Full wwPDB NMR Structure Validation Report (i)

Jan 29, 2024 – 02:09 PM JST

PDB ID	:	8K6Z
BMRB ID	:	36585
Title	:	NMR structure of human leptin
Authors	:	Fan, X.; Qin, R.; Yuan, W.; Fan, J.; Huang, W.; Lin, Z.
Deposited on	:	2023-07-26

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 (i) 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 (i)) were used in the production of this report:

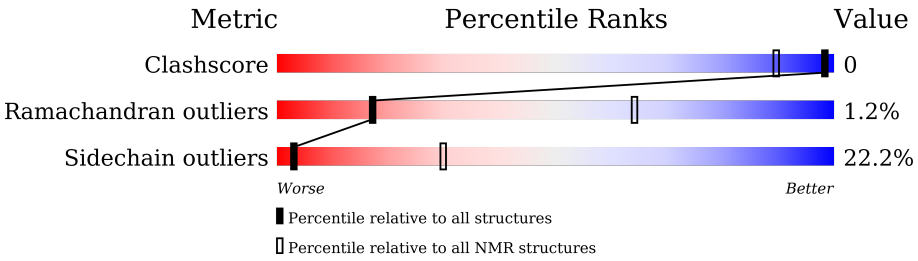
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	146	77% 12% • 10%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:26, A:40-A:146 (132)	0.55	8

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 1 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2276 atoms, of which 1153 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Leptin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	146	2276	709	1153	190	219	5	0

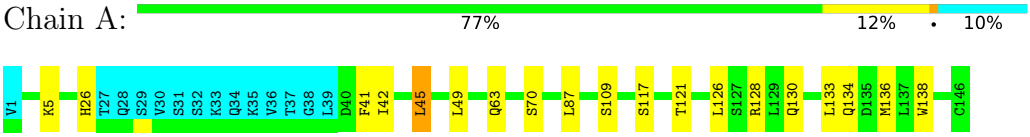
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Leptin

Chain A:



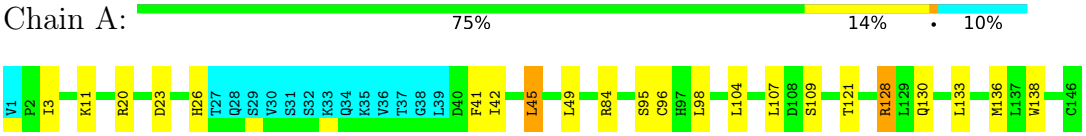
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Leptin

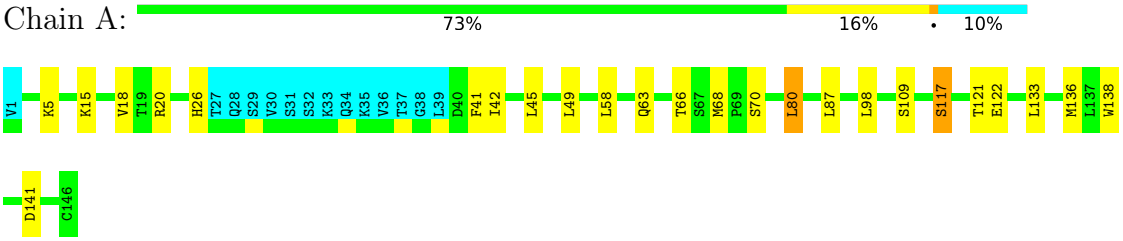
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Leptin

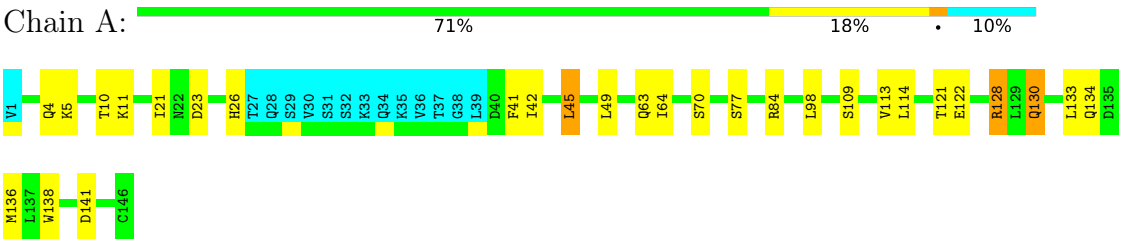
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Leptin

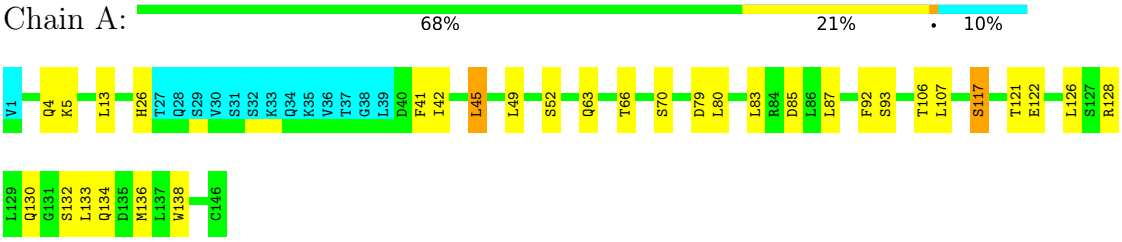
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Leptin

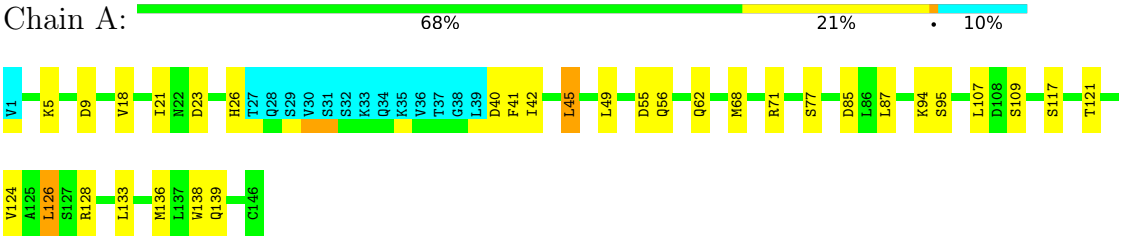
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Leptin

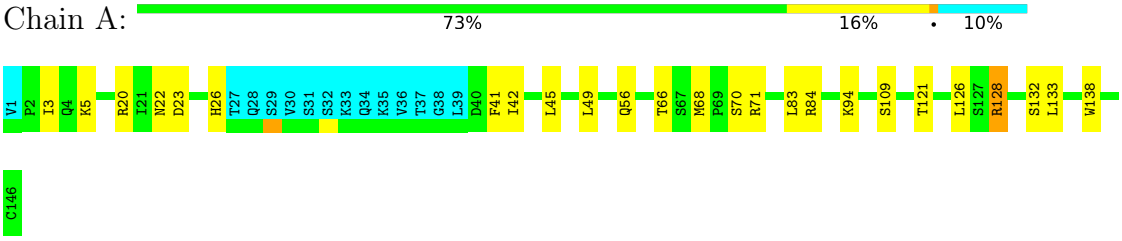
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Leptin

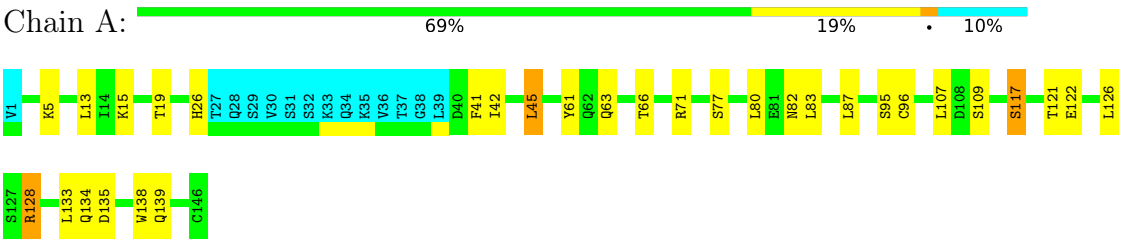
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Leptin

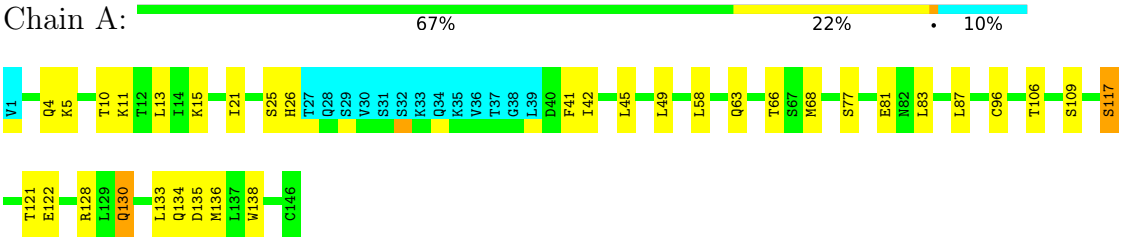
Chain A:



4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: Leptin

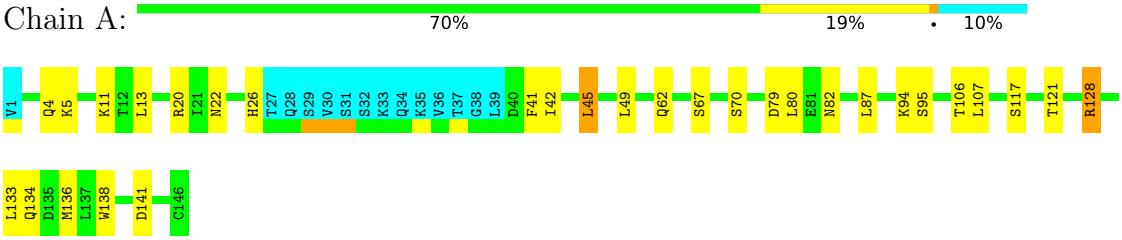
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Leptin

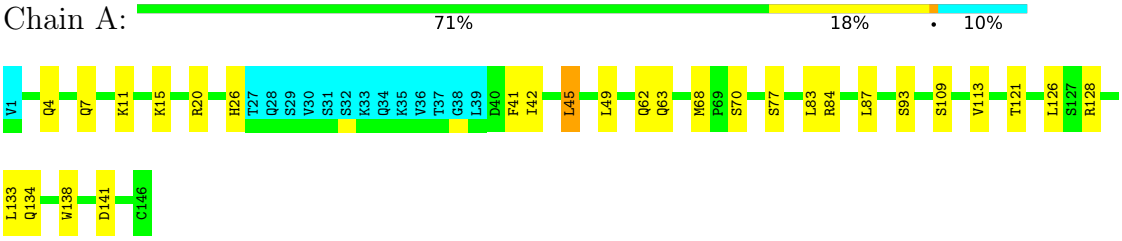
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Leptin

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

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

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

Software name	Classification	Version
CNS	structure calculation	
Amber	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	1768
Number of shifts mapped to atoms	1747
Number of unparsed shifts	0
Number of shifts with mapping errors	21
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.62±0.02	0±0/1039 (0.0± 0.0%)	0.97±0.03	2±1/1413 (0.1± 0.1%)
All	All	0.62	0/10390 (0.0%)	0.97	18/14130 (0.1%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	128	ARG	NE-CZ-NH1	7.47	124.03	120.30	6	9
1	A	84	ARG	NE-CZ-NH1	6.56	123.58	120.30	10	4
1	A	61	TYR	CB-CG-CD1	-5.56	117.67	121.00	7	1
1	A	20	ARG	NE-CZ-NH1	5.34	122.97	120.30	1	2
1	A	84	ARG	NE-CZ-NH2	-5.27	117.67	120.30	3	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1022	1041	1041	0±1
All	All	10220	10410	10410	5

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:HG23	1:A:126:LEU:HD22	0.50	1.82	5	1
1:A:21:ILE:HG21	1:A:130:GLN:HB2	0.43	1.91	8	2
1:A:58:LEU:HD22	1:A:80:LEU:HD11	0.43	1.89	2	1
1:A:64:ILE:HD13	1:A:114:LEU:HD12	0.42	1.90	3	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/146 (90%)	120±1 (92±1%)	9±1 (7±1%)	2±1 (1±1%)	17	64
All	All	1310/1460 (90%)	1203 (92%)	91 (7%)	16 (1%)	17	64

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	45	LEU	7
1	A	117	SER	4
1	A	130	GLN	3
1	A	40	ASP	1
1	A	124	VAL	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/133 (90%)	93±3 (78±3%)	27±3 (22±3%)	3	30
All	All	1200/1330 (90%)	934 (78%)	266 (22%)	3	30

All 64 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	26	HIS	10
1	A	41	PHE	10
1	A	42	ILE	10
1	A	45	LEU	10
1	A	121	THR	10
1	A	133	LEU	10
1	A	138	TRP	10
1	A	49	LEU	9
1	A	109	SER	8
1	A	5	LYS	8
1	A	136	MET	7
1	A	87	LEU	7
1	A	63	GLN	6
1	A	70	SER	6
1	A	117	SER	6
1	A	134	GLN	6
1	A	11	LYS	5
1	A	107	LEU	5
1	A	128	ARG	5
1	A	66	THR	5
1	A	68	MET	5
1	A	122	GLU	5
1	A	4	GLN	5
1	A	77	SER	5
1	A	83	LEU	5
1	A	126	LEU	5
1	A	23	ASP	4
1	A	95	SER	4
1	A	15	LYS	4
1	A	80	LEU	4
1	A	141	ASP	4
1	A	13	LEU	4
1	A	96	CYS	3
1	A	98	LEU	3
1	A	20	ARG	3
1	A	106	THR	3
1	A	62	GLN	3
1	A	71	ARG	3
1	A	94	LYS	3
1	A	3	ILE	2
1	A	18	VAL	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	10	THR	2
1	A	113	VAL	2
1	A	79	ASP	2
1	A	85	ASP	2
1	A	93	SER	2
1	A	132	SER	2
1	A	56	GLN	2
1	A	139	GLN	2
1	A	22	ASN	2
1	A	82	ASN	2
1	A	135	ASP	2
1	A	104	LEU	1
1	A	130	GLN	1
1	A	52	SER	1
1	A	92	PHE	1
1	A	9	ASP	1
1	A	55	ASP	1
1	A	19	THR	1
1	A	25	SER	1
1	A	58	LEU	1
1	A	81	GLU	1
1	A	67	SER	1
1	A	7	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

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

Total number of shifts	1768
Number of shifts mapped to atoms	1747
Number of unparsed shifts	0
Number of shifts with mapping errors	21
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 21 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	GLY	H	8.522	0.02	1
1	A	147	GLY	HA2	3.847	0.02	2
1	A	147	GLY	HA3	4.139	0.02	2
1	A	147	GLY	CA	44.895	0.3	1
1	A	147	GLY	N	106.278	0.2	1
1	A	148	GLY	H	8.092	0.02	1
1	A	148	GLY	HA2	3.882	0.02	2
1	A	148	GLY	CA	44.89	0.3	1
1	A	148	GLY	N	108.232	0.2	1
1	A	149	LYS	H	8.229	0.02	1
1	A	149	LYS	HA	4.234	0.02	1
1	A	149	LYS	HB2	1.664	0.02	2
1	A	149	LYS	HD2	1.342	0.02	2
1	A	149	LYS	HE2	2.905	0.02	2

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	149	LYS	HG2	1.62	0.02	2
1	A	149	LYS	CA	56.168	0.3	1
1	A	149	LYS	CB	33.4	0.3	1
1	A	149	LYS	CD	24.788	0.3	1
1	A	149	LYS	CE	42.276	0.3	1
1	A	149	LYS	CG	28.764	0.3	1
1	A	149	LYS	N	120.967	0.2	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	149	-0.58 ± 0.06	Should be checked
$^{13}C_{\beta}$	139	0.27 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	143	-0.00 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1584 atoms were assigned a chemical shift out of a possible 1800. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	523/655 (80%)	265/265 (100%)	132/264 (50%)	126/126 (100%)
Sidechain	987/1055 (94%)	671/694 (97%)	301/331 (91%)	15/30 (50%)
Aromatic	74/90 (82%)	37/46 (80%)	35/38 (92%)	2/6 (33%)
Overall	1584/1800 (88%)	973/1005 (97%)	468/633 (74%)	143/162 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1746 atoms were assigned a chemical shift out of a possible 1981. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	579/726 (80%)	293/294 (100%)	146/292 (50%)	140/140 (100%)
Sidechain	1093/1165 (94%)	743/766 (97%)	333/365 (91%)	17/34 (50%)
Aromatic	74/90 (82%)	37/46 (80%)	35/38 (92%)	2/6 (33%)
Overall	1746/1981 (88%)	1073/1106 (97%)	514/695 (74%)	159/180 (88%)

7.1.4 Statistically unusual chemical shifts (i)

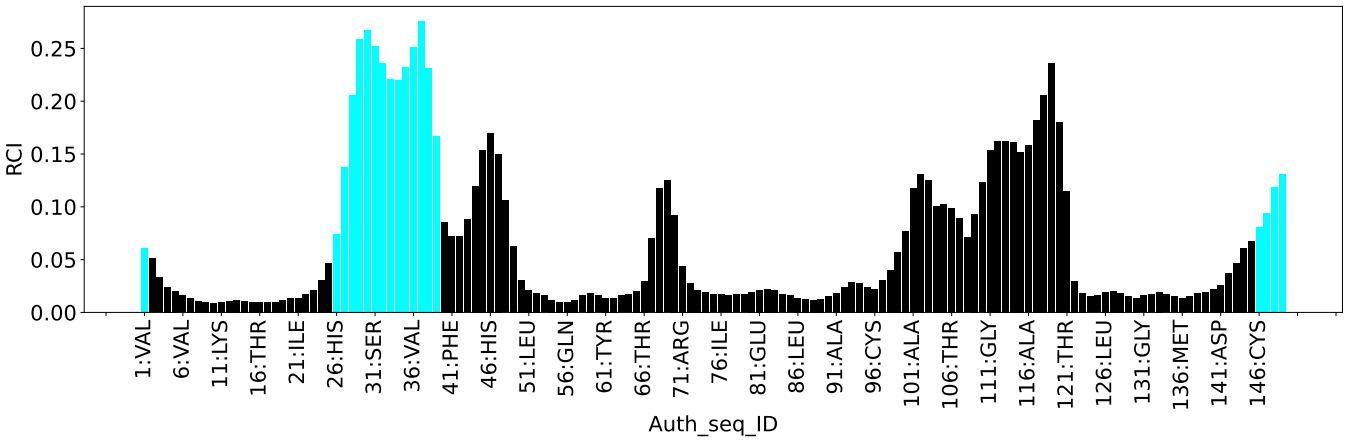
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	78	ASN	CG	2.83	164.52 – 188.90	-71.3

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	7121
Intra-residue (|i-j|=0)	2978
Sequential (|i-j|=1)	1508
Medium range (|i-j|>1 and |i-j|<5)	1487
Long range (|i-j|≥5)	1147
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	1
Total dihedral-angle restraints	219
Number of unmapped restraints	10
Number of restraints per residue	50.3
Number of long range restraints per residue[1]	7.9

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	42.7	0.2
0.2-0.5 (Medium)	56.3	0.5
>0.5 (Large)	10.3	1.96

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)	46.3	9.94
10.0-20.0 (Medium)	4.6	19.92
>20.0 (Large)	0.2	21.74

