	1:45:A:GLN:HA	1:45:A:GLN:HG3	18	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	2	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	2	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	2	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	2	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	2	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	2	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	5	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	5	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	5	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	5	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	5	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	5	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	6	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	6	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	6	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	6	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	6	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	6	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	7	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	7	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	7	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	7	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	7	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	7	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	8	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	8	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	8	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	8	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	8	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	8	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	12	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	12	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	12	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	12	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	12	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	12	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	17	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	17	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	17	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	17	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	17	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	17	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD11	18	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD12	18	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD13	18	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD21	18	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD22	18	0.1
(1,348)	1:23:A:LEU:HA	1:23:A:LEU:HD23	18	0.1
(1,325)	1:41:A:LEU:HB2	1:25:A:CYS:HA	3	0.1
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	9	0.1
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	9	0.1
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG2	14	0.1
(1,319)	1:47:A:LEU:H	1:46:A:ARG:HG3	14	0.1
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD21	11	0.1
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD22	11	0.1
(1,312)	1:26:A:GLY:H	1:41:A:LEU:HD23	11	0.1
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG11	2	0.1
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG12	2	0.1
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG13	2	0.1
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG11	7	0.1
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG12	7	0.1
(1,305)	1:38:A:VAL:H	1:38:A:VAL:HG13	7	0.1
(1,243)	1:61:A:PHE:H	1:57:A:ARG:HA	13	0.1
(1,242)	1:56:A:PHE:HD1	1:60:A:HIS:HD2	3	0.1
(1,242)	1:56:A:PHE:HD2	1:60:A:HIS:HD2	3	0.1
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	3	0.1
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	3	0.1
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	13	0.1
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	13	0.1
(1,239)	1:30:A:PHE:HE1	1:34:A:ALA:HA	20	0.1
(1,239)	1:30:A:PHE:HE2	1:34:A:ALA:HA	20	0.1
(1,193)	1:55:A:HIS:HD2	1:55:A:HIS:HB2	9	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	13	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	13	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	13	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	14	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	14	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	14	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD21	19	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD22	19	0.1
(1,178)	1:27:A:GLU:H	1:41:A:LEU:HD23	19	0.1
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD11	15	0.1
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD12	15	0.1
(1,170)	1:55:A:HIS:H	1:47:A:LEU:HD13	15	0.1
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	5	0.1
(1,146)	1:39:A:SER:HA	1:46:A:ARG:HA	8	0.1
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD1	12	0.1
(1,121)	1:61:A:PHE:HB3	1:56:A:PHE:HD2	12	0.1
(1,116)	1:38:A:VAL:HG21	1:52:A:TYR:HE1	12	0.1
(1,116)	1:38:A:VAL:HG21	1:52:A:TYR:HE2	12	0.1
(1,116)	1:38:A:VAL:HG22	1:52:A:TYR:HE1	12	0.1
(1,116)	1:38:A:VAL:HG22	1:52:A:TYR:HE2	12	0.1
(1,116)	1:38:A:VAL:HG23	1:52:A:TYR:HE1	12	0.1
(1,116)	1:38:A:VAL:HG23	1:52:A:TYR:HE2	12	0.1
(1,112)	1:55:A:HIS:HD2	1:56:A:PHE:HA	6	0.1
(1,93)	1:49:A:LEU:HA	1:38:A:VAL:HB	15	0.1
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD1	11	0.1
(1,90)	1:34:A:ALA:HA	1:36:A:TYR:HD2	11	0.1
(1,76)	1:22:B:ASN:H	1:32:A:ALA:H	6	0.1
(1,72)	1:32:B:ALA:H	1:20:A:TYR:HB3	19	0.1
(1,70)	1:32:B:ALA:H	1:20:A:TYR:HB2	19	0.1
(1,69)	1:32:A:ALA:H	1:20:B:TYR:HB2	7	0.1
(1,58)	1:26:B:GLY:H	1:28:A:VAL:H	15	0.1
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	6	0.1
(1,57)	1:26:A:GLY:H	1:28:B:VAL:H	8	0.1
(1,54)	1:25:B:CYS:H	1:28:A:VAL:HB	5	0.1
(1,53)	1:25:A:CYS:H	1:28:B:VAL:HB	2	0.1
(1,53)	1:25:A:CYS:H	1:28:B:VAL:HB	13	0.1
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	9	0.1
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	9	0.1
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	9	0.1
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	12	0.1
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	12	0.1
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	12	0.1
(1,46)	1:49:B:LEU:HD11	1:53:A:PRO:HD2	17	0.1
(1,46)	1:49:B:LEU:HD12	1:53:A:PRO:HD2	17	0.1
(1,46)	1:49:B:LEU:HD13	1:53:A:PRO:HD2	17	0.1
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	3	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	3	0.1
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	3	0.1
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	8	0.1
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	8	0.1
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	8	0.1
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	10	0.1
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	10	0.1
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	10	0.1
(1,45)	1:49:A:LEU:HD11	1:53:B:PRO:HD2	15	0.1
(1,45)	1:49:A:LEU:HD12	1:53:B:PRO:HD2	15	0.1
(1,45)	1:49:A:LEU:HD13	1:53:B:PRO:HD2	15	0.1
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD21	11	0.1
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD22	11	0.1
(1,42)	1:22:B:ASN:HB2	1:29:A:LEU:HD23	11	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	4	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	4	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	4	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	10	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	10	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	10	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD21	16	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD22	16	0.1
(1,41)	1:22:A:ASN:HB2	1:29:B:LEU:HD23	16	0.1
(1,21)	1:30:A:PHE:HD1	1:23:B:LEU:HG	2	0.1
(1,21)	1:30:A:PHE:HD2	1:23:B:LEU:HG	2	0.1
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	2	0.1
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	3	0.1
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	8	0.1
(1,19)	1:21:A:HIS:HA	1:31:B:SER:HA	10	0.1
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	7	0.1
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	7	0.1
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	7	0.1
(1,13)	1:29:B:LEU:HD21	1:24:A:ARG:HA	13	0.1
(1,13)	1:29:B:LEU:HD22	1:24:A:ARG:HA	13	0.1
(1,13)	1:29:B:LEU:HD23	1:24:A:ARG:HA	13	0.1
(1,4)	1:49:B:LEU:HD11	1:50:A:ASP:HA	16	0.1
(1,4)	1:49:B:LEU:HD12	1:50:A:ASP:HA	16	0.1
(1,4)	1:49:B:LEU:HD13	1:50:A:ASP:HA	16	0.1