9 Distance violation analysis (i)

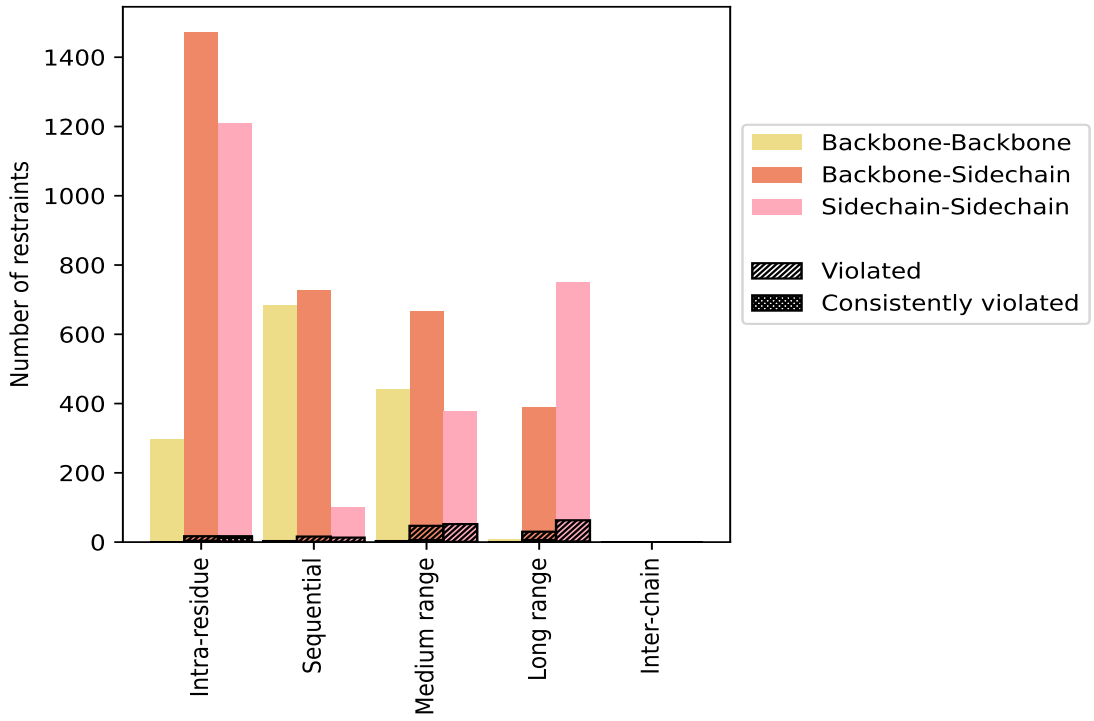
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	2978	41.8	34	1.1	0.5	17	0.6	0.2
Backbone-Backbone	296	4.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1472	20.7	17	1.2	0.2	4	0.3	0.1
Sidechain-Sidechain	1210	17.0	17	1.4	0.2	13	1.1	0.2
Sequential (|i-j|=1)	1508	21.2	32	2.1	0.4	2	0.1	0.0
Backbone-Backbone	682	9.6	3	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	726	10.2	16	2.2	0.2	1	0.1	0.0
Sidechain-Sidechain	100	1.4	13	13.0	0.2	1	1.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1487	20.9	102	6.9	1.4	7	0.5	0.1
Backbone-Backbone	442	6.2	3	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	667	9.4	47	7.0	0.7	6	0.9	0.1
Sidechain-Sidechain	378	5.3	52	13.8	0.7	1	0.3	0.0
Long range (|i-j|≥5)	1147	16.1	93	8.1	1.3	8	0.7	0.1
Backbone-Backbone	8	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	390	5.5	30	7.7	0.4	6	1.5	0.1
Sidechain-Sidechain	749	10.5	63	8.4	0.9	2	0.3	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	1	0.0	0	0.0	0.0	0	0.0	0.0
Total	7121	100.0	261	3.7	3.7	34	0.5	0.5
Backbone-Backbone	1428	20.1	6	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	3255	45.7	110	3.4	1.5	17	0.5	0.2
Sidechain-Sidechain	2438	34.2	145	5.9	2.0	17	0.7	0.2

[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



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

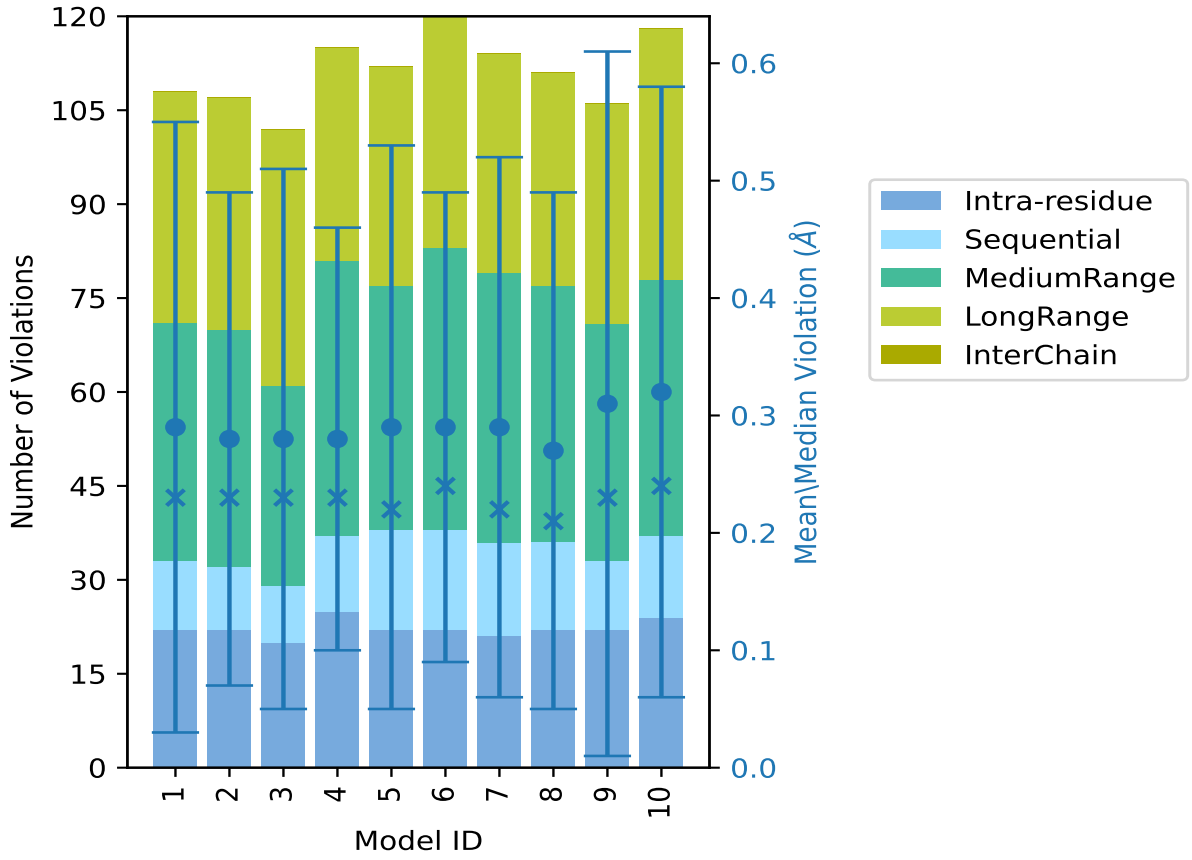
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	22	11	38	37	0	108	0.29	1.96	0.26	0.23
2	22	10	38	37	0	107	0.28	1.51	0.21	0.23
3	20	9	32	41	0	102	0.28	1.49	0.23	0.23
4	25	12	44	34	0	115	0.28	1.58	0.18	0.23
5	22	16	39	35	0	112	0.29	1.59	0.24	0.22
6	22	16	45	37	0	120	0.29	1.45	0.2	0.24
7	21	15	43	35	0	114	0.29	1.55	0.23	0.22
8	22	14	41	34	0	111	0.27	1.44	0.22	0.21
9	22	11	38	35	0	106	0.31	1.69	0.3	0.23
10	24	13	41	40	0	118	0.32	1.56	0.26	0.24

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

[5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6859(IR:2944, SQ:1476, MR:1385, LR:1054, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
3	9	25	31	0	68	1	10.0
6	4	24	13	0	47	2	20.0
3	3	9	13	0	28	3	30.0
1	3	7	3	0	14	4	40.0

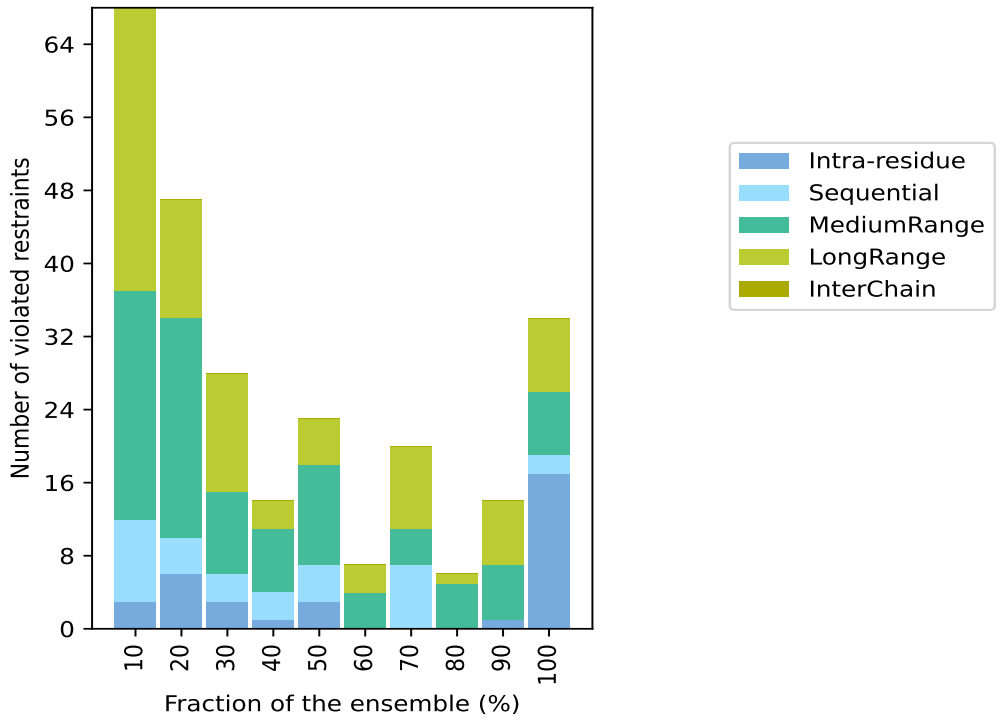
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
3	4	11	5	0	23	5	50.0
0	0	4	3	0	7	6	60.0
0	7	4	9	0	20	7	70.0
0	0	5	1	0	6	8	80.0
1	0	6	7	0	14	9	90.0
17	2	7	8	0	34	10	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

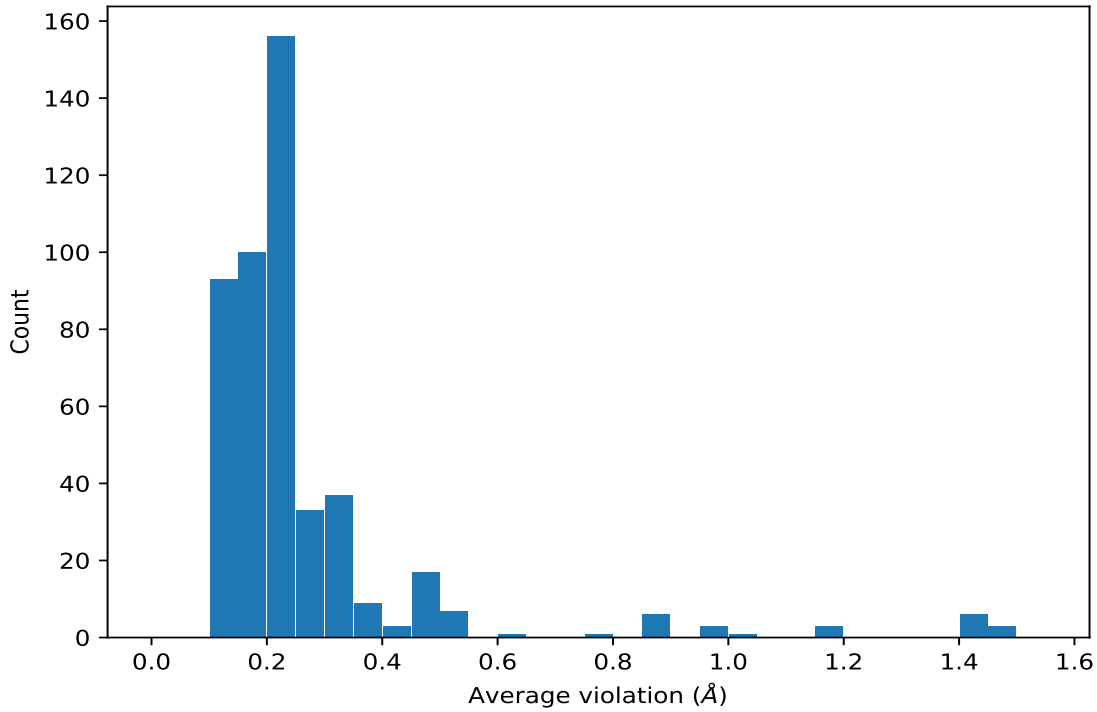
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	10	1.17	0.47	1.12
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	10	1.17	0.47	1.12
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	10	1.17	0.47	1.12
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	10	0.98	0.47	0.86
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	10	0.75	0.16	0.69
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	10	0.63	0.21	0.67
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	10	0.54	0.1	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	10	0.54	0.1	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	10	0.54	0.1	0.54
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	10	0.5	0.09	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	10	0.5	0.09	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	10	0.5	0.09	0.5
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	10	0.47	0.06	0.45
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	10	0.46	0.13	0.48
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	10	0.45	0.1	0.45
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	10	0.45	0.1	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	10	0.45	0.1	0.45
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	10	0.44	0.06	0.43
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	10	0.37	0.1	0.36
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	10	0.33	0.17	0.28
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	10	0.33	0.05	0.32
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	10	0.32	0.03	0.31
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	10	0.27	0.12	0.26
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	10	0.27	0.06	0.27
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	10	0.25	0.06	0.26
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	10	0.25	0.06	0.26
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	10	0.25	0.06	0.26
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	10	0.25	0.05	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	10	0.24	0.01	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	10	0.24	0.01	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	10	0.24	0.01	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	10	0.24	0.01	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	10	0.24	0.01	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	10	0.24	0.01	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	10	0.24	0.01	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	10	0.24	0.01	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	10	0.24	0.01	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	10	0.24	0.01	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	10	0.23	0.0	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	10	0.23	0.0	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	10	0.23	0.01	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	10	0.23	0.01	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	10	0.23	0.01	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	10	0.23	0.01	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	10	0.23	0.01	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	10	0.23	0.01	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	10	0.23	0.03	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	10	0.23	0.0	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	10	0.23	0.0	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	10	0.22	0.0	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	10	0.22	0.0	0.22
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	10	0.21	0.0	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	10	0.21	0.0	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	10	0.21	0.0	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	10	0.21	0.0	0.21
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	10	0.2	0.02	0.2
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	10	0.2	0.02	0.2
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	10	0.17	0.03	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	9	0.48	0.13	0.53
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	9	0.48	0.13	0.53
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	9	0.48	0.13	0.53
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	9	0.38	0.08	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	9	0.38	0.08	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	9	0.38	0.08	0.41
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	9	0.34	0.1	0.36
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	9	0.34	0.1	0.36
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	9	0.34	0.1	0.36
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	9	0.31	0.06	0.32
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	9	0.31	0.06	0.32
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	9	0.27	0.03	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	9	0.27	0.03	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	9	0.27	0.03	0.27
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	9	0.25	0.1	0.22
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	9	0.22	0.07	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	9	0.22	0.07	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	9	0.22	0.07	0.27
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	9	0.2	0.06	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	9	0.2	0.06	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	9	0.2	0.06	0.18
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	9	0.2	0.06	0.19
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	9	0.19	0.02	0.19
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	9	0.19	0.02	0.19
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	9	0.19	0.02	0.19
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	9	0.18	0.04	0.18
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	9	0.16	0.04	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.14	0.02	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.14	0.02	0.14
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	8	0.3	0.06	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	8	0.3	0.06	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	8	0.3	0.06	0.3
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	8	0.27	0.07	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	8	0.27	0.07	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	8	0.27	0.07	0.28
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	8	0.22	0.04	0.21
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	8	0.22	0.04	0.21
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	8	0.22	0.04	0.21
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	8	0.21	0.08	0.18
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	8	0.21	0.08	0.18
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	8	0.21	0.08	0.18
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	8	0.2	0.05	0.2
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	8	0.2	0.05	0.2
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	8	0.2	0.05	0.2
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	8	0.2	0.05	0.2
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	8	0.2	0.05	0.2
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	8	0.2	0.05	0.2
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	7	0.5	0.12	0.48
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	7	0.35	0.1	0.33
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	7	0.33	0.13	0.32
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	7	0.33	0.13	0.32
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	7	0.33	0.13	0.32
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	7	0.31	0.04	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	7	0.31	0.04	0.29
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	7	0.25	0.08	0.25
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	7	0.24	0.05	0.22
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	7	0.24	0.05	0.22
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	7	0.24	0.05	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	7	0.24	0.05	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	7	0.24	0.05	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	7	0.24	0.05	0.22
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	7	0.23	0.09	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	7	0.23	0.09	0.2
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	7	0.22	0.07	0.24
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	7	0.21	0.07	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	7	0.21	0.07	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	7	0.21	0.07	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	7	0.21	0.06	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	7	0.21	0.06	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	7	0.21	0.06	0.2
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	7	0.2	0.11	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	7	0.2	0.11	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	7	0.2	0.11	0.14
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	7	0.19	0.03	0.2
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	7	0.19	0.04	0.19
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	7	0.18	0.03	0.18
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	7	0.18	0.03	0.18
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	7	0.18	0.03	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	7	0.18	0.02	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	7	0.18	0.02	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	7	0.18	0.02	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	7	0.16	0.03	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	7	0.16	0.03	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	7	0.16	0.03	0.16
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	7	0.14	0.01	0.14
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	7	0.14	0.01	0.14
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	6	1.03	0.62	1.43
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	6	0.35	0.07	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	6	0.35	0.07	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	6	0.35	0.07	0.36
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	6	0.32	0.09	0.29
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	6	0.32	0.09	0.29
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	6	0.32	0.09	0.29
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	6	0.19	0.04	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	6	0.19	0.04	0.18
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	6	0.18	0.06	0.16
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	6	0.18	0.06	0.16
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	6	0.18	0.06	0.16
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	6	0.18	0.05	0.16
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	6	0.18	0.05	0.16
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	6	0.18	0.05	0.16
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	6	0.16	0.02	0.16
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	6	0.16	0.02	0.16
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	6	0.16	0.02	0.16
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	5	1.48	0.09	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	5	1.48	0.09	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	5	1.48	0.09	1.51
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	5	0.88	0.22	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	5	0.88	0.22	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	5	0.88	0.22	0.8
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	5	0.44	0.18	0.45
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	5	0.42	0.1	0.43
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	5	0.37	0.34	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	5	0.37	0.34	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	5	0.37	0.34	0.19
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	5	0.35	0.15	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	5	0.35	0.15	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	5	0.35	0.15	0.39
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	5	0.34	0.06	0.34
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	5	0.33	0.04	0.34
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	5	0.24	0.16	0.15
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	5	0.23	0.03	0.24
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	5	0.22	0.07	0.2
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	5	0.22	0.07	0.2
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	5	0.22	0.07	0.2
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	5	0.22	0.05	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	5	0.21	0.1	0.17
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	5	0.21	0.1	0.17
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	5	0.21	0.1	0.17
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	5	0.19	0.05	0.18
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	5	0.19	0.06	0.19
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	5	0.19	0.05	0.17
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	5	0.19	0.05	0.17
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	5	0.19	0.05	0.17
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	5	0.18	0.09	0.16
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	5	0.17	0.06	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	5	0.15	0.03	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	5	0.15	0.03	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	5	0.15	0.03	0.15
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	5	0.15	0.05	0.15
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	5	0.15	0.04	0.15
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	5	0.14	0.05	0.12
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	5	0.14	0.05	0.12
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	5	0.14	0.05	0.12
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	5	0.12	0.01	0.12
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	4	0.32	0.12	0.34
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	4	0.32	0.12	0.34
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	4	0.29	0.05	0.31
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	4	0.29	0.05	0.31
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	4	0.29	0.05	0.31
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	4	0.22	0.09	0.22
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	4	0.22	0.05	0.2
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	4	0.22	0.05	0.2
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	4	0.22	0.05	0.2
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	4	0.22	0.05	0.2
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	4	0.19	0.1	0.15
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	4	0.19	0.05	0.17
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	4	0.17	0.04	0.18
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	4	0.17	0.04	0.18
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	4	0.17	0.04	0.18
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	4	0.16	0.06	0.14
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	4	0.16	0.06	0.14
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	4	0.16	0.06	0.14
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	4	0.16	0.05	0.15
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	4	0.16	0.05	0.15
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	4	0.16	0.05	0.15
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	4	0.15	0.04	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	4	0.15	0.04	0.15
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	4	0.15	0.04	0.15
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	4	0.15	0.03	0.15
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	4	0.15	0.03	0.14
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	4	0.15	0.03	0.14
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	3	0.48	0.27	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	3	0.48	0.27	0.55
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	3	0.36	0.1	0.32
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	3	0.34	0.01	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	3	0.34	0.01	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	3	0.34	0.01	0.35
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	3	0.34	0.15	0.42
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	3	0.32	0.02	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	3	0.32	0.02	0.33
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	3	0.26	0.04	0.24
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	3	0.26	0.04	0.24
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	3	0.26	0.04	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	3	0.23	0.03	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	3	0.23	0.03	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	3	0.23	0.03	0.24
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	3	0.23	0.03	0.24
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	3	0.23	0.03	0.24
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	3	0.23	0.03	0.24
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	3	0.23	0.03	0.22
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	3	0.21	0.01	0.21
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	3	0.21	0.07	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	3	0.21	0.07	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	3	0.21	0.07	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	3	0.21	0.07	0.26
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	3	0.2	0.05	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	3	0.2	0.05	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	3	0.2	0.05	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	3	0.2	0.04	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	3	0.2	0.04	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	3	0.2	0.04	0.17
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	3	0.2	0.09	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	3	0.2	0.09	0.14
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	3	0.2	0.03	0.19
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	3	0.2	0.03	0.19
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	3	0.2	0.03	0.19
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	3	0.19	0.05	0.17
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	3	0.17	0.05	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	3	0.17	0.05	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	3	0.17	0.05	0.18
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	3	0.17	0.05	0.18
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	3	0.17	0.05	0.18
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	3	0.17	0.05	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	3	0.17	0.02	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	3	0.17	0.02	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	3	0.17	0.02	0.18
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	3	0.17	0.05	0.14
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	3	0.17	0.05	0.14
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	3	0.16	0.02	0.15
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	3	0.15	0.03	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	3	0.15	0.03	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	3	0.15	0.03	0.13
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	3	0.15	0.03	0.13
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	3	0.15	0.03	0.13
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	3	0.15	0.03	0.13
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	3	0.14	0.0	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	3	0.14	0.0	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	3	0.14	0.0	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	3	0.13	0.01	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	3	0.13	0.01	0.13
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	3	0.12	0.01	0.11
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	3	0.12	0.02	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	3	0.12	0.02	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	3	0.12	0.02	0.12
(2,3461)	1:142:A:LEU:HD11	1:139:A:GLN:HE21	2	1.45	0.11	1.45
(2,3461)	1:142:A:LEU:HD12	1:139:A:GLN:HE21	2	1.45	0.11	1.45
(2,3461)	1:142:A:LEU:HD13	1:139:A:GLN:HE21	2	1.45	0.11	1.45
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD11	2	1.45	0.11	1.45
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD12	2	1.45	0.11	1.45
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD13	2	1.45	0.11	1.45
(2,3347)	1:135:A:ASP:HB2	1:139:A:GLN:HE21	2	0.96	0.56	0.96
(2,3348)	1:139:A:GLN:HE21	1:135:A:ASP:HB2	2	0.96	0.56	0.96
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD11	2	0.86	0.07	0.86
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD12	2	0.86	0.07	0.86
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD13	2	0.86	0.07	0.86
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG21	2	0.47	0.28	0.47
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG22	2	0.47	0.28	0.47
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG23	2	0.47	0.28	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,325)	1:12:A:THR:H	1:11:A:LYS:HE2	2	0.36	0.11	0.36
(2,2414)	1:105:A:GLU:H	1:56:A:GLN:HE22	2	0.26	0.11	0.26
(2,2415)	1:56:A:GLN:HE22	1:105:A:GLU:H	2	0.26	0.11	0.26
(2,2765)	1:120:A:SER:H	1:124:A:VAL:HB	2	0.26	0.06	0.26
(2,203)	1:7:A:GLN:HE21	1:7:A:GLN:HA	2	0.26	0.08	0.26
(2,1143)	1:49:A:LEU:HD21	1:53:A:LYS:HE2	2	0.25	0.01	0.25
(2,1143)	1:49:A:LEU:HD22	1:53:A:LYS:HE2	2	0.25	0.01	0.25
(2,1143)	1:49:A:LEU:HD23	1:53:A:LYS:HE2	2	0.25	0.01	0.25
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD21	2	0.25	0.01	0.25
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD22	2	0.25	0.01	0.25
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD23	2	0.25	0.01	0.25
(2,755)	1:30:A:VAL:HB	1:32:A:SER:HB2	2	0.24	0.1	0.24
(2,3173)	1:136:A:MET:HE1	1:57:A:THR:HA	2	0.24	0.05	0.24
(2,3173)	1:136:A:MET:HE2	1:57:A:THR:HA	2	0.24	0.05	0.24
(2,3173)	1:136:A:MET:HE3	1:57:A:THR:HA	2	0.24	0.05	0.24
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG21	2	0.22	0.06	0.22
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG22	2	0.22	0.06	0.22
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG23	2	0.22	0.06	0.22
(2,141)	1:5:A:LYS:H	1:5:A:LYS:HE2	2	0.22	0.08	0.22
(2,3058)	1:132:A:SER:H	1:130:A:GLN:HG3	2	0.21	0.05	0.21
(2,989)	1:45:A:LEU:H	1:42:A:ILE:HB	2	0.2	0.0	0.2
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD21	2	0.2	0.02	0.2
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD22	2	0.2	0.02	0.2
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD23	2	0.2	0.02	0.2
(2,1656)	1:73:A:VAL:H	1:71:A:ARG:HB2	2	0.19	0.05	0.19
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD21	2	0.18	0.04	0.18
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD22	2	0.18	0.04	0.18
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD23	2	0.18	0.04	0.18
(2,730)	1:29:A:SER:H	1:27:A:THR:HG21	2	0.18	0.02	0.18
(2,730)	1:29:A:SER:H	1:27:A:THR:HG22	2	0.18	0.02	0.18
(2,730)	1:29:A:SER:H	1:27:A:THR:HG23	2	0.18	0.02	0.18
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG21	2	0.18	0.02	0.18
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG22	2	0.18	0.02	0.18
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG23	2	0.18	0.02	0.18
(2,1175)	1:53:A:LYS:H	1:53:A:LYS:HE2	2	0.18	0.0	0.18
(2,3234)	1:137:A:LEU:HD21	1:11:A:LYS:HE2	2	0.17	0.05	0.17
(2,3234)	1:137:A:LEU:HD22	1:11:A:LYS:HE2	2	0.17	0.05	0.17
(2,3234)	1:137:A:LEU:HD23	1:11:A:LYS:HE2	2	0.17	0.05	0.17
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD21	2	0.17	0.05	0.17
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD22	2	0.17	0.05	0.17
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD23	2	0.17	0.05	0.17
(2,2616)	1:117:A:SER:HB2	1:117:A:SER:HA	2	0.16	0.02	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,1567)	1:68:A:MET:HG2	1:69:A:PRO:HD2	2	0.16	0.01	0.16
(2,2696)	1:68:A:MET:HE1	1:122:A:GLU:HG2	2	0.16	0.04	0.16
(2,2696)	1:68:A:MET:HE2	1:122:A:GLU:HG2	2	0.16	0.04	0.16
(2,2696)	1:68:A:MET:HE3	1:122:A:GLU:HG2	2	0.16	0.04	0.16
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE1	2	0.16	0.04	0.16
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE2	2	0.16	0.04	0.16
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE3	2	0.16	0.04	0.16
(2,589)	1:24:A:ILE:HD11	1:21:A:ILE:HA	2	0.16	0.02	0.16
(2,589)	1:24:A:ILE:HD12	1:21:A:ILE:HA	2	0.16	0.02	0.16
(2,589)	1:24:A:ILE:HD13	1:21:A:ILE:HA	2	0.16	0.02	0.16
(2,2693)	1:68:A:MET:HE1	1:122:A:GLU:HB3	2	0.16	0.05	0.16
(2,2693)	1:68:A:MET:HE2	1:122:A:GLU:HB3	2	0.16	0.05	0.16
(2,2693)	1:68:A:MET:HE3	1:122:A:GLU:HB3	2	0.16	0.05	0.16
(2,293)	1:11:A:LYS:HE2	1:11:A:LYS:HA	2	0.15	0.01	0.15
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD21	2	0.15	0.01	0.15
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD22	2	0.15	0.01	0.15
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD23	2	0.15	0.01	0.15
(2,1030)	1:46:A:HIS:HD2	1:47:A:PRO:HD3	2	0.15	0.04	0.15
(2,832)	1:37:A:THR:H	1:35:A:LYS:HD2	2	0.15	0.04	0.15
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG21	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG22	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG23	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG21	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG22	2	0.14	0.04	0.14
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG23	2	0.14	0.04	0.14
(2,2817)	1:76:A:ILE:HD11	1:126:A:LEU:HA	2	0.14	0.01	0.14
(2,2817)	1:76:A:ILE:HD12	1:126:A:LEU:HA	2	0.14	0.01	0.14
(2,2817)	1:76:A:ILE:HD13	1:126:A:LEU:HA	2	0.14	0.01	0.14
(2,3122)	1:134:A:GLN:HE21	1:134:A:GLN:HA	2	0.14	0.01	0.14
(2,655)	1:26:A:HIS:HD2	1:23:A:ASP:HA	2	0.13	0.02	0.13
(2,1014)	1:46:A:HIS:HD2	1:45:A:LEU:HB2	2	0.12	0.02	0.12
(2,1011)	1:46:A:HIS:HD2	1:42:A:ILE:HG13	2	0.12	0.02	0.12
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD21	2	0.12	0.02	0.12
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD22	2	0.12	0.02	0.12
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD23	2	0.12	0.02	0.12
(2,2395)	1:104:A:LEU:HD21	1:63:A:GLN:HE21	2	0.12	0.0	0.12
(2,2395)	1:104:A:LEU:HD22	1:63:A:GLN:HE21	2	0.12	0.0	0.12
(2,2395)	1:104:A:LEU:HD23	1:63:A:GLN:HE21	2	0.12	0.0	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD21	2	0.12	0.0	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD22	2	0.12	0.0	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD23	2	0.12	0.0	0.12
(2,2626)	1:119:A:TYR:HE1	1:38:A:GLY:HA2	2	0.12	0.0	0.12

Continued on next page...

Continued from previous page...

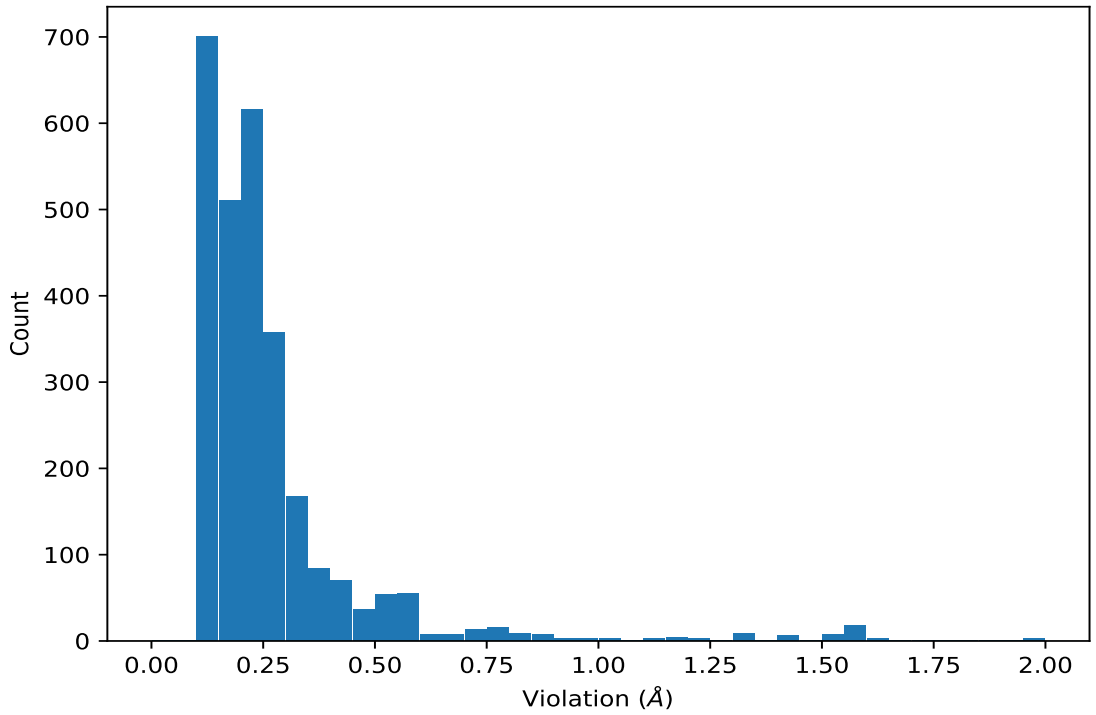
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2626)	1:119:A:TYR:HE2	1:38:A:GLY:HA2	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