10 Dihedral-angle violation analysis ⓘ

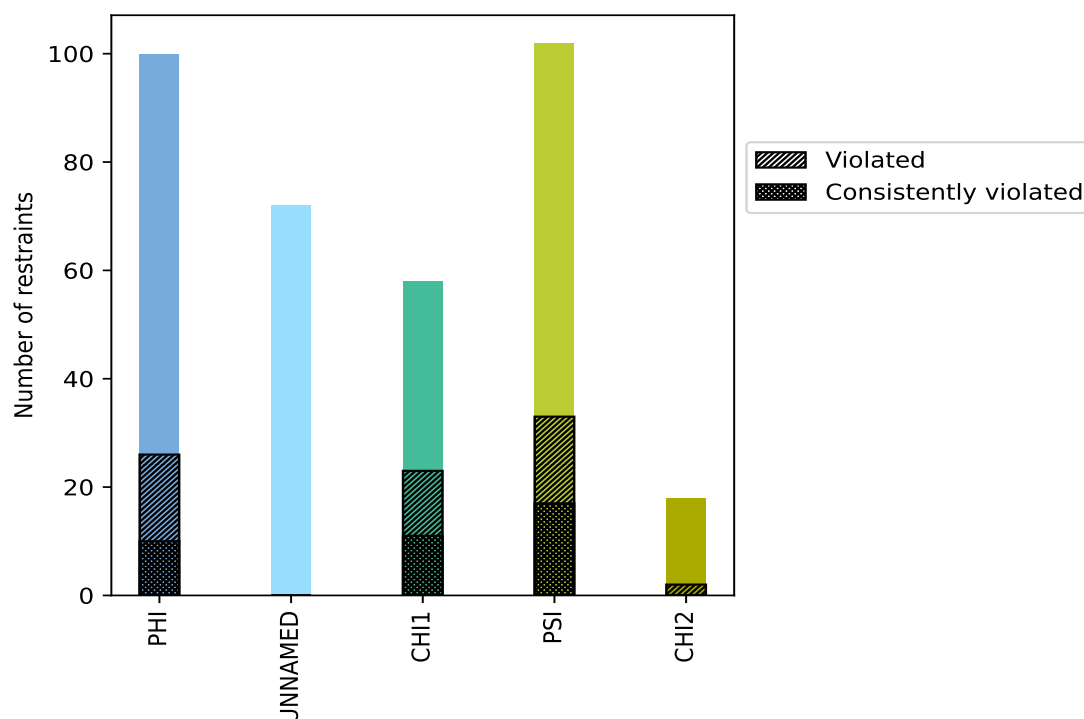
10.1 Summary of dihedral-angle violations ⓘ

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
PHI	100	28.6	26	26.0	7.4	10	10.0	2.9
UNNAMED	72	20.6	0	0.0	0.0	0	0.0	0.0
CHI1	58	16.6	23	39.7	6.6	11	19.0	3.1
PSI	102	29.1	33	32.4	9.4	17	16.7	4.9
CHI2	18	5.1	2	11.1	0.6	0	0.0	0.0
Total	350	100.0	84	24.0	24.0	38	10.9	10.9

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 ⓘ



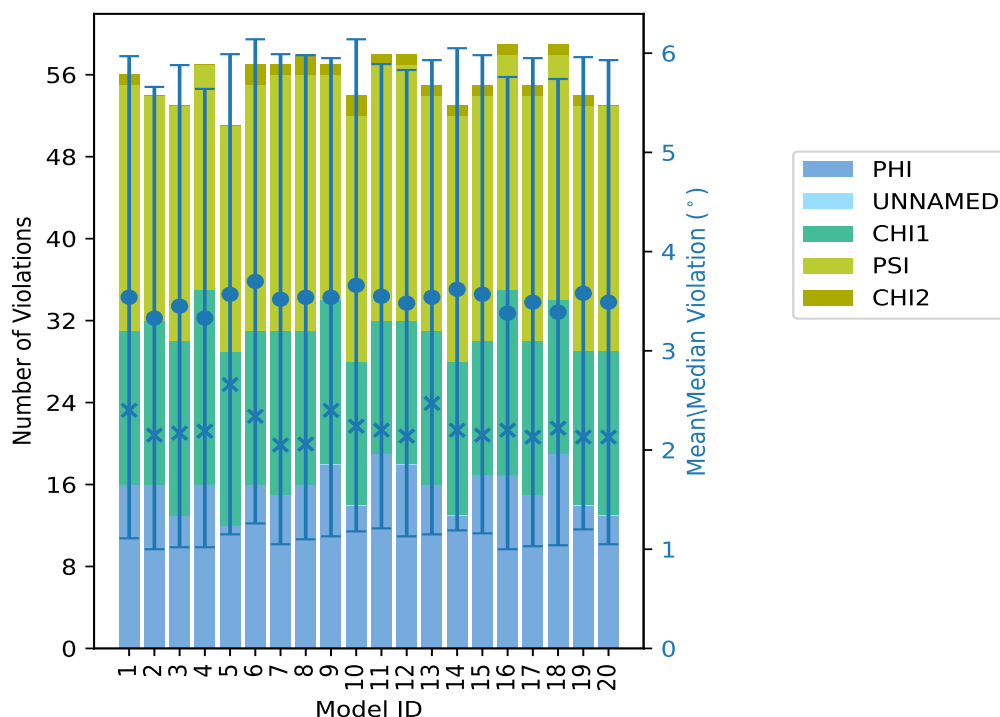
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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
	PHI	UNNAMED	CHI1	PSI	CHI2	Total				
1	16	0	15	24	1	56	3.54	9.31	2.43	2.4
2	16	0	16	22	0	54	3.33	8.09	2.33	2.15
3	13	0	17	23	0	53	3.45	9.77	2.43	2.17
4	16	0	19	22	0	57	3.33	8.13	2.31	2.19
5	12	0	17	22	0	51	3.57	8.26	2.42	2.66
6	16	0	15	24	2	57	3.7	8.54	2.44	2.34
7	15	0	16	25	1	57	3.52	9.73	2.47	2.05
8	16	0	15	25	2	58	3.54	8.53	2.44	2.06
9	18	0	16	22	1	57	3.54	9.47	2.41	2.4
10	14	0	14	24	2	54	3.66	8.43	2.48	2.24
11	19	0	13	25	1	58	3.55	8.41	2.34	2.2
12	18	0	14	25	1	58	3.48	8.4	2.35	2.14
13	16	0	15	23	1	55	3.54	8.38	2.39	2.47
14	13	0	15	24	1	53	3.62	8.53	2.43	2.2
15	17	0	13	24	1	55	3.57	8.93	2.41	2.15
16	17	0	18	23	1	59	3.38	8.78	2.38	2.2
17	15	0	15	24	1	55	3.49	9.23	2.46	2.13
18	19	0	15	24	1	59	3.39	8.27	2.35	2.22
19	14	0	15	24	1	54	3.58	8.26	2.38	2.13
20	13	0	16	24	0	53	3.49	9.58	2.44	2.13

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

Number of violated restraints						Fraction of the ensemble	
PHI	UNNAMED	CHI1	PSI	CHI2	Total	Count ¹	%
2	0	4	2	0	8	1	5.0
1	0	0	0	0	1	2	10.0
3	0	0	3	0	6	3	15.0
3	0	2	1	0	6	4	20.0
0	0	1	0	0	1	5	25.0
0	0	1	0	0	1	6	30.0
1	0	0	3	1	5	7	35.0
1	0	0	0	0	1	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
1	0	0	2	1	4	11	55.0

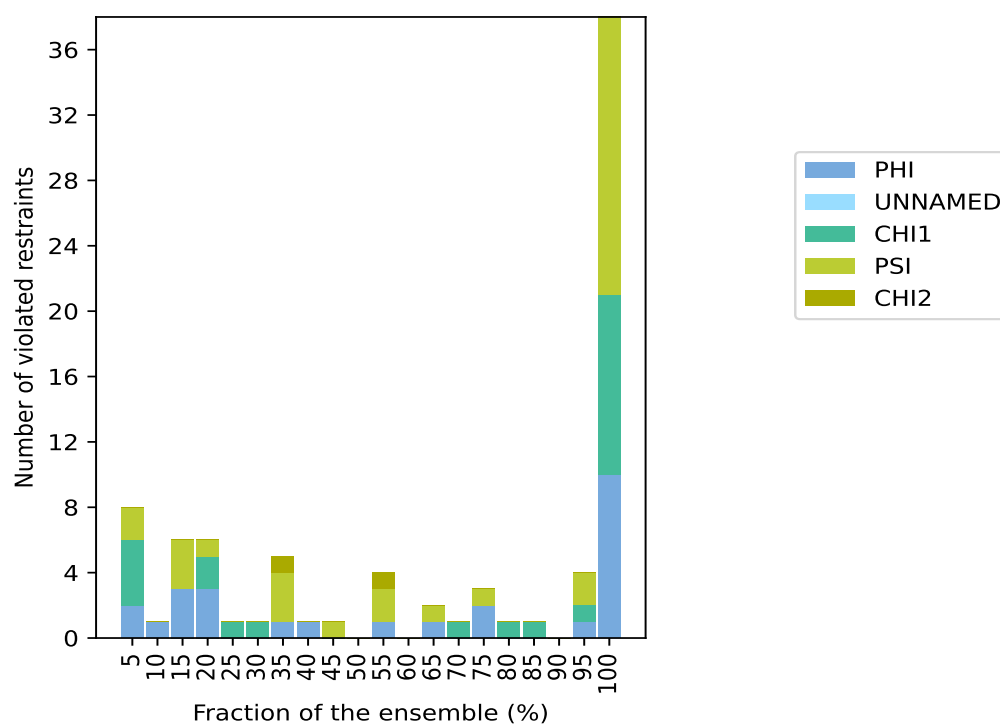
Continued on next page...

Continued from previous page...

PHI	Number of violated restraints					Fraction of the ensemble	
	UNNAMED	CHI1	PSI	CHI2	Total	Count ¹	%
0	0	0	0	0	0	12	60.0
1	0	0	1	0	2	13	65.0
0	0	1	0	0	1	14	70.0
2	0	0	1	0	3	15	75.0
0	0	1	0	0	1	16	80.0
0	0	1	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
1	0	1	2	0	4	19	95.0
10	0	11	17	0	38	20	100.0

¹ Number of models with violations

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

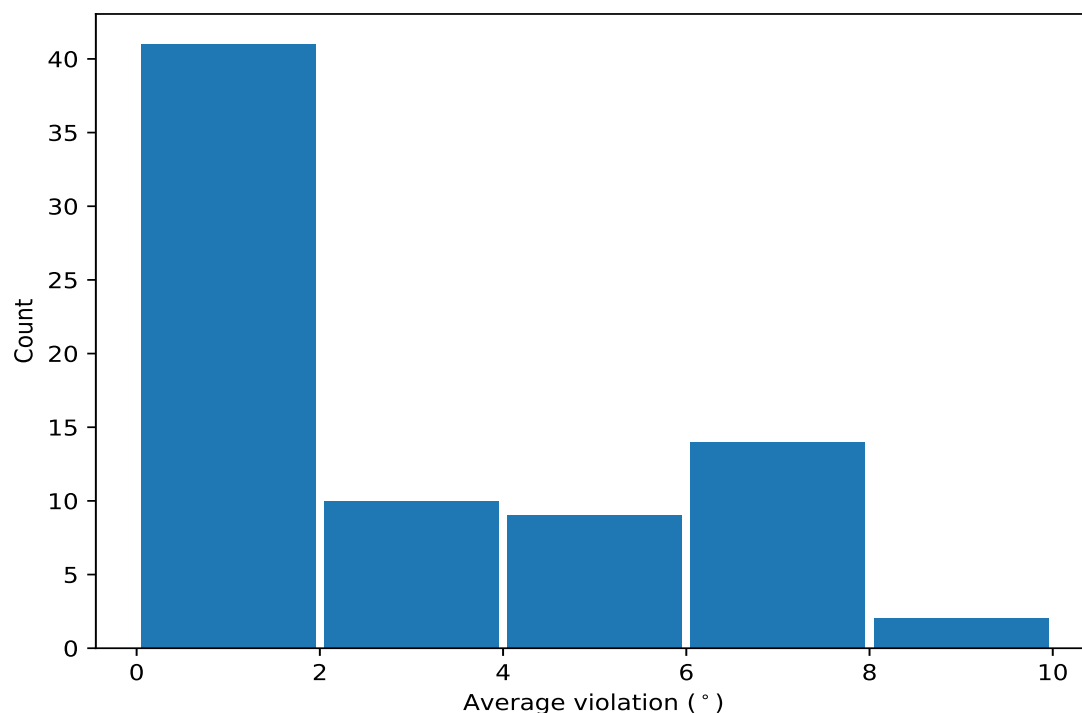


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	20	7.64	0.28	7.6
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	20	7.61	1.07	7.62
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	20	7.56	0.34	7.56
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	20	7.32	0.98	6.71
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	20	7.21	0.76	7.56
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	20	7.02	0.71	6.61
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	20	6.63	0.23	6.56
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	20	6.63	0.32	6.7
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	20	6.57	0.15	6.54
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	20	6.55	0.14	6.52
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	20	6.13	0.68	6.2
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	20	6.08	0.35	6.11
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	20	5.28	0.28	5.32
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	20	5.22	0.38	5.3
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	20	5.15	0.28	5.19
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	20	5.04	0.38	4.97
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	20	4.77	0.43	4.9
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	20	4.71	0.18	4.68
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	20	4.38	0.23	4.38
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	20	4.29	0.27	4.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	20	4.11	0.51	4.34
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	20	3.8	0.49	3.72
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	20	2.65	0.75	2.76
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	20	2.23	0.62	2.35
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	20	2.19	0.76	1.94
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	20	2.16	0.43	2.12
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	20	2.0	0.36	1.88
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	20	1.98	0.17	1.94
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	20	1.93	0.16	1.96
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	20	1.63	0.18	1.63
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	20	1.62	0.19	1.6
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	20	1.6	0.15	1.6
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	20	1.52	0.19	1.5
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	20	1.43	0.24	1.37
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	20	1.27	0.09	1.25
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	20	1.24	0.1	1.23
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	20	1.22	0.16	1.2
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	20	1.16	0.06	1.15
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	19	2.46	0.75	2.17
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	19	2.0	0.65	2.12
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	19	1.34	0.18	1.3
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	19	1.18	0.1	1.14
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	17	1.28	0.19	1.22
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	16	1.24	0.16	1.21
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	15	1.74	0.52	1.58
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	15	1.45	0.2	1.37
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	15	1.2	0.15	1.17
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	14	1.66	0.31	1.71
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	13	1.59	0.45	1.37
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	13	1.57	0.3	1.67
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	11	8.4	0.14	8.4
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	11	7.27	0.12	7.26
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	11	1.58	0.2	1.56
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	11	1.31	0.11	1.29
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	9	1.44	0.48	1.19
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	8	1.52	0.51	1.27
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	7	8.53	0.22	8.43
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	7	7.4	0.2	7.37
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	7	1.62	0.16	1.71
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	7	1.23	0.2	1.21
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	7	1.22	0.09	1.18
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	6	1.55	0.15	1.5
(1,256)	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:CB	1:40:B:CYS:SG	5	1.07	0.04	1.05
(1,114)	1:54:B:GLU:C	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:C	4	1.4	0.39	1.35
(1,123)	1:60:A:HIS:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	4	1.35	0.11	1.37
(1,145)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:LEU:N	4	1.26	0.42	1.03
(1,276)	1:59:B:LYS:N	1:59:B:LYS:CA	1:59:B:LYS:CB	1:59:B:LYS:CG	4	1.14	0.07	1.14
(1,102)	1:45:B:GLN:C	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	4	1.12	0.08	1.1
(1,255)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:CB	1:40:A:CYS:SG	4	1.11	0.03	1.1
(1,115)	1:56:A:PHE:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	3	2.22	0.12	2.22
(1,149)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	3	1.23	0.07	1.19

Continued on next page...