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)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	1	1.96
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	1	1.96
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	1	1.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	9	1.69
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	9	1.63
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	9	1.63
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	9	1.63
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	5	1.59
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	5	1.59
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	5	1.59
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	4	1.58
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	4	1.58
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	4	1.58
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD11	10	1.56
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD12	10	1.56
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD13	10	1.56
(2,3461)	1:142:A:LEU:HD11	1:139:A:GLN:HE21	10	1.56
(2,3461)	1:142:A:LEU:HD12	1:139:A:GLN:HE21	10	1.56
(2,3461)	1:142:A:LEU:HD13	1:139:A:GLN:HE21	10	1.56
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	10	1.56
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	10	1.56
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	10	1.56
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	7	1.55
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	7	1.55
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	7	1.55
(2,3348)	1:139:A:GLN:HE21	1:135:A:ASP:HB2	9	1.52
(2,3347)	1:135:A:ASP:HB2	1:139:A:GLN:HE21	9	1.52
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	5	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	2	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	2	1.51
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	2	1.51
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	1	1.5
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	3	1.49
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	6	1.45
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	8	1.44
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	8	1.42
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	8	1.42
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	8	1.42
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	2	1.41
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	1	1.4
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD11	7	1.34
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD12	7	1.34
(2,3462)	1:139:A:GLN:HE21	1:142:A:LEU:HD13	7	1.34
(2,3461)	1:142:A:LEU:HD11	1:139:A:GLN:HE21	7	1.34
(2,3461)	1:142:A:LEU:HD12	1:139:A:GLN:HE21	7	1.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3461)	1:142:A:LEU:HD13	1:139:A:GLN:HE21	7	1.34
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB1	6	1.33
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB2	6	1.33
(2,1376)	1:63:A:GLN:HE21	1:59:A:ALA:HB3	6	1.33
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	3	1.24
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	3	1.24
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	3	1.24
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	3	1.18
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	3	1.18
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	3	1.18
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	5	1.16
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	5	1.1
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	5	1.1
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	5	1.1
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	10	1.06
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	9	1.04
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	9	1.04
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	9	1.04
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	8	0.99
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	8	0.99
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	8	0.99
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD11	3	0.94
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD12	3	0.94
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD13	3	0.94
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	8	0.88
(2,3337)	1:139:A:GLN:HE21	1:48:A:ILE:HD11	7	0.87
(2,3337)	1:139:A:GLN:HE21	1:48:A:ILE:HD12	7	0.87
(2,3337)	1:139:A:GLN:HE21	1:48:A:ILE:HD13	7	0.87
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	7	0.87
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	10	0.87
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	6	0.87
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	2	0.85
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	4	0.82
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	4	0.82
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	4	0.82
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	3	0.81
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	4	0.81
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	10	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	10	0.8
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	10	0.8
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD11	10	0.79
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD12	10	0.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2816)	1:28:A:GLN:HE22	1:126:A:LEU:HD13	10	0.79
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	10	0.77
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	10	0.77
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	6	0.75
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	6	0.75
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	6	0.75
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	8	0.75
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG21	1	0.75
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG22	1	0.75
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG23	1	0.75
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	2	0.74
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	2	0.74
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	2	0.74
(2,3389)	1:140:A:LEU:HD21	1:11:A:LYS:HE2	9	0.73
(2,3389)	1:140:A:LEU:HD22	1:11:A:LYS:HE2	9	0.73
(2,3389)	1:140:A:LEU:HD23	1:11:A:LYS:HE2	9	0.73
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	9	0.72
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	1	0.71
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	1	0.71
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	1	0.71
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	8	0.71
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	8	0.71
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	8	0.71
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	4	0.7
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	6	0.69
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	2	0.68
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	3	0.68
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	10	0.65
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	10	0.65
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	10	0.65
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	4	0.65
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	1	0.64
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	7	0.64
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	4	0.62
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	5	0.62
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	5	0.62
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	5	0.62
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	8	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	9	0.61
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	6	0.6
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	6	0.6
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	6	0.6
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	7	0.6
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	7	0.6
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	7	0.6
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD21	9	0.6
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD22	9	0.6
(2,2437)	1:63:A:GLN:HE21	1:107:A:LEU:HD23	9	0.6
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	2	0.6
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	2	0.6
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	2	0.6
(2,1249)	1:56:A:GLN:HE21	1:56:A:GLN:H	10	0.6
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	2	0.59
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	8	0.59
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	8	0.59
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	8	0.59
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	5	0.59
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	5	0.58
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	3	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	3	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	3	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	9	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	9	0.57
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	9	0.57
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	6	0.57
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	6	0.57
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	6	0.57
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	10	0.57
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	1	0.57
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	3	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	3	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	3	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	8	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	8	0.56
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	8	0.56
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	6	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	3	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	3	0.55
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	3	0.55
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	10	0.55
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	10	0.55
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	10	0.55
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	5	0.55
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	10	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	2	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	2	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	2	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	9	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	9	0.55
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	9	0.55
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	7	0.55
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	5	0.54
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	4	0.54
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	4	0.54
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	4	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	7	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	7	0.54
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	7	0.54
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	9	0.53
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	9	0.53
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	9	0.53
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	3	0.53
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	3	0.53
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	3	0.53
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	5	0.53
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	6	0.53
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	1	0.52
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	1	0.52
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	1	0.52
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	4	0.52
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	6	0.52
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	6	0.52
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	6	0.52
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	2	0.51
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	2	0.51
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	2	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	4	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	4	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	4	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	9	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	9	0.51
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	9	0.51
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	10	0.51
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	2	0.51
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	5	0.51
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	5	0.51
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	5	0.51
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	8	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	8	0.5
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	8	0.5
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	2	0.5
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	2	0.5
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	2	0.5
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	2	0.5
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	2	0.5
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	2	0.5
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	6	0.5
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	6	0.5
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	6	0.5
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	10	0.5
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	10	0.5
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	10	0.5
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	3	0.5
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	4	0.5
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	2	0.5
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	10	0.49
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	7	0.49
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	5	0.49
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	5	0.49
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	5	0.49
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	1	0.48
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	1	0.48
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	1	0.48
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	1	0.48
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	4	0.48
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	6	0.48
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	4	0.48
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	7	0.48
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	1	0.48
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD21	7	0.47
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD22	7	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2487)	1:63:A:GLN:HE21	1:110:A:LEU:HD23	7	0.47
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	10	0.47
(2,325)	1:12:A:THR:H	1:11:A:LYS:HE2	9	0.47
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	4	0.46
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	4	0.46
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	4	0.46
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	4	0.46
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	6	0.46
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	6	0.46
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	6	0.46
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	7	0.46
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	9	0.46
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	4	0.46
(2,270)	1:7:A:GLN:HE21	1:11:A:LYS:HG2	7	0.46
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	5	0.45
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	4	0.45
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	4	0.45
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	4	0.45
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	7	0.45
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	7	0.45
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	8	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	6	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	6	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	6	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	9	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	9	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	9	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	10	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	10	0.44
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	10	0.44
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	4	0.44
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	4	0.44
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	4	0.44
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	5	0.44
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	5	0.44
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	5	0.44
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	8	0.44
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	6	0.44
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	6	0.44
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	5	0.43
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	7	0.43
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	9	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	6	0.43
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	6	0.43
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	6	0.43
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	6	0.43
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	7	0.43
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	10	0.43
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	10	0.43
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	10	0.43
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	10	0.43
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	10	0.43
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	10	0.43
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	10	0.43
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	10	0.43
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	10	0.43
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	7	0.43
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	8	0.43
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	9	0.43
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	6	0.43
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	7	0.43
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	10	0.43
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	1	0.42
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	1	0.42
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	6	0.42
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	9	0.42
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	7	0.41
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	7	0.41
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	7	0.41
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	1	0.41
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	1	0.41
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	1	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	5	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	5	0.41
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	5	0.41
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	3	0.41
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	1	0.41
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	10	0.41
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	10	0.41
(2,3348)	1:139:A:GLN:HE21	1:135:A:ASP:HB2	5	0.4
(2,3347)	1:135:A:ASP:HB2	1:139:A:GLN:HE21	5	0.4
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	5	0.4
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	10	0.4
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	1	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	1	0.4
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	1	0.4
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	10	0.4
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	10	0.4
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	10	0.4
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	9	0.4
(2,3354)	1:138:A:TRP:HE3	1:139:A:GLN:HA	3	0.39
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	2	0.39
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	6	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	1	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	1	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	1	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	8	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	8	0.39
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	8	0.39
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	1	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	2	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	2	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	2	0.39
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	9	0.39
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	10	0.39
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	10	0.39
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	10	0.39
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	7	0.38
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	7	0.38
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	7	0.38
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	2	0.38
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	2	0.38
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	4	0.38
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	4	0.38
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	4	0.38
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	1	0.38
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	3	0.38
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	3	0.38
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	2	0.38
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	4	0.37
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	4	0.37
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	4	0.37
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	5	0.37
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	5	0.37
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	3	0.37
(2,2415)	1:56:A:GLN:HE22	1:105:A:GLU:H	6	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2414)	1:105:A:GLU:H	1:56:A:GLN:HE22	6	0.37
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	1	0.37
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	1	0.37
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	9	0.37
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	9	0.37
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	9	0.37
(2,1032)	1:46:A:HIS:HD2	1:47:A:PRO:HD2	3	0.37
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	3	0.37
(2,3139)	1:134:A:GLN:HE21	1:134:A:GLN:H	6	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	8	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	8	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	8	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	9	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	9	0.36
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	9	0.36
(2,2927)	1:129:A:LEU:HD11	1:61:A:TYR:HE1	3	0.36
(2,2927)	1:129:A:LEU:HD11	1:61:A:TYR:HE2	3	0.36
(2,2927)	1:129:A:LEU:HD12	1:61:A:TYR:HE1	3	0.36
(2,2927)	1:129:A:LEU:HD12	1:61:A:TYR:HE2	3	0.36
(2,2927)	1:129:A:LEU:HD13	1:61:A:TYR:HE1	3	0.36
(2,2927)	1:129:A:LEU:HD13	1:61:A:TYR:HE2	3	0.36
(2,2926)	1:61:A:TYR:HE1	1:129:A:LEU:HD11	3	0.36
(2,2926)	1:61:A:TYR:HE1	1:129:A:LEU:HD12	3	0.36
(2,2926)	1:61:A:TYR:HE1	1:129:A:LEU:HD13	3	0.36
(2,2926)	1:61:A:TYR:HE2	1:129:A:LEU:HD11	3	0.36
(2,2926)	1:61:A:TYR:HE2	1:129:A:LEU:HD12	3	0.36
(2,2926)	1:61:A:TYR:HE2	1:129:A:LEU:HD13	3	0.36
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	6	0.36
(2,2664)	1:68:A:MET:HE1	1:120:A:SER:HB2	3	0.36
(2,2664)	1:68:A:MET:HE2	1:120:A:SER:HB2	3	0.36
(2,2664)	1:68:A:MET:HE3	1:120:A:SER:HB2	3	0.36
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	7	0.36
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	7	0.36
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	5	0.36
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	5	0.36
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	5	0.36
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	7	0.36
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	7	0.36
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	7	0.36
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	3	0.36
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	7	0.36
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	7	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	7	0.36
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	5	0.36
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	9	0.36
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	7	0.36
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	7	0.36
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	7	0.36
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	2	0.35
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	4	0.35
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	6	0.35
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	6	0.35
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	10	0.35
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	10	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	2	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	2	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	2	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	6	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	6	0.35
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	6	0.35
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	6	0.35
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	6	0.35
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	6	0.35
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	6	0.35
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	6	0.35
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	6	0.35
(2,755)	1:30:A:VAL:HB	1:32:A:SER:HB2	6	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	1	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	1	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	1	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	4	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	4	0.35
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	4	0.35
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	4	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	6	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	6	0.35
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	6	0.35
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	10	0.34
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	10	0.34
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	10	0.34
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	10	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	10	0.34
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	10	0.34
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	8	0.34
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	8	0.34
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	8	0.34
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	2	0.34
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	9	0.34
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	9	0.34
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	8	0.34
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	8	0.34
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	8	0.34
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	6	0.34
(2,2527)	1:41:A:PHE:HE2	1:113:A:VAL:HG21	5	0.34
(2,2527)	1:41:A:PHE:HE2	1:113:A:VAL:HG22	5	0.34
(2,2527)	1:41:A:PHE:HE2	1:113:A:VAL:HG23	5	0.34
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	5	0.34
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	5	0.34
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	7	0.34
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	7	0.34
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	7	0.34
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	2	0.34
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	2	0.34
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	2	0.34
(2,203)	1:7:A:GLN:HE21	1:7:A:GLN:HA	9	0.34
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD11	6	0.34
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD12	6	0.34
(2,158)	1:6:A:VAL:H	1:3:A:ILE:HD13	6	0.34
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	9	0.34
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	9	0.33
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	5	0.33
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	5	0.33
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	5	0.33
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	5	0.33
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	5	0.33
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	5	0.33
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	5	0.33
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	5	0.33
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	5	0.33
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	5	0.33
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	5	0.33
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	5	0.33
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	5	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	5	0.33
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	5	0.33
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	5	0.33
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	5	0.33
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	5	0.33
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	2	0.33
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	2	0.33
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	2	0.33
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	10	0.33
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	10	0.33
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	10	0.33
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	7	0.33
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	7	0.33
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	7	0.33
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	4	0.33
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	6	0.33
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	6	0.33
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	10	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	8	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	8	0.33
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	8	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	8	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	8	0.33
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	8	0.33
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	6	0.33
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	6	0.33
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	6	0.33
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG11	7	0.33
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG12	7	0.33
(2,113)	1:5:A:LYS:HD2	1:1:A:VAL:HG13	7	0.33
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	1	0.32
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	1	0.32
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	1	0.32
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	1	0.32
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	5	0.32
(2,2765)	1:120:A:SER:H	1:124:A:VAL:HB	10	0.32
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	8	0.32
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	8	0.32
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	10	0.32
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	10	0.32
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	10	0.32
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	10	0.32
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	10	0.32
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	8	0.32
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	1	0.32
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	8	0.32
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	7	0.32
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	4	0.32
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	4	0.32
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	4	0.32
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	1	0.32
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	5	0.32
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	5	0.32
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	5	0.32
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	4	0.32
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	4	0.32
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	4	0.32
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	2	0.32
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	2	0.32
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	2	0.32
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	7	0.32
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	7	0.32
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	7	0.32
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	8	0.32
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	7	0.32
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	10	0.31
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	10	0.31
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	10	0.31
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	3	0.31
(2,2705)	1:122:A:GLU:HB3	1:121:A:THR:HB	1	0.31
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	6	0.31
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	6	0.31
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	3	0.31
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	1	0.31
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	8	0.31
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	10	0.31
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	10	0.31
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	10	0.31
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	10	0.31
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	10	0.31
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	10	0.31
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	10	0.31
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	8	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	8	0.31
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	8	0.31
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	1	0.31
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	1	0.31
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	1	0.31
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	3	0.31
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	5	0.3
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	2	0.3
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	9	0.3
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	9	0.3
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	9	0.3
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	4	0.3
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	8	0.3
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	10	0.3
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	10	0.3
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	10	0.3
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	10	0.3
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	10	0.3
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	10	0.3
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	10	0.3
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	10	0.3
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	10	0.3
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	10	0.3
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	10	0.3
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	10	0.3
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	10	0.3
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	10	0.3
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	10	0.3
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	10	0.3
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	10	0.3
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	10	0.3
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	4	0.3
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	4	0.3
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	10	0.3
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	4	0.3
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	1	0.3
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	5	0.3
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	10	0.3
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	5	0.3
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	9	0.3
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	3	0.3
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	3	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	3	0.3
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD11	1	0.3
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD12	1	0.3
(2,1975)	1:8:A:ASP:HB3	1:86:A:LEU:HD13	1	0.3
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	2	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	7	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	7	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	7	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	8	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	8	0.3