Continued from previous page...

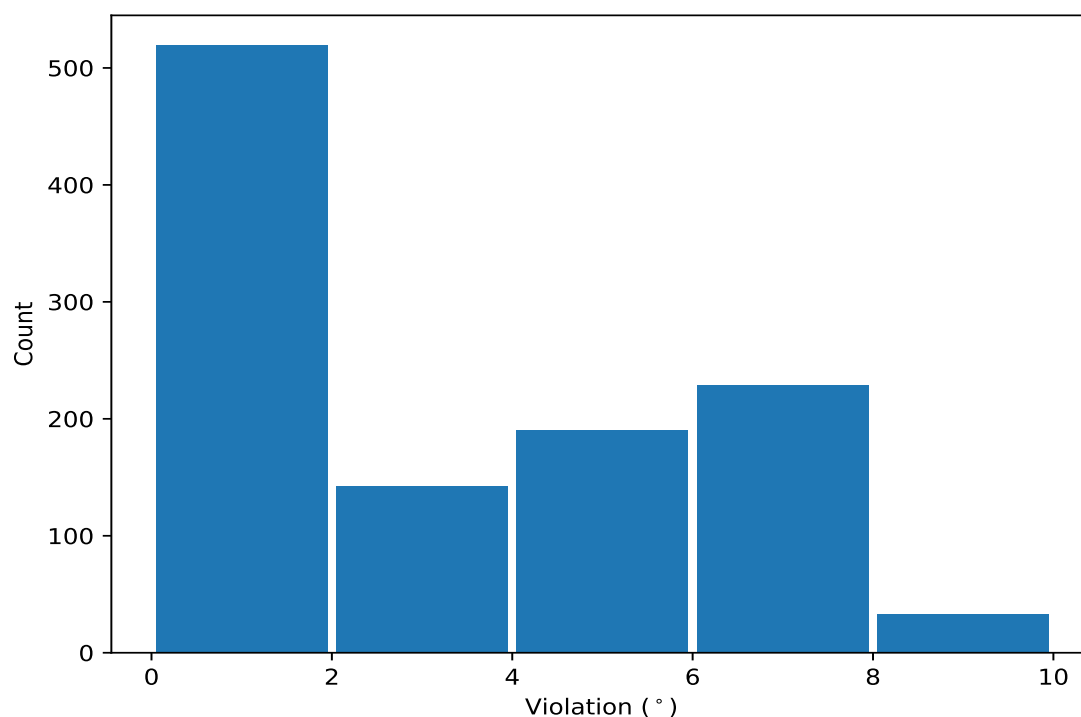
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,101)	1:45:A:GLN:C	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	3	1.22	0.11	1.26
(1,199)	1:26:B:GLY:N	1:26:B:GLY:CA	1:26:B:GLY:C	1:27:B:GLU:N	3	1.19	0.12	1.23
(1,143)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:HIS:N	3	1.14	0.1	1.12
(1,54)	1:17:B:ALA:C	1:18:B:GLY:N	1:18:B:GLY:CA	1:18:B:GLY:C	3	1.11	0.06	1.13
(1,116)	1:56:B:PHE:C	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:C	2	2.24	0.02	2.24

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 (°)
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	3	9.77
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	7	9.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	20	9.58
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	9	9.47
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1	9.31
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	17	9.23
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	15	8.93
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	16	8.78
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	9	8.67
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	6	8.54
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	14	8.53
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	8	8.53
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	16	8.46
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1	8.44
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	10	8.43
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	11	8.41
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	12	8.4
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	17	8.4
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	6	8.4
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	13	8.38
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	6	8.37
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	8	8.32
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	10	8.27
(1,95)	1:42:A:LEU:C	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	18	8.27
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	5	8.26
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	19	8.26
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	15	8.25
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	7	8.22
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	3	8.13
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	4	8.13
(1,96)	1:42:B:LEU:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	7	8.13
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	2	8.09
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	5	8.08
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	14	7.96
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	15	7.92
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	10	7.91
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	3	7.89
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	16	7.88
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	4	7.87
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	18	7.86
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	4	7.86
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	3	7.85
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	15	7.85
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	5	7.84
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	13	7.82
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	14	7.81
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	16	7.79
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	19	7.79
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	19	7.78
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	20	7.78
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	2	7.76
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	5	7.76
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	20	7.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	13	7.75
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	5	7.75
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	12	7.74
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	18	7.72
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	2	7.7
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1	7.69
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	13	7.69
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	8	7.69
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	14	7.68
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	16	7.67
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	4	7.65
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	15	7.64
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	7	7.63
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	6	7.63
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	16	7.63
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	2	7.62
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	17	7.62
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	20	7.62
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	18	7.61
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	15	7.6
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	11	7.6
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	12	7.6
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	10	7.6
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	11	7.57
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	19	7.56
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	8	7.56
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	4	7.56
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	9	7.55
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	12	7.54
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	9	7.54
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	17	7.53
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	17	7.53
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	4	7.52
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	8	7.5
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1	7.49
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	20	7.47
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	18	7.47
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	9	7.46
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	11	7.46
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	7	7.44
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	2	7.44
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	11	7.42
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	6	7.37
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	14	7.37
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	13	7.37
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	17	7.36
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	8	7.34
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	10	7.34
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	3	7.32
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	20	7.32
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	12	7.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	10	7.26
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	3	7.25
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	1	7.24
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	7	7.23
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	19	7.21
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	12	7.2
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	6	7.2
(1,71)	1:28:A:VAL:C	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	13	7.2
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	9	7.18
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	7	7.17
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	1	7.17
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	5	7.17
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	14	7.15
(1,72)	1:28:B:VAL:C	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	2	7.12
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	11	7.11
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	19	7.09
(1,162)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:CYS:N	18	7.08
(1,212)	1:42:B:LEU:N	1:42:B:LEU:CA	1:42:B:LEU:C	1:43:B:CYS:N	11	7.02
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	4	7.02
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	6	7.01
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	13	6.93
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	19	6.93
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	14	6.93
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	20	6.91
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	5	6.91
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	5	6.89
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	18	6.88
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	14	6.86
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	8	6.86
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	13	6.85
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	5	6.84
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	15	6.83
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	18	6.83
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	9	6.82
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	1	6.82
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	3	6.81
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	14	6.8
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	7	6.77
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	10	6.76
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	1	6.74
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	7	6.74
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	10	6.73
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	7	6.71
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	17	6.69
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	12	6.69
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	11	6.68
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	8	6.67
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	9	6.67
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	12	6.66
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	7	6.66
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	4	6.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	19	6.66
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	17	6.66
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	11	6.66
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	19	6.66
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	20	6.66
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	20	6.65
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	12	6.65
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	15	6.63
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	20	6.63
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	3	6.63
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	13	6.59
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	1	6.59
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	6	6.59
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	7	6.58
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1	6.58
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	19	6.58
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	11	6.57
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	7	6.57
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	10	6.56
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	11	6.56
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	19	6.56
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	6	6.56
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	10	6.56
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	17	6.55
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	6	6.55
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	12	6.55
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	5	6.54
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	6	6.54
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	14	6.54
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	6	6.54
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	10	6.54
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	16	6.54
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	5	6.54
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	4	6.53
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	17	6.53
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	14	6.53
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	9	6.53
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	13	6.52
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	12	6.51
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	2	6.51
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	3	6.51
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	14	6.51
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	13	6.51
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	6	6.5
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	15	6.5
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	1	6.49
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	18	6.49
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	8	6.49
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	20	6.49
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	9	6.49
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	9	6.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	18	6.48
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	16	6.48
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	1	6.47
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	2	6.47
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	2	6.47
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	1	6.46
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	9	6.45
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	19	6.44
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	19	6.43
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	15	6.43
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	10	6.42
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	11	6.41
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	16	6.41
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	8	6.4
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	6	6.39
(1,219)	1:51:B:GLY:N	1:51:B:GLY:CA	1:51:B:GLY:C	1:52:B:TYR:N	16	6.39
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	12	6.39
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	3	6.39
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	17	6.36
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	5	6.36
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	8	6.36
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	11	6.35
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	13	6.34
(1,98)	1:43:B:CYS:C	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	8	6.34
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	2	6.34
(1,169)	1:51:A:GLY:N	1:51:A:GLY:CA	1:51:A:GLY:C	1:52:A:TYR:N	4	6.33
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	17	6.33
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	6	6.32
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	12	6.31
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	10	6.28
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	8	6.27
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	8	6.27
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	13	6.27
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	10	6.26
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	16	6.25
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	9	6.24
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	18	6.24
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	4	6.23
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	2	6.22
(1,97)	1:43:A:CYS:C	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	16	6.22
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	4	6.19
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	8	6.19
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	15	6.18
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	14	6.18
(1,158)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:VAL:N	15	6.17
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	20	6.17
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	18	6.16
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	6	6.15
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	15	6.14
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	16	6.12
(1,163)	1:43:A:CYS:N	1:43:A:CYS:CA	1:43:A:CYS:C	1:44:A:ASP:N	18	6.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	3	6.1
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	17	6.08
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	10	6.06
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	18	6.04
(1,208)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:C	1:38:B:VAL:N	3	6.0
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	12	5.98
(1,213)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASP:N	11	5.94
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	13	5.93
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	9	5.89
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	1	5.88
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	8	5.85
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	7	5.84
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	10	5.84
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	19	5.76
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	11	5.75
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	17	5.74
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	19	5.65
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	14	5.65
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	12	5.64
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	4	5.64
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	8	5.64
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	15	5.63
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	14	5.63
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	20	5.61