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	8	0.3
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	2	0.3
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	3	0.3
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	3	0.3
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	3	0.3
(2,833)	1:36:A:VAL:HA	1:37:A:THR:HB	9	0.3
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	4	0.3
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	4	0.3
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	4	0.3
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	6	0.3
(2,141)	1:5:A:LYS:H	1:5:A:LYS:HE2	10	0.3
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	6	0.29
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	6	0.29
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	6	0.29
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	9	0.29
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	10	0.29
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	4	0.29
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	4	0.29
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	4	0.29
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	5	0.29
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	5	0.29
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	5	0.29
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG21	7	0.29
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG22	7	0.29
(2,2725)	1:26:A:HIS:H	1:123:A:VAL:HG23	7	0.29
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	2	0.29
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	4	0.29
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	4	0.29
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	4	0.29
(2,2107)	1:90:A:LEU:HD21	1:7:A:GLN:HB3	9	0.29
(2,2107)	1:90:A:LEU:HD22	1:7:A:GLN:HB3	9	0.29
(2,2107)	1:90:A:LEU:HD23	1:7:A:GLN:HB3	9	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2106)	1:7:A:GLN:HB3	1:90:A:LEU:HD21	9	0.29
(2,2106)	1:7:A:GLN:HB3	1:90:A:LEU:HD22	9	0.29
(2,2106)	1:7:A:GLN:HB3	1:90:A:LEU:HD23	9	0.29
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	7	0.29
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	7	0.29
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	6	0.29
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	6	0.29
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	6	0.29
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	6	0.29
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	6	0.29
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	6	0.29
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	5	0.29
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	5	0.29
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	5	0.29
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD21	2	0.29
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD22	2	0.29
(2,1321)	1:61:A:TYR:HE1	1:45:A:LEU:HD23	2	0.29
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD21	2	0.29
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD22	2	0.29
(2,1321)	1:61:A:TYR:HE2	1:45:A:LEU:HD23	2	0.29
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG21	4	0.29
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG22	4	0.29
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG23	4	0.29
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	2	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	2	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	2	0.28
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	3	0.28
(2,3173)	1:136:A:MET:HE1	1:57:A:THR:HA	10	0.28
(2,3173)	1:136:A:MET:HE2	1:57:A:THR:HA	10	0.28
(2,3173)	1:136:A:MET:HE3	1:57:A:THR:HA	10	0.28
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	2	0.28
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	2	0.28
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	2	0.28
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	5	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	1	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	1	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	1	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	3	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	3	0.28
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	3	0.28
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	5	0.28
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	8	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	4	0.28
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	5	0.28
(2,1651)	1:70:A:SER:H	1:73:A:VAL:HB	8	0.28
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	4	0.28
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	5	0.28
(2,1650)	1:73:A:VAL:HB	1:70:A:SER:H	8	0.28
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	5	0.28
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	5	0.28
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	5	0.28
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	5	0.28
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	5	0.28
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	5	0.28
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	5	0.28
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	6	0.28
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	6	0.28
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	6	0.28
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	1	0.28
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	7	0.28
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	4	0.28
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	4	0.28
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	4	0.28
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	9	0.28
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	9	0.28
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	9	0.28
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	10	0.28
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	10	0.28
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	10	0.28
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	8	0.27
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	8	0.27
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	8	0.27
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	7	0.27
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	10	0.27
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	7	0.27
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	7	0.27
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	7	0.27
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	7	0.27
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	8	0.27
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	8	0.27
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	8	0.27
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	10	0.27
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	10	0.27
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	10	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	6	0.27
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	6	0.27
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	6	0.27
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	6	0.27
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	6	0.27
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	9	0.27
(2,2299)	1:100:A:TRP:HZ2	1:84:A:ARG:HA	2	0.27
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	4	0.27
(2,2260)	1:98:A:LEU:HD11	1:55:A:ASP:HB2	4	0.27
(2,2260)	1:98:A:LEU:HD12	1:55:A:ASP:HB2	4	0.27
(2,2260)	1:98:A:LEU:HD13	1:55:A:ASP:HB2	4	0.27
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	9	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	2	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	2	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	2	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	5	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	5	0.27
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	5	0.27
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	10	0.27
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	3	0.27
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	3	0.27
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	3	0.27
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	3	0.27
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	3	0.27
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	3	0.27
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	1	0.27
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	1	0.27
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	1	0.27
(2,811)	1:35:A:LYS:H	1:35:A:LYS:HE2	8	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	2	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	2	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	2	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	5	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	5	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	5	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	6	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	6	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	6	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	7	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	7	0.27
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	7	0.27
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	9	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	3	0.26
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	3	0.26
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	3	0.26
(2,3058)	1:132:A:SER:H	1:130:A:GLN:HG3	7	0.26
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	3	0.26
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	2	0.26
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	3	0.26
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	3	0.26
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	2	0.26
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	2	0.26
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	2	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	1	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	1	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	1	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	1	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	1	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	1	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	1	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	1	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	1	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	10	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	10	0.26
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	10	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	10	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	10	0.26
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	10	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	10	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	10	0.26
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	10	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	1	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	1	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	1	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	1	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	1	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	1	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	1	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	1	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	1	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	10	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	10	0.26
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	10	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	10	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	10	0.26
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	10	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	10	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	10	0.26
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	10	0.26
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	3	0.26
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	3	0.26
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	3	0.26
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	3	0.26
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	3	0.26
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	3	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	5	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	5	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	5	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	5	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	5	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	5	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	5	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	5	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	5	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	6	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	6	0.26
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	6	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	6	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	6	0.26
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	6	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	6	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	6	0.26
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	6	0.26
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	1	0.26
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	1	0.26
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	1	0.26
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	5	0.26
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	5	0.26
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	5	0.26
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	3	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	6	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	6	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	6	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	8	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	8	0.26
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	8	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2056)	1:88:A:HIS:HD2	1:87:A:LEU:HB3	8	0.26
(2,1539)	1:67:A:SER:H	1:68:A:MET:HB2	2	0.26
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	1	0.26
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	2	0.26
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	7	0.26
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	4	0.26
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	7	0.26
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	7	0.26
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	7	0.26
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD21	4	0.26
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD22	4	0.26
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD23	4	0.26
(2,1143)	1:49:A:LEU:HD21	1:53:A:LYS:HE2	4	0.26
(2,1143)	1:49:A:LEU:HD22	1:53:A:LYS:HE2	4	0.26
(2,1143)	1:49:A:LEU:HD23	1:53:A:LYS:HE2	4	0.26
(2,937)	1:41:A:PHE:HZ	1:43:A:PRO:HA	4	0.26
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	3	0.26
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	3	0.26
(2,776)	1:28:A:GLN:HG2	1:34:A:GLN:HB2	9	0.26
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	1	0.25
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	6	0.25
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	6	0.25
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	6	0.25
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	1	0.25
(2,2828)	1:126:A:LEU:H	1:123:A:VAL:HB	7	0.25
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	9	0.25
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	9	0.25
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	9	0.25
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	9	0.25
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	9	0.25
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	9	0.25
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	4	0.25
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	4	0.25
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	4	0.25
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	2	0.25
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	3	0.25
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	8	0.25
(2,1350)	1:59:A:ALA:HB1	1:62:A:GLN:HB3	6	0.25
(2,1350)	1:59:A:ALA:HB2	1:62:A:GLN:HB3	6	0.25
(2,1350)	1:59:A:ALA:HB3	1:62:A:GLN:HB3	6	0.25
(2,700)	1:28:A:GLN:HG2	1:25:A:SER:HB2	10	0.25
(2,325)	1:12:A:THR:H	1:11:A:LYS:HE2	10	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	2	0.25
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	2	0.25
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	4	0.25
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	9	0.25
(2,118)	1:2:A:PRO:HB2	1:5:A:LYS:HG2	10	0.25
(2,100)	1:4:A:GLN:HE21	1:4:A:GLN:HA	4	0.25
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	2	0.25
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	2	0.25
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	10	0.25
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	10	0.25
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	2	0.25
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	2	0.25
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	9	0.25
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	9	0.25
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	2	0.25
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	2	0.25
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	9	0.25
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	9	0.25
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	8	0.25
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	8	0.25
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	10	0.25
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	10	0.25
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	5	0.25
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	5	0.25
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	6	0.25
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	6	0.25
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	1	0.25
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	1	0.25
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	9	0.24
(2,3161)	1:49:A:LEU:HD11	1:136:A:MET:HB3	10	0.24
(2,3161)	1:49:A:LEU:HD12	1:136:A:MET:HB3	10	0.24
(2,3161)	1:49:A:LEU:HD13	1:136:A:MET:HB3	10	0.24
(2,3160)	1:136:A:MET:HB3	1:49:A:LEU:HD11	10	0.24
(2,3160)	1:136:A:MET:HB3	1:49:A:LEU:HD12	10	0.24
(2,3160)	1:136:A:MET:HB3	1:49:A:LEU:HD13	10	0.24
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD11	6	0.24
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD12	6	0.24
(2,3074)	1:80:A:LEU:HB2	1:133:A:LEU:HD13	6	0.24
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	4	0.24
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	4	0.24
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	4	0.24
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	2	0.24
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	2	0.24
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	2	0.24
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	10	0.24
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	10	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	1	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	1	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	1	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	10	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	10	0.24
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	10	0.24
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	1	0.24
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	1	0.24
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	1	0.24
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	10	0.24
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	10	0.24
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	10	0.24
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	6	0.24
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	8	0.24
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	6	0.24
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	4	0.24
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	4	0.24
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	4	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	4	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	4	0.24
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	4	0.24
(2,1791)	1:77:A:SER:H	1:75:A:GLN:HB2	6	0.24
(2,1656)	1:73:A:VAL:H	1:71:A:ARG:HB2	4	0.24
(2,1500)	1:67:A:SER:H	1:63:A:GLN:HA	2	0.24
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	4	0.24
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	4	0.24
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	4	0.24
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	1	0.24
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	1	0.24
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	1	0.24
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	6	0.24
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD21	1	0.24
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD22	1	0.24
(2,1144)	1:53:A:LYS:HE2	1:49:A:LEU:HD23	1	0.24
(2,1143)	1:49:A:LEU:HD21	1:53:A:LYS:HE2	1	0.24
(2,1143)	1:49:A:LEU:HD22	1:53:A:LYS:HE2	1	0.24
(2,1143)	1:49:A:LEU:HD23	1:53:A:LYS:HE2	1	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	3	0.24
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	3	0.24
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	3	0.24
(2,586)	1:24:A:ILE:H	1:20:A:ARG:HA	3	0.24
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	5	0.24
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	4	0.24
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	4	0.24
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	7	0.24
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	7	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	3	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	3	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	4	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	4	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	6	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	6	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	7	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	7	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	8	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	8	0.24
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	10	0.24
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	10	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	2	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	2	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	4	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	4	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	9	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	9	0.24
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	10	0.24
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	10	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	1	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	1	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	6	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	6	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	8	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	8	0.24
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	10	0.24
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	10	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	1	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	1	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	2	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	2	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	4	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	6	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	6	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	9	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	9	0.24
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	10	0.24
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	10	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	2	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	2	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	4	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	4	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	5	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	5	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	6	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	6	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	7	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	7	0.24
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	8	0.24
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	8	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	3	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	3	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	5	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	5	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	6	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	6	0.24
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	8	0.24
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	8	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	2	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	2	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	3	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	3	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	7	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	7	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	8	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	8	0.24
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	9	0.24
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	9	0.24
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	5	0.24
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	5	0.24
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	6	0.24
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	6	0.24
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	1	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	1	0.23
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	1	0.23
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	2	0.23
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	2	0.23
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	2	0.23
(2,3188)	1:136:A:MET:HE1	1:132:A:SER:HB2	6	0.23
(2,3188)	1:136:A:MET:HE2	1:132:A:SER:HB2	6	0.23
(2,3188)	1:136:A:MET:HE3	1:132:A:SER:HB2	6	0.23
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	3	0.23
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	4	0.23
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	9	0.23
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	9	0.23
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	9	0.23
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	10	0.23
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	10	0.23
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	10	0.23
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	9	0.23
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	9	0.23
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	9	0.23
(2,2455)	1:108:A:ASP:HB3	1:107:A:LEU:HB2	8	0.23
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	7	0.23
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	2	0.23
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	8	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	1	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	1	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	1	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB1	9	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB2	9	0.23
(2,2238)	1:97:A:HIS:HE1	1:91:A:ALA:HB3	9	0.23
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	9	0.23
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	9	0.23
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	9	0.23
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	6	0.23
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	6	0.23
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	6	0.23
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	9	0.23
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	9	0.23
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	9	0.23
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	1	0.23
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	4	0.23
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	7	0.23
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	4	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	4	0.23
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	4	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	3	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	8	0.23
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	10	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	1	0.23
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	1	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	2	0.23
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	2	0.23
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	3	0.23
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	3	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	3	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	3	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	5	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	5	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	8	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	8	0.23
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	9	0.23
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	9	0.23
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	1	0.23
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	1	0.23
(1,1856)	1:80:A:LEU:HB2	1:80:A:LEU:HB3	5	0.23
(1,1856)	1:80:A:LEU:HB3	1:80:A:LEU:HB2	5	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	1	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	1	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	3	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	3	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	6	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	6	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	7	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	7	0.23
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	8	0.23
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	8	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	3	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	3	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	4	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	4	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	5	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	5	0.23
(1,1102)	1:51:A:LEU:HB2	1:51:A:LEU:HB3	7	0.23
(1,1102)	1:51:A:LEU:HB3	1:51:A:LEU:HB2	7	0.23
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	3	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	3	0.23
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	5	0.23
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	5	0.23
(1,1053)	1:48:A:ILE:HG13	1:48:A:ILE:HG12	7	0.23
(1,1053)	1:48:A:ILE:HG12	1:48:A:ILE:HG13	7	0.23
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	1	0.23
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	1	0.23
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	3	0.23
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	3	0.23
(1,916)	1:42:A:ILE:HG13	1:42:A:ILE:HG12	9	0.23
(1,916)	1:42:A:ILE:HG12	1:42:A:ILE:HG13	9	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	2	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	2	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	4	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	4	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	7	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	7	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	8	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	8	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	9	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	9	0.23
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	10	0.23
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	10	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	1	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	1	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	2	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	2	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	4	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	4	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	7	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	7	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	9	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	9	0.23
(1,340)	1:13:A:LEU:HB2	1:13:A:LEU:HB3	10	0.23
(1,340)	1:13:A:LEU:HB3	1:13:A:LEU:HB2	10	0.23
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	1	0.23
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	1	0.23
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	4	0.23
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	4	0.23
(1,309)	1:11:A:LYS:HG2	1:11:A:LYS:HG3	10	0.23
(1,309)	1:11:A:LYS:HG3	1:11:A:LYS:HG2	10	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	2	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	3	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	3	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	4	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	4	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	8	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	8	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	9	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	9	0.23
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	10	0.23
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	10	0.23
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD21	6	0.22
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD22	6	0.22
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD23	6	0.22
(2,3234)	1:137:A:LEU:HD21	1:11:A:LYS:HE2	6	0.22
(2,3234)	1:137:A:LEU:HD22	1:11:A:LYS:HE2	6	0.22
(2,3234)	1:137:A:LEU:HD23	1:11:A:LYS:HE2	6	0.22
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	4	0.22
(2,3172)	1:54:A:MET:HE1	1:136:A:MET:HG2	7	0.22
(2,3172)	1:54:A:MET:HE2	1:136:A:MET:HG2	7	0.22
(2,3172)	1:54:A:MET:HE3	1:136:A:MET:HG2	7	0.22
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	7	0.22
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	7	0.22
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	7	0.22
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	7	0.22
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	7	0.22
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	7	0.22
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	4	0.22
(2,2992)	1:21:A:ILE:HD11	1:130:A:GLN:HG2	7	0.22
(2,2992)	1:21:A:ILE:HD12	1:130:A:GLN:HG2	7	0.22
(2,2992)	1:21:A:ILE:HD13	1:130:A:GLN:HG2	7	0.22
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	8	0.22
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	2	0.22
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	2	0.22
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	2	0.22
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	9	0.22
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	9	0.22
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	9	0.22
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	9	0.22
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	9	0.22
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	9	0.22
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	9	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	9	0.22
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	9	0.22
(2,2695)	1:122:A:GLU:HG3	1:68:A:MET:HE1	2	0.22
(2,2695)	1:122:A:GLU:HG3	1:68:A:MET:HE2	2	0.22
(2,2695)	1:122:A:GLU:HG3	1:68:A:MET:HE3	2	0.22
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	1	0.22
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	1	0.22
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	1	0.22
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	1	0.22
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	1	0.22
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	1	0.22
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	7	0.22
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	7	0.22
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	7	0.22
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	2	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	1	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	5	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	9	0.22
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	10	0.22
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	1	0.22
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	6	0.22
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	5	0.22
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	5	0.22
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	5	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	4	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	4	0.22
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	4	0.22
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	4	0.22
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	4	0.22
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	4	0.22
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	3	0.22