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	17	5.61
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	2	5.6
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	4	5.53
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	18	5.53
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	10	5.53
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	1	5.51
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	14	5.5
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	19	5.5
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	13	5.48
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	6	5.47
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	5	5.47
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	11	5.43
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	16	5.42
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	15	5.42
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	16	5.42
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	3	5.4
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	5	5.39
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	7	5.38
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	20	5.38
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	13	5.36
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	9	5.36
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	1	5.34
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	10	5.33
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	17	5.33
(1,73)	1:29:A:LEU:C	1:30:A:PHE:N	1:30:A:PHE:CA	1:30:A:PHE:C	12	5.33
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	8	5.31
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	2	5.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	11	5.28
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	9	5.28
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	1	5.27
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	3	5.26
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	7	5.25
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	9	5.24
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	18	5.21
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	15	5.2
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	2	5.2
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	3	5.19
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	13	5.18
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	20	5.18
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	5	5.18
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	17	5.17
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	20	5.14
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	12	5.13
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	19	5.12
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	11	5.12
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	18	5.11
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	5	5.1
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	20	5.1
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	20	5.09
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	2	5.08
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	3	5.02
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	9	5.01
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	5	5.01
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	2	5.0
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	14	4.98
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	11	4.97
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	16	4.96
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	3	4.96
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	6	4.96
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	18	4.95
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	5	4.95
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	11	4.95
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	11	4.94
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	7	4.94
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	2	4.94
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	12	4.94
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	19	4.94
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	7	4.92
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	15	4.91
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	18	4.91
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	6	4.91
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	1	4.9
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	4	4.9
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	14	4.9
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	15	4.9
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	14	4.89
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	6	4.87
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	13	4.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	9	4.82
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	3	4.82
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	15	4.82
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	16	4.76
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	16	4.75
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	2	4.75
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	13	4.74
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	8	4.73
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	8	4.72
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	17	4.72
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	15	4.71
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	1	4.71
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	12	4.7
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	6	4.7
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	16	4.69
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	16	4.69
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	6	4.68
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	7	4.67
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	14	4.67
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	8	4.65
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	1	4.65
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	19	4.65
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	4	4.64
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	18	4.64
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	6	4.63
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	10	4.63
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	7	4.63
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	19	4.62
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	17	4.62
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	8	4.61
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	17	4.58
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	8	4.57
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	1	4.57
(1,221)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:C	1:55:B:HIS:N	7	4.57
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	13	4.57
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	14	4.55
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	15	4.55
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	10	4.55
(1,171)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:C	1:55:A:HIS:N	10	4.54
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	9	4.54
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	14	4.54
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	19	4.53
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	12	4.53
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	12	4.52
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	13	4.52
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	11	4.52
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	2	4.52
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	18	4.51
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	2	4.51
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	20	4.51
(1,200)	1:27:B:GLU:N	1:27:B:GLU:CA	1:27:B:GLU:C	1:28:B:VAL:N	4	4.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	20	4.51
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	10	4.51
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	3	4.49
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	9	4.46
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	1	4.45
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	12	4.44
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	17	4.43
(1,152)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:C	1:30:A:PHE:N	12	4.42
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	11	4.41
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	18	4.41
(1,150)	1:27:A:GLU:N	1:27:A:GLU:CA	1:27:A:GLU:C	1:28:A:VAL:N	4	4.41
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	8	4.39
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	10	4.38
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	3	4.38
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	5	4.37
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	19	4.36
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	7	4.34
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	12	4.34
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	10	4.34
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	16	4.34
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	6	4.32
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	17	4.32
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	10	4.31
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	4	4.3
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	9	4.29
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	6	4.29
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	15	4.29
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	17	4.27
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	5	4.24
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	16	4.24
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	12	4.22
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	4	4.18
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	13	4.14
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	1	4.13
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	14	4.13
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	11	4.11
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	6	4.1
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	9	4.08
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	6	4.06
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	7	4.04
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	19	4.04
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	15	4.0
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	8	3.98
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	18	3.98
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	10	3.97
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	8	3.95
(1,74)	1:29:B:LEU:C	1:30:B:PHE:N	1:30:B:PHE:CA	1:30:B:PHE:C	15	3.9
(1,159)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:SER:N	13	3.89
(1,209)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:SER:N	11	3.85
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	2	3.81
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	16	3.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	19	3.77
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	9	3.7
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	14	3.67
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	5	3.66
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	16	3.66
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	20	3.61
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	20	3.59
(1,202)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:C	1:30:B:PHE:N	15	3.58
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	4	3.57
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	13	3.53
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	3	3.52
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	16	3.47
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	7	3.46
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	3	3.45
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	18	3.43
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	17	3.43
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	2	3.31
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	4	3.24
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	9	3.2
(1,270)	1:56:B:PHE:N	1:56:B:PHE:CA	1:56:B:PHE:CB	1:56:B:PHE:CG	5	3.18
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	9	3.14
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	14	3.11
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	1	3.1
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	4	3.04
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	19	3.03
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	1	3.02
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	4	2.98
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	13	2.96
(1,269)	1:56:A:PHE:N	1:56:A:PHE:CA	1:56:A:PHE:CB	1:56:A:PHE:CG	4	2.95
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	2	2.95
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	20	2.95
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	16	2.94
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	17	2.9
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	5	2.89
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	9	2.89
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	1	2.89
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	13	2.86
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	5	2.83
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	4	2.79
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	3	2.78
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	4	2.78
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	2	2.78
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	16	2.77
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	16	2.74
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	5	2.74
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	11	2.74
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	18	2.73
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1	2.73
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	7	2.71
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	9	2.7
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	18	2.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	2	2.68
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	5	2.66
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	13	2.65
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	18	2.65
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	5	2.63
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	11	2.63
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	15	2.62
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	18	2.61
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	7	2.6
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	1	2.57
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	19	2.57
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	2	2.56
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	11	2.55
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	20	2.55
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	8	2.49
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	3	2.49
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	20	2.49
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	3	2.48
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	13	2.47
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	12	2.47
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	17	2.43
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	10	2.42
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	9	2.4
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	14	2.4
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	2	2.38
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	6	2.38
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	3	2.37
(1,115)	1:56:A:PHE:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	12	2.37
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	16	2.37
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	17	2.35
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	12	2.35
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	6	2.34
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	18	2.34
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	9	2.32
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	7	2.32
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	8	2.29
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	20	2.27
(1,116)	1:56:B:PHE:C	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:C	11	2.26
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	4	2.24
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	1	2.23
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	9	2.22
(1,115)	1:56:A:PHE:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	18	2.22
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	12	2.22
(1,116)	1:56:B:PHE:C	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:C	15	2.21
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	19	2.21
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	16	2.2
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	14	2.2
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	4	2.19
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	7	2.18
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	3	2.17
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	14	2.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	15	2.15
(1,141)	1:18:A:GLY:N	1:18:A:GLY:CA	1:18:A:GLY:C	1:19:A:GLY:N	11	2.14
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	8	2.14
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	20	2.13
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	17	2.13
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	5	2.13
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	14	2.13
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	4	2.13
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	6	2.12
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	20	2.11
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	6	2.1
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	11	2.09
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	5	2.09
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	13	2.08
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	9	2.07
(1,115)	1:56:A:PHE:C	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:C	11	2.07
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	10	2.07
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	12	2.06
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	16	2.06
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	4	2.06
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	7	2.05
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	17	2.05
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	19	2.05
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	6	2.05
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	5	2.05
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	10	2.04
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	15	2.04
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	15	2.04
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	13	2.03
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	11	2.03
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	4	2.0
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	3	1.99
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	4	1.99
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	3	1.99
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	8	1.98
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	20	1.98
(1,145)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:LEU:N	15	1.98
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	1	1.97
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	19	1.97
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	12	1.97
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	16	1.96
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	10	1.96
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	18	1.96
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	5	1.95
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	12	1.94
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	14	1.94
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	1	1.93
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	2	1.93
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	4	1.93
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	15	1.93
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	11	1.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	18	1.92
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	5	1.92
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	16	1.92
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	15	1.91
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	19	1.91
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	14	1.91
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	3	1.91
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	1	1.9
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	11	1.9
(1,114)	1:54:B:GLU:C	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:C	11	1.9
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	7	1.89
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	9	1.89
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	13	1.89
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	6	1.89
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	12	1.89
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	9	1.88
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	20	1.88
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	6	1.88
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	8	1.88
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	9	1.88
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	19	1.88
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	13	1.87
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	18	1.87
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	3	1.86
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	6	1.86
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	6	1.86
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	19	1.85
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	20	1.84
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	18	1.84
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	5	1.83
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	3	1.83
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	11	1.83
(1,55)	1:18:A:GLY:C	1:19:A:GLY:N	1:19:A:GLY:CA	1:19:A:GLY:C	11	1.83
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	19	1.82
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	12	1.82
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	15	1.82
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	2	1.82
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	3	1.82
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	1	1.82
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	5	1.8
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	7	1.8
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	7	1.8
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	7	1.8
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1	1.8
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	12	1.8
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	17	1.8
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	2	1.79
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	20	1.79
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	10	1.79
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	14	1.78
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	4	1.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	4	1.78
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	2	1.77
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	14	1.77
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	4	1.76
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	8	1.76
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	2	1.76
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	14	1.75
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	15	1.75
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	8	1.75
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	20	1.75
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	8	1.74
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	14	1.72
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	18	1.72
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	19	1.72
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	8	1.72
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	13	1.72
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	6	1.71
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	13	1.71
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	18	1.71
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	1	1.71
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	7	1.7
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	11	1.7
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	16	1.7
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	14	1.69
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	16	1.69
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	11	1.69
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	20	1.69
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	18	1.69
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	20	1.68
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	17	1.68
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	13	1.68
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	3	1.68
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	9	1.68
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	12	1.67
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	2	1.67
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	15	1.67
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	12	1.67
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	13	1.67
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	13	1.67
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	1	1.66
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	17	1.66
(1,114)	1:54:B:GLU:C	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:C	15	1.66
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	11	1.66
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	12	1.66
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	19	1.66
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	4	1.65
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	11	1.65
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	8	1.65
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	12	1.65
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	14	1.64
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	7	1.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	7	1.63
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	1	1.63
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	20	1.63
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	2	1.62
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	3	1.62
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	10	1.62
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	5	1.62
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	6	1.62
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	7	1.62
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	4	1.62
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	10	1.62
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	17	1.62
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	13	1.61
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	6	1.61
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	10	1.6
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	14	1.6
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	7	1.6
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	12	1.59
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	18	1.59
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	8	1.59
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	7	1.58
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	20	1.58
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	19	1.58
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	17	1.58
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	16	1.58
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	6	1.57
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	19	1.57
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	8	1.57
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	9	1.57
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	7	1.57
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	1	1.56
(1,244)	1:29:B:LEU:N	1:29:B:LEU:CA	1:29:B:LEU:CB	1:29:B:LEU:CG	15	1.56
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	3	1.56
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	8	1.56
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	12	1.56
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	16	1.56
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	7	1.56
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	5	1.56
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	20	1.56
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	8	1.55
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	3	1.55
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	9	1.55
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	8	1.55
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	6	1.54
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	2	1.54
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	3	1.54
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	15	1.54
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	5	1.53
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	6	1.53
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	13	1.53
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	11	1.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	18	1.53
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	19	1.53
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	20	1.52
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	12	1.52
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	7	1.52
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	12	1.52
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	12	1.52
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	19	1.51
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	1	1.51
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	13	1.5
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	16	1.5
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	13	1.5
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	17	1.5
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	7	1.5
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	9	1.5
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	19	1.5
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	14	1.5
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	10	1.5
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	16	1.5
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	10	1.49
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	10	1.49
(1,123)	1:60:A:HIS:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	6	1.49
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	18	1.49
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	11	1.48
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	6	1.47
(1,243)	1:29:A:LEU:N	1:29:A:LEU:CA	1:29:A:LEU:CB	1:29:A:LEU:CG	15	1.47
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	7	1.47
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	18	1.47
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	5	1.47
(1,87)	1:37:A:GLU:C	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	17	1.47
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	7	1.47
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	7	1.47
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	9	1.46
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	17	1.46
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	10	1.46
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	15	1.46
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	19	1.46
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	17	1.46
(1,177)	1:60:A:HIS:N	1:60:A:HIS:CA	1:60:A:HIS:C	1:61:A:PHE:N	17	1.46
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	2	1.45
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	16	1.45
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	8	1.45
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	2	1.45
(1,88)	1:37:B:GLU:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	15	1.45
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	1	1.44
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	1	1.44
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	14	1.44
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	9	1.43
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	15	1.43
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	8	1.43
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	20	1.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	15	1.43
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	4	1.43
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	12	1.43
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	6	1.42
(1,268)	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:CB	1:55:B:HIS:CG	10	1.42
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	17	1.42
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	9	1.42
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	17	1.42
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	20	1.42
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	19	1.41
(1,234)	1:20:B:TYR:N	1:20:B:TYR:CA	1:20:B:TYR:CB	1:20:B:TYR:CG	4	1.41
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	10	1.41
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	18	1.39
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	20	1.39
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	1	1.39
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	4	1.39
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	13	1.39
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	2	1.39
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	17	1.39
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	15	1.39
(1,278)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:CB	1:61:B:PHE:CG	18	1.38
(1,267)	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:CB	1:55:A:HIS:CG	10	1.38
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	6	1.38
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	12	1.38
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	10	1.37
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	19	1.37