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	3	0.22
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	9	0.22
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	9	0.22
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	3	0.22
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD21	4	0.22
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD22	4	0.22
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD23	4	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	4	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	4	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	5	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	5	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	6	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	6	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	7	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	7	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	8	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	8	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	9	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	9	0.22
(1,3194)	1:136:A:MET:HB2	1:136:A:MET:HB3	10	0.22
(1,3194)	1:136:A:MET:HB3	1:136:A:MET:HB2	10	0.22
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	1	0.22
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	1	0.22
(1,2031)	1:87:A:LEU:HB2	1:87:A:LEU:HB3	6	0.22
(1,2031)	1:87:A:LEU:HB3	1:87:A:LEU:HB2	6	0.22
(1,1365)	1:62:A:GLN:HG3	1:62:A:GLN:HG2	5	0.22
(1,1365)	1:62:A:GLN:HG2	1:62:A:GLN:HG3	5	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	1	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	1	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	3	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	3	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	5	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	5	0.22
(1,401)	1:15:A:LYS:HD2	1:15:A:LYS:HD3	6	0.22
(1,401)	1:15:A:LYS:HD3	1:15:A:LYS:HD2	6	0.22
(1,68)	1:3:A:ILE:HG13	1:3:A:ILE:HG12	7	0.22
(1,68)	1:3:A:ILE:HG12	1:3:A:ILE:HG13	7	0.22
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	5	0.21
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	5	0.21
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	5	0.21
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	2	0.21
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	2	0.21
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	2	0.21
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	5	0.21
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	5	0.21
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	5	0.21
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	1	0.21
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	1	0.21
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	1	0.21
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	8	0.21
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	2	0.21
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	9	0.21
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	9	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	9	0.21
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	7	0.21
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	7	0.21
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	7	0.21
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	2	0.21
(2,2693)	1:68:A:MET:HE1	1:122:A:GLU:HB3	1	0.21
(2,2693)	1:68:A:MET:HE2	1:122:A:GLU:HB3	1	0.21
(2,2693)	1:68:A:MET:HE3	1:122:A:GLU:HB3	1	0.21
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	6	0.21
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	6	0.21
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	6	0.21
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	8	0.21
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	8	0.21
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	8	0.21
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	8	0.21
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	8	0.21
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	8	0.21
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	10	0.21
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	1	0.21
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD21	7	0.21
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD22	7	0.21
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD23	7	0.21
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	4	0.21
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	4	0.21
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	4	0.21
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	7	0.21
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	7	0.21
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	7	0.21
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	7	0.21
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	7	0.21
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	7	0.21
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	4	0.21
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	7	0.21
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	1	0.21
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	1	0.21
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	7	0.21
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	7	0.21
(2,774)	1:33:A:LYS:H	1:33:A:LYS:HE2	6	0.21
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	10	0.21
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	10	0.21
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	10	0.21
(2,391)	1:12:A:THR:HG21	1:15:A:LYS:HB2	8	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:12:A:THR:HG22	1:15:A:LYS:HB2	8	0.21
(2,391)	1:12:A:THR:HG23	1:15:A:LYS:HB2	8	0.21
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	1	0.21
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	7	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	1	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	1	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	2	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	2	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	3	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	3	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	6	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	6	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	7	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	7	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	9	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	9	0.21
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	10	0.21
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	10	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	1	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	1	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	2	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	2	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	3	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	3	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	4	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	4	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	5	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	5	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	6	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	6	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	7	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	7	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	8	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	8	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	9	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	9	0.21
(1,25)	1:2:A:PRO:HB3	1:2:A:PRO:HB2	10	0.21
(1,25)	1:2:A:PRO:HB2	1:2:A:PRO:HB3	10	0.21
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	4	0.2
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	4	0.2
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	4	0.2
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	4	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	4	0.2
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	4	0.2
(2,3364)	1:139:A:GLN:HE21	1:139:A:GLN:HA	10	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	6	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	6	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	6	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	9	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	9	0.2
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	9	0.2
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	1	0.2
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	1	0.2
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	1	0.2
(2,3190)	1:136:A:MET:HB3	1:133:A:LEU:HA	10	0.2
(2,3183)	1:136:A:MET:HE1	1:83:A:LEU:HD21	10	0.2
(2,3183)	1:136:A:MET:HE1	1:83:A:LEU:HD22	10	0.2
(2,3183)	1:136:A:MET:HE1	1:83:A:LEU:HD23	10	0.2
(2,3183)	1:136:A:MET:HE2	1:83:A:LEU:HD21	10	0.2
(2,3183)	1:136:A:MET:HE2	1:83:A:LEU:HD22	10	0.2
(2,3183)	1:136:A:MET:HE2	1:83:A:LEU:HD23	10	0.2
(2,3183)	1:136:A:MET:HE3	1:83:A:LEU:HD21	10	0.2
(2,3183)	1:136:A:MET:HE3	1:83:A:LEU:HD22	10	0.2
(2,3183)	1:136:A:MET:HE3	1:83:A:LEU:HD23	10	0.2
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	5	0.2
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	5	0.2
(2,2911)	1:128:A:ARG:HG2	1:128:A:ARG:HD2	5	0.2
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	9	0.2
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	9	0.2
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	9	0.2
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	4	0.2
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB1	3	0.2
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB2	3	0.2
(2,2801)	1:122:A:GLU:HB3	1:125:A:ALA:HB3	3	0.2
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	7	0.2
(2,2765)	1:120:A:SER:H	1:124:A:VAL:HB	3	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	2	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	2	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	2	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	2	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	2	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	2	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	2	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	2	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	2	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	8	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	8	0.2
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	8	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	8	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	8	0.2
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	8	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	8	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	8	0.2
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	8	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	2	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	2	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	2	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	2	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	2	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	2	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	2	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	2	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	2	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	8	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	8	0.2
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	8	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	8	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	8	0.2
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	8	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	8	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	8	0.2
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	8	0.2
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE1	10	0.2
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE2	10	0.2
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE3	10	0.2
(2,2696)	1:68:A:MET:HE1	1:122:A:GLU:HG2	10	0.2
(2,2696)	1:68:A:MET:HE2	1:122:A:GLU:HG2	10	0.2
(2,2696)	1:68:A:MET:HE3	1:122:A:GLU:HG2	10	0.2
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	7	0.2
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	7	0.2
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	7	0.2
(2,2558)	1:114:A:LEU:HG	1:111:A:GLY:HA3	1	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	2	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	2	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	2	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	2	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	2	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	2	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	2	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	2	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	2	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	8	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	8	0.2
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	8	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	8	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	8	0.2
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	8	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	8	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	8	0.2
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	8	0.2
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	9	0.2
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	9	0.2
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	9	0.2
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	4	0.2
(2,2288)	1:98:A:LEU:HD11	1:99:A:PRO:HG2	8	0.2
(2,2288)	1:98:A:LEU:HD12	1:99:A:PRO:HG2	8	0.2
(2,2288)	1:98:A:LEU:HD13	1:99:A:PRO:HG2	8	0.2
(2,2095)	1:6:A:VAL:H	1:90:A:LEU:HD11	5	0.2
(2,2095)	1:6:A:VAL:H	1:90:A:LEU:HD12	5	0.2
(2,2095)	1:6:A:VAL:H	1:90:A:LEU:HD13	5	0.2
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	3	0.2
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	3	0.2
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	3	0.2
(2,1723)	1:71:A:ARG:HD2	1:75:A:GLN:HG2	6	0.2
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	2	0.2
(2,989)	1:45:A:LEU:H	1:42:A:ILE:HB	6	0.2
(2,989)	1:45:A:LEU:H	1:42:A:ILE:HB	8	0.2
(2,988)	1:45:A:LEU:HD11	1:42:A:ILE:HB	9	0.2
(2,988)	1:45:A:LEU:HD12	1:42:A:ILE:HB	9	0.2
(2,988)	1:45:A:LEU:HD13	1:42:A:ILE:HB	9	0.2
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	6	0.2
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	6	0.2
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	10	0.2
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	10	0.2
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	1	0.2
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	1	0.2
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	1	0.2
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	6	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	6	0.2
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	6	0.2
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	10	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	7	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	7	0.2
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	7	0.2
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	9	0.2
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	1	0.2
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	4	0.2
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	4	0.2
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	5	0.2
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	5	0.2
(1,2280)	1:99:A:PRO:HB3	1:99:A:PRO:HB2	8	0.2
(1,2280)	1:99:A:PRO:HB2	1:99:A:PRO:HB3	8	0.2
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	1	0.19
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	1	0.19
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	1	0.19
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	6	0.19
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	6	0.19
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	6	0.19
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	8	0.19
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	8	0.19
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	8	0.19
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	10	0.19
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	10	0.19
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	10	0.19
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	10	0.19
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	10	0.19
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	10	0.19
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	1	0.19
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	1	0.19
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	1	0.19
(2,3173)	1:136:A:MET:HE1	1:57:A:THR:HA	8	0.19
(2,3173)	1:136:A:MET:HE2	1:57:A:THR:HA	8	0.19
(2,3173)	1:136:A:MET:HE3	1:57:A:THR:HA	8	0.19
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	2	0.19
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	4	0.19
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	5	0.19
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	5	0.19
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	5	0.19
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	8	0.19
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	8	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	8	0.19
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	7	0.19
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	7	0.19
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	7	0.19
(2,2648)	1:119:A:TYR:H	1:117:A:SER:HB2	6	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	2	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	2	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	2	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	7	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	7	0.19
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	7	0.19
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	2	0.19
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	2	0.19
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	2	0.19
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	7	0.19
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	7	0.19
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	7	0.19
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	2	0.19
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	7	0.19
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	2	0.19
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	2	0.19
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	2	0.19
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	7	0.19
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	5	0.19
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	7	0.19
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	4	0.19
(2,2109)	1:90:A:LEU:HD21	1:7:A:GLN:HB2	1	0.19
(2,2109)	1:90:A:LEU:HD22	1:7:A:GLN:HB2	1	0.19
(2,2109)	1:90:A:LEU:HD23	1:7:A:GLN:HB2	1	0.19
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD21	1	0.19
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD22	1	0.19
(2,2108)	1:7:A:GLN:HB2	1:90:A:LEU:HD23	1	0.19
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	10	0.19
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	10	0.19
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	10	0.19
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	3	0.19
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	10	0.19
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG21	1	0.19
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG22	1	0.19
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG23	1	0.19
(2,1030)	1:46:A:HIS:HD2	1:47:A:PRO:HD3	5	0.19
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	4	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	4	0.19
(2,832)	1:37:A:THR:H	1:35:A:LYS:HD2	5	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	10	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	10	0.19
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	10	0.19
(2,815)	1:36:A:VAL:H	1:35:A:LYS:HA	9	0.19
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG21	4	0.19
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG22	4	0.19
(2,777)	1:34:A:GLN:HE22	1:30:A:VAL:HG23	4	0.19
(2,730)	1:29:A:SER:H	1:27:A:THR:HG21	5	0.19
(2,730)	1:29:A:SER:H	1:27:A:THR:HG22	5	0.19
(2,730)	1:29:A:SER:H	1:27:A:THR:HG23	5	0.19
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	6	0.19
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	6	0.19
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	6	0.19
(2,697)	1:28:A:GLN:HB2	1:25:A:SER:HB3	7	0.19
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	6	0.19
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	8	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	8	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	8	0.18
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	3	0.18
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	3	0.18
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	3	0.18
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	7	0.18
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	7	0.18
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	7	0.18
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	10	0.18
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	10	0.18
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	10	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	4	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	4	0.18
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	4	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	5	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	5	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	5	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	6	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	6	0.18
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	6	0.18
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	9	0.18
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	9	0.18
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	9	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	9	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	9	0.18
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	9	0.18
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	8	0.18
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	3	0.18
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	3	0.18
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	3	0.18
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	3	0.18
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	7	0.18
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	4	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	3	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	3	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	3	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	3	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	3	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	3	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	3	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	3	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	3	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	4	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	4	0.18
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	4	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	4	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	4	0.18
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	4	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	4	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	4	0.18
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	4	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	3	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	3	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	3	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	3	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	3	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	3	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	3	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	3	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	3	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	4	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	4	0.18
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	4	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	4	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	4	0.18
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	4	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	4	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	4	0.18
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	4	0.18
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	1	0.18
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	1	0.18
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	1	0.18
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	8	0.18
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	8	0.18
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	8	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	3	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	3	0.18
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	3	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	3	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	3	0.18
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	3	0.18
(2,2637)	1:119:A:TYR:HE1	1:115:A:GLU:HG2	1	0.18
(2,2637)	1:119:A:TYR:HE2	1:115:A:GLU:HG2	1	0.18
(2,2616)	1:117:A:SER:HB2	1:117:A:SER:HA	4	0.18
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	6	0.18
(2,2492)	1:106:A:THR:HG21	1:110:A:LEU:HA	1	0.18
(2,2492)	1:106:A:THR:HG22	1:110:A:LEU:HA	1	0.18
(2,2492)	1:106:A:THR:HG23	1:110:A:LEU:HA	1	0.18
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	10	0.18
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	10	0.18
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	10	0.18
(2,2398)	1:63:A:GLN:HE22	1:104:A:LEU:HD21	3	0.18
(2,2398)	1:63:A:GLN:HE22	1:104:A:LEU:HD22	3	0.18
(2,2398)	1:63:A:GLN:HE22	1:104:A:LEU:HD23	3	0.18
(2,2397)	1:104:A:LEU:HD21	1:63:A:GLN:HE22	3	0.18
(2,2397)	1:104:A:LEU:HD22	1:63:A:GLN:HE22	3	0.18
(2,2397)	1:104:A:LEU:HD23	1:63:A:GLN:HE22	3	0.18
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	6	0.18
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	7	0.18
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	10	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	2	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	2	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	2	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	2	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	2	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	2	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	2	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	2	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	4	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	4	0.18
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	4	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	4	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	4	0.18
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	4	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	4	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	4	0.18
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	4	0.18
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD21	9	0.18
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD22	9	0.18
(2,1918)	1:83:A:LEU:H	1:80:A:LEU:HD23	9	0.18
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	8	0.18
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	8	0.18
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	8	0.18
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	8	0.18
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	8	0.18
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	8	0.18
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	2	0.18
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	2	0.18
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	2	0.18
(2,1393)	1:63:A:GLN:HE21	1:63:A:GLN:HA	8	0.18
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	9	0.18
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	2	0.18
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	2	0.18
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	2	0.18
(2,1175)	1:53:A:LYS:H	1:53:A:LYS:HE2	2	0.18
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	5	0.18
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	1	0.18
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	2	0.18
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	2	0.18
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	8	0.18
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	8	0.18
(2,882)	1:41:A:PHE:HD1	1:39:A:LEU:HD11	7	0.18
(2,882)	1:41:A:PHE:HD1	1:39:A:LEU:HD12	7	0.18
(2,882)	1:41:A:PHE:HD1	1:39:A:LEU:HD13	7	0.18
(2,882)	1:41:A:PHE:HD2	1:39:A:LEU:HD11	7	0.18
(2,882)	1:41:A:PHE:HD2	1:39:A:LEU:HD12	7	0.18
(2,882)	1:41:A:PHE:HD2	1:39:A:LEU:HD13	7	0.18
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	9	0.18
(2,712)	1:28:A:GLN:HE21	1:28:A:GLN:HA	9	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	5	0.18
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	6	0.17
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	6	0.17
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	6	0.17
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	2	0.17
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	2	0.17
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	2	0.17
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	2	0.17
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	2	0.17
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	2	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	4	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	4	0.17
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	4	0.17
(2,2975)	1:130:A:GLN:H	1:18:A:VAL:HG21	9	0.17
(2,2975)	1:130:A:GLN:H	1:18:A:VAL:HG22	9	0.17
(2,2975)	1:130:A:GLN:H	1:18:A:VAL:HG23	9	0.17
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD11	3	0.17
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD12	3	0.17
(2,2863)	1:128:A:ARG:HD3	1:42:A:ILE:HD13	3	0.17
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	7	0.17
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	7	0.17
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	7	0.17
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	7	0.17
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	7	0.17
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	7	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	10	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	10	0.17
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	10	0.17
(2,2469)	1:109:A:SER:H	1:107:A:LEU:HB2	9	0.17
(2,2320)	1:100:A:TRP:HH2	1:88:A:HIS:HA	10	0.17
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	3	0.17
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	10	0.17
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	10	0.17
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	10	0.17
(2,1567)	1:68:A:MET:HG2	1:69:A:PRO:HD2	4	0.17
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	3	0.17
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	4	0.17
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	4	0.17
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	4	0.17
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	7	0.17
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	7	0.17
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	7	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG21	5	0.17
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG22	5	0.17
(2,1480)	1:63:A:GLN:HE22	1:66:A:THR:HG23	5	0.17
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG21	2	0.17
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG22	2	0.17
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG23	2	0.17
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG21	2	0.17
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG22	2	0.17
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG23	2	0.17
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	3	0.17
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	3	0.17
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	3	0.17
(2,1269)	1:55:A:ASP:H	1:58:A:LEU:HG	10	0.17
(2,1175)	1:53:A:LYS:H	1:53:A:LYS:HE2	5	0.17
(2,1163)	1:53:A:LYS:HD2	1:53:A:LYS:HB2	4	0.17
(2,1092)	1:48:A:ILE:HG21	1:50:A:THR:HG21	10	0.17
(2,1092)	1:48:A:ILE:HG21	1:50:A:THR:HG22	10	0.17
(2,1092)	1:48:A:ILE:HG21	1:50:A:THR:HG23	10	0.17
(2,1092)	1:48:A:ILE:HG22	1:50:A:THR:HG21	10	0.17
(2,1092)	1:48:A:ILE:HG22	1:50:A:THR:HG22	10	0.17
(2,1092)	1:48:A:ILE:HG22	1:50:A:THR:HG23	10	0.17
(2,1092)	1:48:A:ILE:HG23	1:50:A:THR:HG21	10	0.17
(2,1092)	1:48:A:ILE:HG23	1:50:A:THR:HG22	10	0.17
(2,1092)	1:48:A:ILE:HG23	1:50:A:THR:HG23	10	0.17
(2,1091)	1:50:A:THR:HG21	1:48:A:ILE:HG21	10	0.17
(2,1091)	1:50:A:THR:HG21	1:48:A:ILE:HG22	10	0.17
(2,1091)	1:50:A:THR:HG21	1:48:A:ILE:HG23	10	0.17
(2,1091)	1:50:A:THR:HG22	1:48:A:ILE:HG21	10	0.17
(2,1091)	1:50:A:THR:HG22	1:48:A:ILE:HG22	10	0.17
(2,1091)	1:50:A:THR:HG22	1:48:A:ILE:HG23	10	0.17
(2,1091)	1:50:A:THR:HG23	1:48:A:ILE:HG21	10	0.17
(2,1091)	1:50:A:THR:HG23	1:48:A:ILE:HG22	10	0.17
(2,1091)	1:50:A:THR:HG23	1:48:A:ILE:HG23	10	0.17
(2,895)	1:41:A:PHE:HE1	1:41:A:PHE:HA	5	0.17
(2,895)	1:41:A:PHE:HE2	1:41:A:PHE:HA	5	0.17
(2,837)	1:37:A:THR:H	1:36:A:VAL:H	7	0.17
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	5	0.17
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	5	0.17
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	5	0.17
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	4	0.17
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	1	0.17
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	1	0.17
(2,589)	1:24:A:ILE:HD11	1:21:A:ILE:HA	1	0.17
(2,589)	1:24:A:ILE:HD12	1:21:A:ILE:HA	1	0.17
(2,589)	1:24:A:ILE:HD13	1:21:A:ILE:HA	1	0.17
(2,203)	1:7:A:GLN:HE21	1:7:A:GLN:HA	4	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	3	0.17
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	3	0.17
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	2	0.16
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	2	0.16
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	2	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	5	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	5	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	5	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	6	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	6	0.16
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	6	0.16
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD21	9	0.16
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD22	9	0.16
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD23	9	0.16
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	7	0.16
(2,3058)	1:132:A:SER:H	1:130:A:GLN:HG3	8	0.16
(2,3057)	1:132:A:SER:H	1:130:A:GLN:HB2	7	0.16
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD11	2	0.16
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD12	2	0.16
(2,2985)	1:130:A:GLN:HE21	1:21:A:ILE:HD13	2	0.16
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	2	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2882)	1:128:A:ARG:HE	1:124:A:VAL:HG21	4	0.16
(2,2882)	1:128:A:ARG:HE	1:124:A:VAL:HG22	4	0.16
(2,2882)	1:128:A:ARG:HE	1:124:A:VAL:HG23	4	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	6	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	6	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	6	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	6	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	6	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	6	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	6	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	6	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	6	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	9	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	9	0.16
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	9	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	9	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	9	0.16
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	9	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	9	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	9	0.16
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	9	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	6	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	6	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	6	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	6	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	6	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	6	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	6	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	6	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	6	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	9	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	9	0.16
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	9	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	9	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	9	0.16
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	9	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	9	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	9	0.16
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	9	0.16
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	5	0.16
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	5	0.16
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	5	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	5	0.16
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	5	0.16
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	5	0.16
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	5	0.16
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	5	0.16
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	5	0.16
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	4	0.16
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	4	0.16
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	4	0.16
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	10	0.16
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	10	0.16
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	10	0.16
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	10	0.16
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	10	0.16
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	10	0.16
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	4	0.16
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	4	0.16
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	4	0.16
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	6	0.16
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	6	0.16
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	6	0.16
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	4	0.16
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	4	0.16
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	4	0.16
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	4	0.16
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	4	0.16
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	4	0.16
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	4	0.16
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	4	0.16
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	4	0.16
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD21	6	0.16
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD22	6	0.16
(2,2524)	1:112:A:GLY:H	1:110:A:LEU:HD23	6	0.16
(2,2413)	1:56:A:GLN:HE21	1:105:A:GLU:H	5	0.16
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	3	0.16
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	10	0.16
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	4	0.16
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	8	0.16
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE1	1	0.16
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE2	1	0.16
(2,1542)	1:67:A:SER:H	1:68:A:MET:HE3	1	0.16
(2,1541)	1:68:A:MET:HE1	1:67:A:SER:H	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1541)	1:68:A:MET:HE2	1:67:A:SER:H	1	0.16
(2,1541)	1:68:A:MET:HE3	1:67:A:SER:H	1	0.16
(2,1538)	1:68:A:MET:HB3	1:67:A:SER:H	8	0.16
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG21	10	0.16
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG22	10	0.16
(2,1406)	1:64:A:ILE:H	1:60:A:VAL:HG23	10	0.16
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	8	0.16
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG21	2	0.16
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG22	2	0.16
(2,1150)	1:53:A:LYS:HE2	1:50:A:THR:HG23	2	0.16
(2,886)	1:41:A:PHE:HD1	1:40:A:ASP:HB3	4	0.16
(2,886)	1:41:A:PHE:HD2	1:40:A:ASP:HB3	4	0.16
(2,730)	1:29:A:SER:H	1:27:A:THR:HG21	6	0.16
(2,730)	1:29:A:SER:H	1:27:A:THR:HG22	6	0.16
(2,730)	1:29:A:SER:H	1:27:A:THR:HG23	6	0.16
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	5	0.16
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	6	0.16
(2,704)	1:27:A:THR:HG21	1:28:A:GLN:HA	7	0.16
(2,704)	1:27:A:THR:HG22	1:28:A:GLN:HA	7	0.16
(2,704)	1:27:A:THR:HG23	1:28:A:GLN:HA	7	0.16
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	9	0.16
(2,293)	1:11:A:LYS:HE2	1:11:A:LYS:HA	10	0.16
(2,272)	1:11:A:LYS:HD2	1:8:A:ASP:HA	10	0.16
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG21	8	0.16
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG22	8	0.16
(2,181)	1:7:A:GLN:HE22	1:3:A:ILE:HG23	8	0.16
(2,157)	1:6:A:VAL:H	1:3:A:ILE:HB	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	2	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	2	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	2	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	5	0.16
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	5	0.16
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG21	10	0.15
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG22	10	0.15
(2,3537)	1:145:A:GLY:H	1:48:A:ILE:HG23	10	0.15
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	1	0.15
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	8	0.15
(2,3489)	1:54:A:MET:HE1	1:143:A:SER:HB2	8	0.15
(2,3489)	1:54:A:MET:HE2	1:143:A:SER:HB2	8	0.15
(2,3489)	1:54:A:MET:HE3	1:143:A:SER:HB2	8	0.15
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	8	0.15
(2,2999)	1:46:A:HIS:HE1	1:130:A:GLN:HA	8	0.15
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	5	0.15
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	3	0.15
(2,2843)	1:46:A:HIS:HE1	1:127:A:SER:HA	6	0.15
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	6	0.15
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	3	0.15
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	3	0.15
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	3	0.15
(2,2730)	1:28:A:GLN:HB2	1:123:A:VAL:HG21	8	0.15
(2,2730)	1:28:A:GLN:HB2	1:123:A:VAL:HG22	8	0.15
(2,2730)	1:28:A:GLN:HB2	1:123:A:VAL:HG23	8	0.15
(2,2616)	1:117:A:SER:HB2	1:117:A:SER:HA	8	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	4	0.15
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	4	0.15
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	4	0.15
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	4	0.15
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	4	0.15
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	4	0.15
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	2	0.15
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD11	3	0.15
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD12	3	0.15
(2,2470)	1:109:A:SER:H	1:107:A:LEU:HD13	3	0.15
(2,2415)	1:56:A:GLN:HE22	1:105:A:GLU:H	7	0.15
(2,2414)	1:105:A:GLU:H	1:56:A:GLN:HE22	7	0.15
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	2	0.15
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	8	0.15
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	2	0.15
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	8	0.15
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	2	0.15
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	5	0.15
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	6	0.15
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	6	0.15
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	6	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	2	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	2	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	2	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	3	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	3	0.15
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	3	0.15
(2,1567)	1:68:A:MET:HG2	1:69:A:PRO:HD2	7	0.15
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	5	0.15
(2,1014)	1:46:A:HIS:HD2	1:45:A:LEU:HB2	6	0.15
(2,655)	1:26:A:HIS:HD2	1:23:A:ASP:HA	10	0.15
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	5	0.15
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	7	0.15
(2,3549)	1:146:A:CYS:H	1:50:A:THR:HG21	7	0.14
(2,3549)	1:146:A:CYS:H	1:50:A:THR:HG22	7	0.14
(2,3549)	1:146:A:CYS:H	1:50:A:THR:HG23	7	0.14
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD21	8	0.14
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD22	8	0.14
(2,3453)	1:138:A:TRP:HD1	1:142:A:LEU:HD23	8	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	3	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	3	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	3	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG21	8	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG22	8	0.14
(2,3293)	1:138:A:TRP:HH2	1:48:A:ILE:HG23	8	0.14
(2,3256)	1:15:A:LYS:HE2	1:137:A:LEU:HD21	8	0.14
(2,3256)	1:15:A:LYS:HE2	1:137:A:LEU:HD22	8	0.14
(2,3256)	1:15:A:LYS:HE2	1:137:A:LEU:HD23	8	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	2	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	2	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	2	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	3	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	3	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	3	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD21	4	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD22	4	0.14
(2,3255)	1:15:A:LYS:HA	1:137:A:LEU:HD23	4	0.14
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	4	0.14
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	4	0.14
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	4	0.14
(2,3122)	1:134:A:GLN:HE21	1:134:A:GLN:HA	3	0.14
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	4	0.14
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	7	0.14
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	7	0.14
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	5	0.14
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	5	0.14
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	5	0.14
(2,3003)	1:126:A:LEU:HD11	1:130:A:GLN:HA	8	0.14
(2,3003)	1:126:A:LEU:HD12	1:130:A:GLN:HA	8	0.14
(2,3003)	1:126:A:LEU:HD13	1:130:A:GLN:HA	8	0.14
(2,2903)	1:128:A:ARG:HE	1:128:A:ARG:HA	2	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	2	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	2	0.14
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	2	0.14
(2,2817)	1:76:A:ILE:HD11	1:126:A:LEU:HA	2	0.14
(2,2817)	1:76:A:ILE:HD12	1:126:A:LEU:HA	2	0.14
(2,2817)	1:76:A:ILE:HD13	1:126:A:LEU:HA	2	0.14
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	8	0.14
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	8	0.14
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	6	0.14
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	6	0.14
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	6	0.14
(2,2679)	1:121:A:THR:HG21	1:120:A:SER:HA	5	0.14
(2,2679)	1:121:A:THR:HG22	1:120:A:SER:HA	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2679)	1:121:A:THR:HG23	1:120:A:SER:HA	5	0.14
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	5	0.14
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	5	0.14
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	5	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	5	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	5	0.14
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	5	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	5	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	5	0.14
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	5	0.14
(2,2515)	1:111:A:GLY:H	1:110:A:LEU:HG	8	0.14
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	3	0.14
(2,2326)	1:100:A:TRP:HZ3	1:88:A:HIS:H	6	0.14
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	5	0.14
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	7	0.14
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	5	0.14
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	7	0.14
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	8	0.14
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB1	10	0.14
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB2	10	0.14
(2,2136)	1:87:A:LEU:HD11	1:91:A:ALA:HB3	10	0.14
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB1	10	0.14
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB2	10	0.14
(2,2136)	1:87:A:LEU:HD12	1:91:A:ALA:HB3	10	0.14
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB1	10	0.14
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB2	10	0.14
(2,2136)	1:87:A:LEU:HD13	1:91:A:ALA:HB3	10	0.14
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	1	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	3	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	3	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	3	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	9	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	9	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	9	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD11	10	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD12	10	0.14
(2,1852)	1:80:A:LEU:H	1:65:A:LEU:HD13	10	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	6	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	6	0.14
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	6	0.14
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	6	0.14
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	6	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	6	0.14
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	6	0.14
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	6	0.14
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	6	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	5	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	5	0.14
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	5	0.14
(2,1656)	1:73:A:VAL:H	1:71:A:ARG:HB2	7	0.14
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	7	0.14
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	7	0.14
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	7	0.14
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	8	0.14
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	8	0.14
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	8	0.14
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	6	0.14
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	9	0.14
(2,755)	1:30:A:VAL:HB	1:32:A:SER:HB2	5	0.14
(2,589)	1:24:A:ILE:HD11	1:21:A:ILE:HA	4	0.14
(2,589)	1:24:A:ILE:HD12	1:21:A:ILE:HA	4	0.14
(2,589)	1:24:A:ILE:HD13	1:21:A:ILE:HA	4	0.14
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	9	0.14
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	9	0.14
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	9	0.14
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	6	0.14
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD21	8	0.14
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD22	8	0.14
(2,422)	1:16:A:THR:H	1:13:A:LEU:HD23	8	0.14
(2,324)	1:12:A:THR:H	1:11:A:LYS:HD2	6	0.14
(2,293)	1:11:A:LYS:HE2	1:11:A:LYS:HA	9	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	4	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	4	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	8	0.14
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	8	0.14
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	5	0.13
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	5	0.13
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	5	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	5	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	5	0.13
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	5	0.13
(2,3122)	1:134:A:GLN:HE21	1:134:A:GLN:HA	10	0.13
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	9	0.13
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	9	0.13
(2,2987)	1:130:A:GLN:HE21	1:21:A:ILE:H	4	0.13
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	1	0.13
(2,2970)	1:130:A:GLN:HE21	1:18:A:VAL:HA	6	0.13
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG11	5	0.13
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG12	5	0.13
(2,2844)	1:127:A:SER:H	1:73:A:VAL:HG13	5	0.13
(2,2817)	1:76:A:ILE:HD11	1:126:A:LEU:HA	5	0.13
(2,2817)	1:76:A:ILE:HD12	1:126:A:LEU:HA	5	0.13
(2,2817)	1:76:A:ILE:HD13	1:126:A:LEU:HA	5	0.13
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	9	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	1	0.13
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	1	0.13
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	1	0.13
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG11	1	0.13
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG12	1	0.13
(2,2736)	1:42:A:ILE:HG21	1:123:A:VAL:HG13	1	0.13
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG11	1	0.13
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG12	1	0.13
(2,2736)	1:42:A:ILE:HG22	1:123:A:VAL:HG13	1	0.13
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG11	1	0.13
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG12	1	0.13
(2,2736)	1:42:A:ILE:HG23	1:123:A:VAL:HG13	1	0.13
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG21	1	0.13
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG22	1	0.13
(2,2735)	1:123:A:VAL:HG11	1:42:A:ILE:HG23	1	0.13
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG21	1	0.13
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG22	1	0.13
(2,2735)	1:123:A:VAL:HG12	1:42:A:ILE:HG23	1	0.13
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG21	1	0.13
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG22	1	0.13
(2,2735)	1:123:A:VAL:HG13	1:42:A:ILE:HG23	1	0.13
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	2	0.13
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	2	0.13
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	2	0.13
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	2	0.13
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	2	0.13
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	2	0.13
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	2	0.13
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	2	0.13
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	2	0.13
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	4	0.13
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	4	0.13
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	4	0.13
(2,2724)	1:26:A:HIS:HD2	1:123:A:VAL:HG21	1	0.13
(2,2724)	1:26:A:HIS:HD2	1:123:A:VAL:HG22	1	0.13
(2,2724)	1:26:A:HIS:HD2	1:123:A:VAL:HG23	1	0.13
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB1	5	0.13
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB2	5	0.13
(2,2642)	1:119:A:TYR:HE1	1:116:A:ALA:HB3	5	0.13
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB1	5	0.13
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB2	5	0.13
(2,2642)	1:119:A:TYR:HE2	1:116:A:ALA:HB3	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2628)	1:64:A:ILE:HD11	1:119:A:TYR:HB2	8	0.13
(2,2628)	1:64:A:ILE:HD12	1:119:A:TYR:HB2	8	0.13
(2,2628)	1:64:A:ILE:HD13	1:119:A:TYR:HB2	8	0.13
(2,2595)	1:64:A:ILE:HD11	1:116:A:ALA:HA	6	0.13
(2,2595)	1:64:A:ILE:HD12	1:116:A:ALA:HA	6	0.13
(2,2595)	1:64:A:ILE:HD13	1:116:A:ALA:HA	6	0.13
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	5	0.13
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD11	3	0.13
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD12	3	0.13
(2,2531)	1:113:A:VAL:HG21	1:64:A:ILE:HD13	3	0.13
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD11	3	0.13
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD12	3	0.13
(2,2531)	1:113:A:VAL:HG22	1:64:A:ILE:HD13	3	0.13
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD11	3	0.13
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD12	3	0.13
(2,2531)	1:113:A:VAL:HG23	1:64:A:ILE:HD13	3	0.13
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG21	1	0.13
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG22	1	0.13
(2,2528)	1:61:A:TYR:HE1	1:113:A:VAL:HG23	1	0.13
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG21	1	0.13
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG22	1	0.13
(2,2528)	1:61:A:TYR:HE2	1:113:A:VAL:HG23	1	0.13
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	3	0.13
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	9	0.13
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	3	0.13
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	9	0.13
(2,2296)	1:100:A:TRP:HE3	1:84:A:ARG:HD3	7	0.13
(2,2240)	1:97:A:HIS:HE1	1:95:A:SER:H	7	0.13
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	1	0.13
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	9	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	2	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	2	0.13
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	2	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	2	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	2	0.13
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	2	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	2	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	2	0.13
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	2	0.13
(2,1733)	1:75:A:GLN:HE21	1:75:A:GLN:HA	5	0.13
(2,1537)	1:68:A:MET:HB3	1:67:A:SER:HB2	9	0.13
(2,1527)	1:68:A:MET:HE1	1:65:A:LEU:H	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1527)	1:68:A:MET:HE2	1:65:A:LEU:H	5	0.13
(2,1527)	1:68:A:MET:HE3	1:65:A:LEU:H	5	0.13
(2,1517)	1:64:A:ILE:HD11	1:68:A:MET:HE1	6	0.13
(2,1517)	1:64:A:ILE:HD11	1:68:A:MET:HE2	6	0.13
(2,1517)	1:64:A:ILE:HD11	1:68:A:MET:HE3	6	0.13
(2,1517)	1:64:A:ILE:HD12	1:68:A:MET:HE1	6	0.13
(2,1517)	1:64:A:ILE:HD12	1:68:A:MET:HE2	6	0.13
(2,1517)	1:64:A:ILE:HD12	1:68:A:MET:HE3	6	0.13
(2,1517)	1:64:A:ILE:HD13	1:68:A:MET:HE1	6	0.13
(2,1517)	1:64:A:ILE:HD13	1:68:A:MET:HE2	6	0.13
(2,1517)	1:64:A:ILE:HD13	1:68:A:MET:HE3	6	0.13
(2,1516)	1:68:A:MET:HE1	1:64:A:ILE:HD11	6	0.13
(2,1516)	1:68:A:MET:HE1	1:64:A:ILE:HD12	6	0.13
(2,1516)	1:68:A:MET:HE1	1:64:A:ILE:HD13	6	0.13
(2,1516)	1:68:A:MET:HE2	1:64:A:ILE:HD11	6	0.13
(2,1516)	1:68:A:MET:HE2	1:64:A:ILE:HD12	6	0.13
(2,1516)	1:68:A:MET:HE2	1:64:A:ILE:HD13	6	0.13
(2,1516)	1:68:A:MET:HE3	1:64:A:ILE:HD11	6	0.13
(2,1516)	1:68:A:MET:HE3	1:64:A:ILE:HD12	6	0.13
(2,1516)	1:68:A:MET:HE3	1:64:A:ILE:HD13	6	0.13
(2,1515)	1:68:A:MET:HE1	1:64:A:ILE:HA	8	0.13
(2,1515)	1:68:A:MET:HE2	1:64:A:ILE:HA	8	0.13
(2,1515)	1:68:A:MET:HE3	1:64:A:ILE:HA	8	0.13
(2,1402)	1:64:A:ILE:HD11	1:60:A:VAL:HG11	5	0.13
(2,1402)	1:64:A:ILE:HD11	1:60:A:VAL:HG12	5	0.13
(2,1402)	1:64:A:ILE:HD11	1:60:A:VAL:HG13	5	0.13
(2,1402)	1:64:A:ILE:HD12	1:60:A:VAL:HG11	5	0.13
(2,1402)	1:64:A:ILE:HD12	1:60:A:VAL:HG12	5	0.13
(2,1402)	1:64:A:ILE:HD12	1:60:A:VAL:HG13	5	0.13
(2,1402)	1:64:A:ILE:HD13	1:60:A:VAL:HG11	5	0.13
(2,1402)	1:64:A:ILE:HD13	1:60:A:VAL:HG12	5	0.13
(2,1402)	1:64:A:ILE:HD13	1:60:A:VAL:HG13	5	0.13
(2,1332)	1:61:A:TYR:HE1	1:58:A:LEU:HD21	3	0.13
(2,1332)	1:61:A:TYR:HE1	1:58:A:LEU:HD22	3	0.13
(2,1332)	1:61:A:TYR:HE1	1:58:A:LEU:HD23	3	0.13
(2,1332)	1:61:A:TYR:HE2	1:58:A:LEU:HD21	3	0.13
(2,1332)	1:61:A:TYR:HE2	1:58:A:LEU:HD22	3	0.13
(2,1332)	1:61:A:TYR:HE2	1:58:A:LEU:HD23	3	0.13
(2,1257)	1:56:A:GLN:H	1:57:A:THR:HB	10	0.13
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD21	7	0.13
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD22	7	0.13
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD23	7	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1011)	1:46:A:HIS:HD2	1:42:A:ILE:HG13	2	0.13
(2,814)	1:36:A:VAL:HG21	1:35:A:LYS:HD2	2	0.13
(2,814)	1:36:A:VAL:HG22	1:35:A:LYS:HD2	2	0.13
(2,814)	1:36:A:VAL:HG23	1:35:A:LYS:HD2	2	0.13
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	10	0.13
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	1	0.13
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	9	0.13
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	9	0.13
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	9	0.13
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	8	0.13
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	8	0.13
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	8	0.13
(2,141)	1:5:A:LYS:H	1:5:A:LYS:HE2	1	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	9	0.13
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	9	0.13
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	4	0.12
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	1	0.12
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	1	0.12
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	1	0.12
(2,3450)	1:142:A:LEU:HD11	1:138:A:TRP:HZ2	1	0.12
(2,3450)	1:142:A:LEU:HD12	1:138:A:TRP:HZ2	1	0.12
(2,3450)	1:142:A:LEU:HD13	1:138:A:TRP:HZ2	1	0.12
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD11	1	0.12
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD12	1	0.12
(2,3449)	1:138:A:TRP:HZ2	1:142:A:LEU:HD13	1	0.12
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD21	2	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD22	2	0.12
(2,3235)	1:11:A:LYS:HE2	1:137:A:LEU:HD23	2	0.12
(2,3234)	1:137:A:LEU:HD21	1:11:A:LYS:HE2	2	0.12
(2,3234)	1:137:A:LEU:HD22	1:11:A:LYS:HE2	2	0.12
(2,3234)	1:137:A:LEU:HD23	1:11:A:LYS:HE2	2	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	2	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	2	0.12
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	2	0.12
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD21	9	0.12
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD22	9	0.12
(2,3191)	1:136:A:MET:HB3	1:133:A:LEU:HD23	9	0.12
(2,3113)	1:134:A:GLN:HE21	1:131:A:GLY:HA2	7	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	1	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	1	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	1	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	4	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	4	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	4	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG21	7	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG22	7	0.12
(2,2862)	1:128:A:ARG:HD2	1:37:A:THR:HG23	7	0.12
(2,2798)	1:119:A:TYR:HE1	1:125:A:ALA:H	2	0.12
(2,2798)	1:119:A:TYR:HE2	1:125:A:ALA:H	2	0.12
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE1	9	0.12
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE2	9	0.12
(2,2697)	1:122:A:GLU:HG2	1:68:A:MET:HE3	9	0.12
(2,2696)	1:68:A:MET:HE1	1:122:A:GLU:HG2	9	0.12
(2,2696)	1:68:A:MET:HE2	1:122:A:GLU:HG2	9	0.12
(2,2696)	1:68:A:MET:HE3	1:122:A:GLU:HG2	9	0.12
(2,2626)	1:119:A:TYR:HE1	1:38:A:GLY:HA2	6	0.12
(2,2626)	1:119:A:TYR:HE2	1:38:A:GLY:HA2	6	0.12
(2,2452)	1:108:A:ASP:H	1:106:A:THR:HB	8	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD21	3	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD22	3	0.12
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD23	3	0.12
(2,2395)	1:104:A:LEU:HD21	1:63:A:GLN:HE21	3	0.12
(2,2395)	1:104:A:LEU:HD22	1:63:A:GLN:HE21	3	0.12
(2,2395)	1:104:A:LEU:HD23	1:63:A:GLN:HE21	3	0.12
(2,2295)	1:100:A:TRP:HE3	1:84:A:ARG:HB2	3	0.12
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	3	0.12
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	9	0.12
(2,2192)	1:94:A:LYS:H	1:92:A:PHE:HB2	2	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	6	0.12
(2,1916)	1:83:A:LEU:HB3	1:80:A:LEU:HD21	10	0.12
(2,1916)	1:83:A:LEU:HB3	1:80:A:LEU:HD22	10	0.12
(2,1916)	1:83:A:LEU:HB3	1:80:A:LEU:HD23	10	0.12
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	6	0.12
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	6	0.12
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	6	0.12
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG21	8	0.12
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG22	8	0.12
(2,1757)	1:76:A:ILE:HG21	1:73:A:VAL:HG23	8	0.12
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG21	8	0.12
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG22	8	0.12
(2,1757)	1:76:A:ILE:HG22	1:73:A:VAL:HG23	8	0.12
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG21	8	0.12
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG22	8	0.12
(2,1757)	1:76:A:ILE:HG23	1:73:A:VAL:HG23	8	0.12
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG21	7	0.12
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG22	7	0.12
(2,1681)	1:70:A:SER:H	1:74:A:ILE:HG23	7	0.12
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	4	0.12
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	4	0.12
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	4	0.12
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	8	0.12
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	1	0.12
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	1	0.12
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	1	0.12
(2,1190)	1:51:A:LEU:HD11	1:54:A:MET:HB2	3	0.12
(2,1190)	1:51:A:LEU:HD12	1:54:A:MET:HB2	3	0.12
(2,1190)	1:51:A:LEU:HD13	1:54:A:MET:HB2	3	0.12
(2,884)	1:41:A:PHE:H	1:39:A:LEU:HB2	3	0.12
(2,813)	1:36:A:VAL:HG11	1:35:A:LYS:HA	7	0.12
(2,813)	1:36:A:VAL:HG12	1:35:A:LYS:HA	7	0.12
(2,813)	1:36:A:VAL:HG13	1:35:A:LYS:HA	7	0.12
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	6	0.12
(2,761)	1:32:A:SER:H	1:33:A:LYS:H	6	0.12
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	8	0.12
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG21	5	0.12
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG22	5	0.12
(2,637)	1:25:A:SER:HB3	1:24:A:ILE:HG23	5	0.12
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD11	1	0.12
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD12	1	0.12
(2,581)	1:23:A:ASP:H	1:21:A:ILE:HD13	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	1	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	1	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	7	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	7	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	10	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD11	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD12	1:64:A:ILE:HD13	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD11	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD12	10	0.12
(1,2542)	1:114:A:LEU:HD13	1:64:A:ILE:HD13	10	0.12
(2,3490)	1:143:A:SER:H	1:141:A:ASP:HA	5	0.11
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD21	3	0.11
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD22	3	0.11
(2,3469)	1:141:A:ASP:H	1:142:A:LEU:HD23	3	0.11
(2,3454)	1:138:A:TRP:HE1	1:142:A:LEU:HD21	9	0.11
(2,3454)	1:138:A:TRP:HE1	1:142:A:LEU:HD22	9	0.11
(2,3454)	1:138:A:TRP:HE1	1:142:A:LEU:HD23	9	0.11
(2,3167)	1:136:A:MET:HB2	1:54:A:MET:HE1	9	0.11
(2,3167)	1:136:A:MET:HB2	1:54:A:MET:HE2	9	0.11
(2,3167)	1:136:A:MET:HB2	1:54:A:MET:HE3	9	0.11
(2,3163)	1:49:A:LEU:HD11	1:136:A:MET:HB2	8	0.11
(2,3163)	1:49:A:LEU:HD12	1:136:A:MET:HB2	8	0.11
(2,3163)	1:49:A:LEU:HD13	1:136:A:MET:HB2	8	0.11
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD11	8	0.11
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD12	8	0.11
(2,3162)	1:136:A:MET:HB2	1:49:A:LEU:HD13	8	0.11
(2,3108)	1:134:A:GLN:HG2	1:18:A:VAL:HA	3	0.11
(2,3088)	1:133:A:LEU:HG	1:130:A:GLN:HA	2	0.11
(2,3087)	1:130:A:GLN:HA	1:133:A:LEU:HG	2	0.11
(2,3009)	1:130:A:GLN:HG3	1:127:A:SER:HA	7	0.11
(2,2948)	1:129:A:LEU:H	1:128:A:ARG:HD2	8	0.11
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG21	10	0.11
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG22	10	0.11
(2,2761)	1:119:A:TYR:HB2	1:124:A:VAL:HG23	10	0.11
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG11	7	0.11
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG12	7	0.11
(2,2733)	1:29:A:SER:H	1:123:A:VAL:HG13	7	0.11
(2,2704)	1:122:A:GLU:H	1:73:A:VAL:HG11	9	0.11
(2,2704)	1:122:A:GLU:H	1:73:A:VAL:HG12	9	0.11
(2,2704)	1:122:A:GLU:H	1:73:A:VAL:HG13	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2626)	1:119:A:TYR:HE1	1:38:A:GLY:HA2	5	0.11
(2,2626)	1:119:A:TYR:HE2	1:38:A:GLY:HA2	5	0.11
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB1	7	0.11
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB2	7	0.11
(2,2597)	1:64:A:ILE:HD11	1:116:A:ALA:HB3	7	0.11
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB1	7	0.11
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB2	7	0.11
(2,2597)	1:64:A:ILE:HD12	1:116:A:ALA:HB3	7	0.11
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB1	7	0.11
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB2	7	0.11
(2,2597)	1:64:A:ILE:HD13	1:116:A:ALA:HB3	7	0.11
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD11	7	0.11
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD12	7	0.11
(2,2596)	1:116:A:ALA:HB1	1:64:A:ILE:HD13	7	0.11
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD11	7	0.11
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD12	7	0.11
(2,2596)	1:116:A:ALA:HB2	1:64:A:ILE:HD13	7	0.11
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD11	7	0.11
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD12	7	0.11
(2,2596)	1:116:A:ALA:HB3	1:64:A:ILE:HD13	7	0.11
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG21	6	0.11
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG22	6	0.11
(2,2580)	1:115:A:GLU:HG2	1:113:A:VAL:HG23	6	0.11
(2,2579)	1:113:A:VAL:HG21	1:115:A:GLU:HG2	6	0.11
(2,2579)	1:113:A:VAL:HG22	1:115:A:GLU:HG2	6	0.11
(2,2579)	1:113:A:VAL:HG23	1:115:A:GLU:HG2	6	0.11
(2,2550)	1:114:A:LEU:H	1:41:A:PHE:HZ	8	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD11	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD12	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD13	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD21	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD22	1	0.11
(2,2481)	1:56:A:GLN:HE21	1:110:A:LEU:HD23	1	0.11
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD21	10	0.11
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD22	10	0.11
(2,2396)	1:63:A:GLN:HE21	1:104:A:LEU:HD23	10	0.11
(2,2395)	1:104:A:LEU:HD21	1:63:A:GLN:HE21	10	0.11
(2,2395)	1:104:A:LEU:HD22	1:63:A:GLN:HE21	10	0.11
(2,2395)	1:104:A:LEU:HD23	1:63:A:GLN:HE21	10	0.11
(2,2305)	1:84:A:ARG:H	1:100:A:TRP:HZ3	10	0.11
(2,2304)	1:100:A:TRP:HZ3	1:84:A:ARG:H	10	0.11
(2,2131)	1:91:A:ALA:HA	1:3:A:ILE:HG13	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD11	9	0.11
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD12	9	0.11
(2,2030)	1:84:A:ARG:HE	1:87:A:LEU:HD13	9	0.11
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD11	8	0.11
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD12	8	0.11
(2,1836)	1:79:A:ASP:HB2	1:76:A:ILE:HD13	8	0.11
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	8	0.11
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	8	0.11
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	8	0.11
(2,1227)	1:56:A:GLN:H	1:53:A:LYS:HB2	6	0.11
(2,1167)	1:53:A:LYS:HD2	1:53:A:LYS:HG2	3	0.11
(2,1030)	1:46:A:HIS:HD2	1:47:A:PRO:HD3	10	0.11
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG21	4	0.11
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG22	4	0.11
(2,829)	1:34:A:GLN:HE21	1:37:A:THR:HG23	4	0.11
(2,656)	1:26:A:HIS:HE1	1:23:A:ASP:HA	2	0.11
(2,655)	1:26:A:HIS:HD2	1:23:A:ASP:HA	6	0.11
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	3	0.11
(2,426)	1:16:A:THR:H	1:15:A:LYS:HD2	5	0.11
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD21	3	0.1
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD22	3	0.1
(2,3198)	1:136:A:MET:HG3	1:133:A:LEU:HD23	3	0.1
(2,3186)	1:136:A:MET:HE1	1:87:A:LEU:HD21	1	0.1
(2,3186)	1:136:A:MET:HE1	1:87:A:LEU:HD22	1	0.1
(2,3186)	1:136:A:MET:HE1	1:87:A:LEU:HD23	1	0.1
(2,3186)	1:136:A:MET:HE2	1:87:A:LEU:HD21	1	0.1
(2,3186)	1:136:A:MET:HE2	1:87:A:LEU:HD22	1	0.1
(2,3186)	1:136:A:MET:HE2	1:87:A:LEU:HD23	1	0.1
(2,3186)	1:136:A:MET:HE3	1:87:A:LEU:HD21	1	0.1
(2,3186)	1:136:A:MET:HE3	1:87:A:LEU:HD22	1	0.1
(2,3186)	1:136:A:MET:HE3	1:87:A:LEU:HD23	1	0.1
(2,2784)	1:61:A:TYR:HE1	1:125:A:ALA:HB1	6	0.1
(2,2784)	1:61:A:TYR:HE1	1:125:A:ALA:HB2	6	0.1
(2,2784)	1:61:A:TYR:HE1	1:125:A:ALA:HB3	6	0.1
(2,2784)	1:61:A:TYR:HE2	1:125:A:ALA:HB1	6	0.1
(2,2784)	1:61:A:TYR:HE2	1:125:A:ALA:HB2	6	0.1
(2,2784)	1:61:A:TYR:HE2	1:125:A:ALA:HB3	6	0.1
(2,2767)	1:124:A:VAL:HB	1:121:A:THR:HA	10	0.1
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD11	4	0.1
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD12	4	0.1
(2,2734)	1:123:A:VAL:HG11	1:42:A:ILE:HD13	4	0.1
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD11	4	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD12	4	0.1
(2,2734)	1:123:A:VAL:HG12	1:42:A:ILE:HD13	4	0.1
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD11	4	0.1
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD12	4	0.1
(2,2734)	1:123:A:VAL:HG13	1:42:A:ILE:HD13	4	0.1
(2,2693)	1:68:A:MET:HE1	1:122:A:GLU:HB3	9	0.1
(2,2693)	1:68:A:MET:HE2	1:122:A:GLU:HB3	9	0.1
(2,2693)	1:68:A:MET:HE3	1:122:A:GLU:HB3	9	0.1
(2,2676)	1:68:A:MET:HE1	1:121:A:THR:HG21	3	0.1
(2,2676)	1:68:A:MET:HE1	1:121:A:THR:HG22	3	0.1
(2,2676)	1:68:A:MET:HE1	1:121:A:THR:HG23	3	0.1
(2,2676)	1:68:A:MET:HE2	1:121:A:THR:HG21	3	0.1
(2,2676)	1:68:A:MET:HE2	1:121:A:THR:HG22	3	0.1
(2,2676)	1:68:A:MET:HE2	1:121:A:THR:HG23	3	0.1
(2,2676)	1:68:A:MET:HE3	1:121:A:THR:HG21	3	0.1
(2,2676)	1:68:A:MET:HE3	1:121:A:THR:HG22	3	0.1
(2,2676)	1:68:A:MET:HE3	1:121:A:THR:HG23	3	0.1
(2,2675)	1:121:A:THR:HG21	1:68:A:MET:HE1	3	0.1
(2,2675)	1:121:A:THR:HG21	1:68:A:MET:HE2	3	0.1
(2,2675)	1:121:A:THR:HG21	1:68:A:MET:HE3	3	0.1
(2,2675)	1:121:A:THR:HG22	1:68:A:MET:HE1	3	0.1
(2,2675)	1:121:A:THR:HG22	1:68:A:MET:HE2	3	0.1
(2,2675)	1:121:A:THR:HG22	1:68:A:MET:HE3	3	0.1
(2,2675)	1:121:A:THR:HG23	1:68:A:MET:HE1	3	0.1
(2,2675)	1:121:A:THR:HG23	1:68:A:MET:HE2	3	0.1
(2,2675)	1:121:A:THR:HG23	1:68:A:MET:HE3	3	0.1
(2,2389)	1:63:A:GLN:HB2	1:104:A:LEU:HD11	6	0.1
(2,2389)	1:63:A:GLN:HB2	1:104:A:LEU:HD12	6	0.1
(2,2389)	1:63:A:GLN:HB2	1:104:A:LEU:HD13	6	0.1
(2,2203)	1:94:A:LYS:HB2	1:94:A:LYS:HD2	10	0.1
(2,1566)	1:68:A:MET:HE1	1:69:A:PRO:HD2	5	0.1
(2,1566)	1:68:A:MET:HE2	1:69:A:PRO:HD2	5	0.1
(2,1566)	1:68:A:MET:HE3	1:69:A:PRO:HD2	5	0.1
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG21	8	0.1
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG22	8	0.1
(2,1418)	1:61:A:TYR:HE1	1:64:A:ILE:HG23	8	0.1
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG21	8	0.1
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG22	8	0.1
(2,1418)	1:61:A:TYR:HE2	1:64:A:ILE:HG23	8	0.1
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD21	9	0.1
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD22	9	0.1
(2,1147)	1:53:A:LYS:H	1:49:A:LEU:HD23	9	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1014)	1:46:A:HIS:HD2	1:45:A:LEU:HB2	2	0.1
(2,1011)	1:46:A:HIS:HD2	1:42:A:ILE:HG13	1	0.1
(2,832)	1:37:A:THR:H	1:35:A:LYS:HD2	9	0.1
(2,779)	1:34:A:GLN:HG2	1:31:A:SER:HB2	8	0.1
(2,729)	1:29:A:SER:H	1:27:A:THR:HB	1	0.1
(2,467)	1:18:A:VAL:H	1:16:A:THR:HB	8	0.1
(2,224)	1:8:A:ASP:HB2	1:5:A:LYS:HB3	4	0.1