(1,123)	1:60:A:HIS:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	9	1.37
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	19	1.37
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	1	1.37
(1,53)	1:17:A:ALA:C	1:18:A:GLY:N	1:18:A:GLY:CA	1:18:A:GLY:C	11	1.37
(1,271)	1:57:A:ARG:N	1:57:A:ARG:CA	1:57:A:ARG:CB	1:57:A:ARG:CG	3	1.36
(1,123)	1:60:A:HIS:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	16	1.36
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	15	1.36
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	18	1.36
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	11	1.35
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	20	1.35
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	12	1.35
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	1	1.35
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	17	1.35
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	3	1.35
(1,1)	1:24:A:ARG:N	1:24:A:ARG:CA	1:24:A:ARG:CB	1:24:A:ARG:CG	3	1.35
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	16	1.34
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	17	1.34
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	19	1.34
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	11	1.34
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	7	1.34
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	19	1.34
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	9	1.34
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	19	1.34
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	16	1.33
(1,165)	1:45:A:GLN:N	1:45:A:GLN:CA	1:45:A:GLN:C	1:46:A:ARG:N	6	1.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,149)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	10	1.33
(1,101)	1:45:A:GLN:C	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	18	1.33
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	2	1.33
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	19	1.33
(1,33)	1:33:A:PRO:N	1:33:A:PRO:CA	1:33:A:PRO:C	1:34:A:ALA:N	3	1.33
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	16	1.32
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	18	1.32
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	8	1.32
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	11	1.32
(1,199)	1:26:B:GLY:N	1:26:B:GLY:CA	1:26:B:GLY:C	1:27:B:GLU:N	19	1.32
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	12	1.32
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	14	1.32
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	1	1.32
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	4	1.32
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	7	1.32
(1,272)	1:57:B:ARG:N	1:57:B:ARG:CA	1:57:B:ARG:CB	1:57:B:ARG:CG	9	1.31
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	5	1.31
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	9	1.31
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	14	1.31
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	2	1.3
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	4	1.3
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	13	1.3
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	13	1.3
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	20	1.3
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	19	1.3
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	14	1.3
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	14	1.29
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	12	1.29
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	11	1.29
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	1	1.29
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	10	1.29
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	16	1.29
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	8	1.28
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	8	1.28
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	5	1.28
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	1	1.28
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	3	1.27
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	16	1.27
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	4	1.27
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	12	1.27
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	8	1.27
(1,143)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:HIS:N	3	1.27
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	6	1.27
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	16	1.27
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	9	1.27
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	13	1.26
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	12	1.26
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	10	1.26
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	1	1.26
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	9	1.26
(1,233)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:CB	1:20:A:TYR:CG	15	1.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	5	1.26
(1,101)	1:45:A:GLN:C	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	15	1.26
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	11	1.26
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	13	1.26
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	2	1.26
(1,34)	1:33:B:PRO:N	1:33:B:PRO:CA	1:33:B:PRO:C	1:34:B:ALA:N	14	1.26
(1,276)	1:59:B:LYS:N	1:59:B:LYS:CA	1:59:B:LYS:CB	1:59:B:LYS:CG	7	1.25
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	3	1.25
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	4	1.25
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	19	1.25
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	16	1.25
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	6	1.24
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	1	1.24
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	18	1.24
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	3	1.24
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	7	1.24
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	15	1.24
(1,215)	1:45:B:GLN:N	1:45:B:GLN:CA	1:45:B:GLN:C	1:46:B:ARG:N	1	1.24
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	6	1.24
(1,102)	1:45:B:GLN:C	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	8	1.24
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	6	1.24
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	6	1.24
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	8	1.24
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	18	1.23
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	5	1.23
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	12	1.23
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	14	1.23
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	18	1.23
(1,199)	1:26:B:GLY:N	1:26:B:GLY:CA	1:26:B:GLY:C	1:27:B:GLU:N	1	1.23
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	9	1.23
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	3	1.23
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	7	1.22
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	18	1.22
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	9	1.22
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	13	1.22
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	15	1.22
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	10	1.22
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	7	1.22
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	8	1.21
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	6	1.21
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	7	1.21
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	9	1.21
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	18	1.21
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	11	1.21
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	7	1.2
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	14	1.2
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	15	1.2
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	4	1.2
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	9	1.2
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	11	1.2
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	15	1.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	17	1.2
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	2	1.2
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	5	1.2
(1,61)	1:22:A:ASN:C	1:23:A:LEU:N	1:23:A:LEU:CA	1:23:A:LEU:C	17	1.2
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	4	1.19
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	2	1.19
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	2	1.19
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	16	1.19
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	16	1.19
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	2	1.19
(1,149)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	8	1.19
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	11	1.19
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	10	1.19
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	4	1.18
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	1	1.18
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	5	1.18
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	16	1.18
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	3	1.18
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	17	1.18
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	6	1.18
(1,276)	1:59:B:LYS:N	1:59:B:LYS:CA	1:59:B:LYS:CB	1:59:B:LYS:CG	16	1.17
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	8	1.17
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	4	1.17
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	8	1.17
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	6	1.17
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	18	1.17
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	2	1.17
(1,149)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:GLU:N	18	1.17
(1,123)	1:60:A:HIS:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	4	1.17
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	8	1.17
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	10	1.17
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	13	1.17
(1,255)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:CB	1:40:A:CYS:SG	3	1.16
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	13	1.16
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	15	1.16
(1,54)	1:17:B:ALA:C	1:18:B:GLY:N	1:18:B:GLY:CA	1:18:B:GLY:C	18	1.16
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	1	1.15
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	2	1.15
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	5	1.15
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	11	1.15
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	20	1.15
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	7	1.15
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	14	1.15
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	17	1.15
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	10	1.15
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	2	1.15
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	12	1.15
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	16	1.15
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	9	1.14
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	20	1.14
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	13	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,256)	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:CB	1:40:B:CYS:SG	16	1.14
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	16	1.14
(1,102)	1:45:B:GLN:C	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	9	1.14
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	13	1.14
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	8	1.13
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	12	1.13
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	1	1.13
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	13	1.13
(1,228)	1:61:B:PHE:N	1:61:B:PHE:CA	1:61:B:PHE:C	1:62:B:THR:N	20	1.13
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	1	1.13
(1,54)	1:17:B:ALA:C	1:18:B:GLY:N	1:18:B:GLY:CA	1:18:B:GLY:C	2	1.13
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	19	1.12
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	9	1.12
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	12	1.12
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	20	1.12
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	5	1.12
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	16	1.12
(1,249)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:CB	1:37:A:GLU:CG	10	1.12
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	14	1.12
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	18	1.12
(1,143)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:HIS:N	11	1.12
(1,276)	1:59:B:LYS:N	1:59:B:LYS:CA	1:59:B:LYS:CB	1:59:B:LYS:CG	17	1.11
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	13	1.11
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	14	1.11
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	17	1.11
(1,255)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:CB	1:40:A:CYS:SG	4	1.11
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	4	1.11
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	4	1.11
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	17	1.1
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	10	1.1
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	2	1.1
(1,255)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:CB	1:40:A:CYS:SG	2	1.1
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	17	1.1
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	13	1.1
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	4	1.1
(1,277)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:CB	1:61:A:PHE:CG	16	1.09
(1,256)	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:CB	1:40:B:CYS:SG	5	1.09
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	7	1.09
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	5	1.09
(1,168)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:ASP:N	9	1.09
(1,91)	1:39:A:SER:C	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:C	15	1.09
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	9	1.09
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	18	1.09
(1,22)	1:47:B:LEU:CA	1:47:B:LEU:CB	1:47:B:LEU:CG	1:47:B:LEU:CD1	8	1.09
(1,214)	1:44:B:ASP:N	1:44:B:ASP:CA	1:44:B:ASP:C	1:45:B:GLN:N	15	1.08
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	3	1.08
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	3	1.07
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	11	1.07
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	14	1.07
(1,255)	1:40:A:CYS:N	1:40:A:CYS:CA	1:40:A:CYS:CB	1:40:A:CYS:SG	5	1.07
(1,218)	1:49:B:LEU:N	1:49:B:LEU:CA	1:49:B:LEU:C	1:50:B:ASP:N	11	1.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	1:44:A:ASP:N	1:44:A:ASP:CA	1:44:A:ASP:C	1:45:A:GLN:N	20	1.07
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	2	1.07
(1,101)	1:45:A:GLN:C	1:46:A:ARG:N	1:46:A:ARG:CA	1:46:A:ARG:C	13	1.07
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	18	1.07
(1,62)	1:22:B:ASN:C	1:23:B:LEU:N	1:23:B:LEU:CA	1:23:B:LEU:C	8	1.07
(1,21)	1:47:A:LEU:CA	1:47:A:LEU:CB	1:47:A:LEU:CG	1:47:A:LEU:CD1	18	1.07
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	19	1.06
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	19	1.06
(1,102)	1:45:B:GLN:C	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	6	1.06
(1,92)	1:39:B:SER:C	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:C	10	1.06
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	20	1.06
(1,276)	1:59:B:LYS:N	1:59:B:LYS:CA	1:59:B:LYS:CB	1:59:B:LYS:CG	4	1.05
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	10	1.05
(1,265)	1:54:A:GLU:N	1:54:A:GLU:CA	1:54:A:GLU:CB	1:54:A:GLU:CG	5	1.05
(1,257)	1:41:A:LEU:N	1:41:A:LEU:CA	1:41:A:LEU:CB	1:41:A:LEU:CG	12	1.05
(1,256)	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:CB	1:40:B:CYS:SG	18	1.05
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	1	1.05
(1,145)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:LEU:N	20	1.05
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	2	1.05
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	20	1.05
(1,266)	1:54:B:GLU:N	1:54:B:GLU:CA	1:54:B:GLU:CB	1:54:B:GLU:CG	3	1.04
(1,250)	1:37:B:GLU:N	1:37:B:GLU:CA	1:37:B:GLU:CB	1:37:B:GLU:CG	6	1.04
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	17	1.04
(1,114)	1:54:B:GLU:C	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:C	5	1.04
(1,102)	1:45:B:GLN:C	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	11	1.04
(1,258)	1:41:B:LEU:N	1:41:B:LEU:CA	1:41:B:LEU:CB	1:41:B:LEU:CG	17	1.03
(1,256)	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:CB	1:40:B:CYS:SG	2	1.03
(1,227)	1:60:B:HIS:N	1:60:B:HIS:CA	1:60:B:HIS:C	1:61:B:PHE:N	10	1.03
(1,199)	1:26:B:GLY:N	1:26:B:GLY:CA	1:26:B:GLY:C	1:27:B:GLU:N	12	1.03
(1,195)	1:22:B:ASN:N	1:22:B:ASN:CA	1:22:B:ASN:C	1:23:B:LEU:N	3	1.03
(1,143)	1:20:A:TYR:N	1:20:A:TYR:CA	1:20:A:TYR:C	1:21:A:HIS:N	7	1.03
(1,113)	1:54:A:GLU:C	1:55:A:HIS:N	1:55:A:HIS:CA	1:55:A:HIS:C	16	1.03
(1,79)	1:33:A:PRO:C	1:34:A:ALA:N	1:34:A:ALA:CA	1:34:A:ALA:C	14	1.03
(1,54)	1:17:B:ALA:C	1:18:B:GLY:N	1:18:B:GLY:CA	1:18:B:GLY:C	12	1.03
(1,275)	1:59:A:LYS:N	1:59:A:LYS:CA	1:59:A:LYS:CB	1:59:A:LYS:CG	20	1.02
(1,256)	1:40:B:CYS:N	1:40:B:CYS:CA	1:40:B:CYS:CB	1:40:B:CYS:SG	4	1.02
(1,80)	1:33:B:PRO:C	1:34:B:ALA:N	1:34:B:ALA:CA	1:34:B:ALA:C	17	1.02
(1,145)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:LEU:N	8	1.01
(1,114)	1:54:B:GLU:C	1:55:B:HIS:N	1:55:B:HIS:CA	1:55:B:HIS:C	16	1.01
(1,145)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:LEU:N	14	1.0