10 Dihedral-angle violation analysis

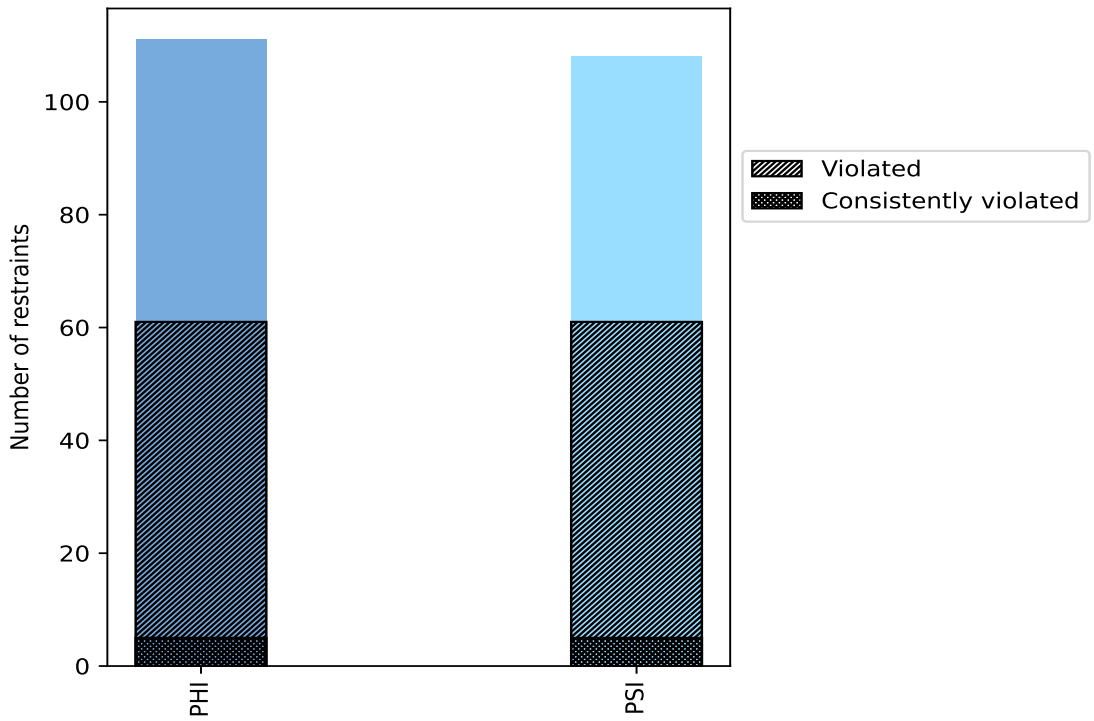
10.1 Summary of dihedral-angle violations

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	111	50.7	61	55.0	27.9	5	4.5	2.3
PSI	108	49.3	61	56.5	27.9	5	4.6	2.3
Total	219	100.0	122	55.7	55.7	10	4.6	4.6

[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



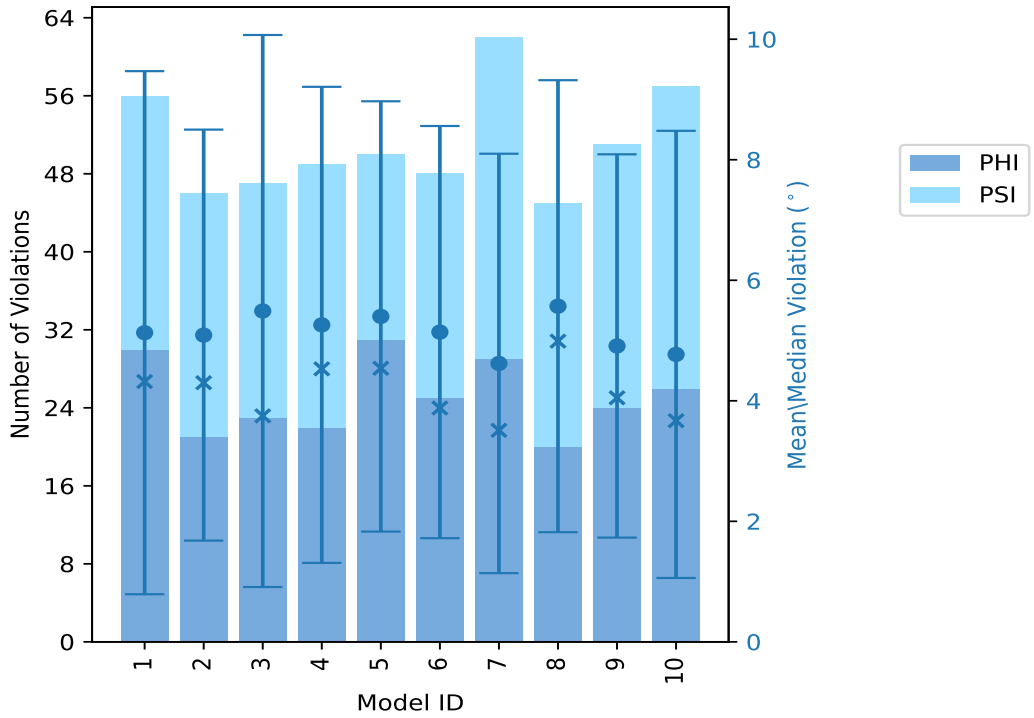
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	PSI	Total				
1	30	26	56	5.13	21.74	4.34	4.32
2	21	25	46	5.09	16.27	3.41	4.3
3	23	24	47	5.49	21.63	4.58	3.75
4	22	27	49	5.26	18.69	3.95	4.53
5	31	19	50	5.4	16.87	3.57	4.54
6	25	23	48	5.14	15.87	3.42	3.88
7	29	33	62	4.62	14.9	3.48	3.51
8	20	25	45	5.57	16.14	3.75	4.99
9	24	27	51	4.91	14.69	3.18	4.05
10	26	31	57	4.77	19.92	3.71	3.67

10.2.1 Bar graph : Dihedral violation statistics for each model



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

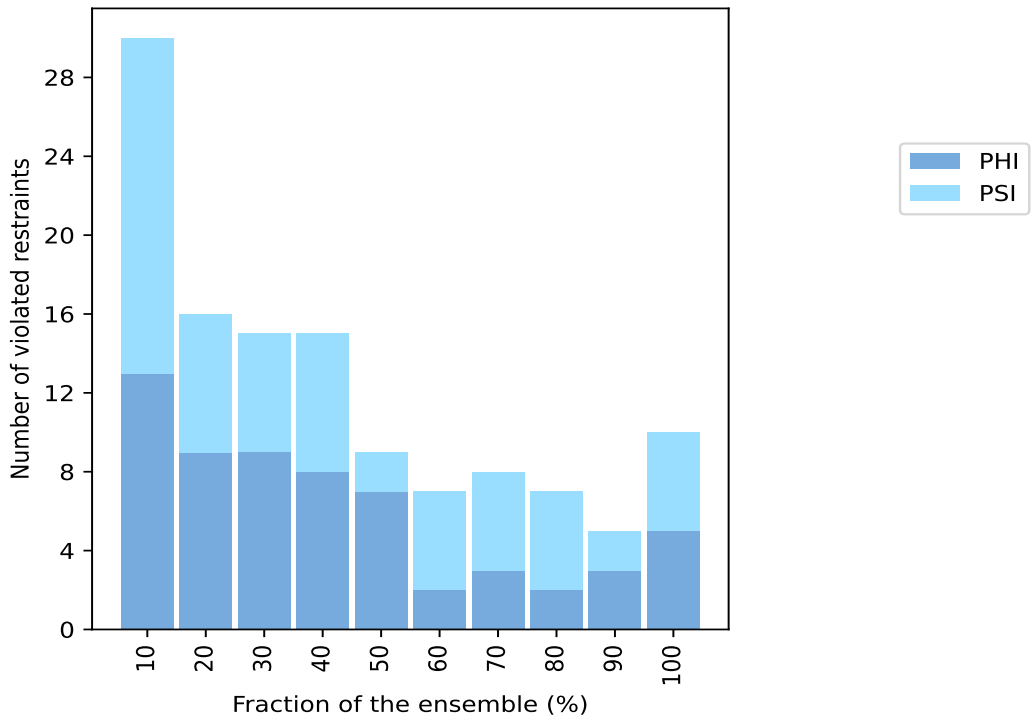
10.3 Dihedral-angle violation statistics for the ensemble

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
13	17	30	1	10.0
9	7	16	2	20.0
9	6	15	3	30.0
8	7	15	4	40.0
7	2	9	5	50.0
2	5	7	6	60.0
3	5	8	7	70.0
2	5	7	8	80.0
3	2	5	9	90.0
5	5	10	10	100.0

[1] Number of models with violations

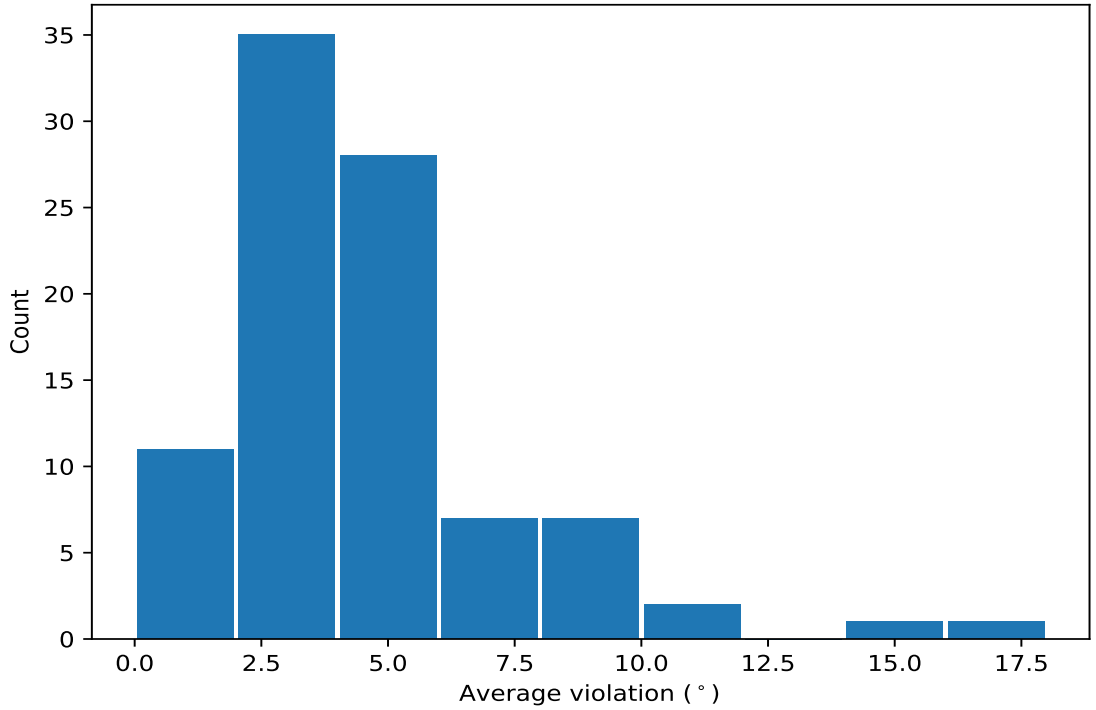
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble



10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

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
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	10	16.65	1.51	16.35
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	10	8.98	1.49	9.2
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	10	8.64	3.28	8.48
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	10	8.43	1.97	8.16
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	10	8.16	2.04	8.42
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	10	6.1	2.32	5.94
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	10	5.76	1.43	5.23
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	10	5.72	1.97	5.62
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	10	5.27	1.47	5.62
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	10	4.03	1.69	4.56
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	9	14.81	4.1	14.33
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	9	10.91	5.09	10.92
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	9	9.5	4.79	7.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	9	6.52	2.46	7.2
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	9	2.49	0.75	2.32
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	8	7.47	3.49	9.59
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	8	5.31	1.66	5.44
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	8	5.24	4.28	3.06
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	8	4.77	2.41	4.69
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	8	4.73	1.83	5.08
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	8	4.57	1.76	4.97
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	8	2.34	0.87	1.95
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	7	5.73	1.76	5.73
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	7	5.17	2.27	4.99
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	7	5.05	1.93	4.74
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	7	4.71	1.71	4.35
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	7	3.78	1.36	3.82
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	7	3.14	1.27	3.5
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	7	3.09	1.07	2.84
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	7	3.02	1.49	2.1
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	6	5.72	1.71	5.43
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	6	4.05	2.39	3.56
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	6	3.3	0.99	3.49
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	6	3.17	1.53	2.46
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	6	3.02	2.37	2.19
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	6	2.6	1.41	1.98
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	6	2.24	0.73	2.04
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	5	9.3	4.41	9.4
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	5	7.0	1.1	6.99
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	5	5.67	2.95	4.69
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	5	5.46	3.54	4.64
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	4.62	1.15	4.53
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	5	4.56	1.64	4.64
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	5	2.32	0.63	2.4
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	5	2.17	0.96	1.75
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	5	2.14	0.77	2.06
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	4	10.45	4.68	11.02
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	4	5.49	3.67	4.92
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	4	4.94	2.25	5.56
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	4	4.42	1.38	4.83
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	4	4.18	1.61	3.94
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	4	4.02	2.35	4.18
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	4	3.78	0.78	3.5
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	4	3.72	0.96	3.45
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	4	3.43	2.08	2.9
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	4	3.15	1.44	3.48
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	4	3.07	1.64	2.66
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	4	2.42	1.67	1.7
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	4	2.37	1.25	1.86
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	4	2.12	0.64	2.33
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	4	1.7	0.45	1.63
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	3	7.36	1.52	8.07
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	3	6.42	0.99	6.21
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	3	5.28	2.04	6.25

Continued on next page...

Continued from previous page...

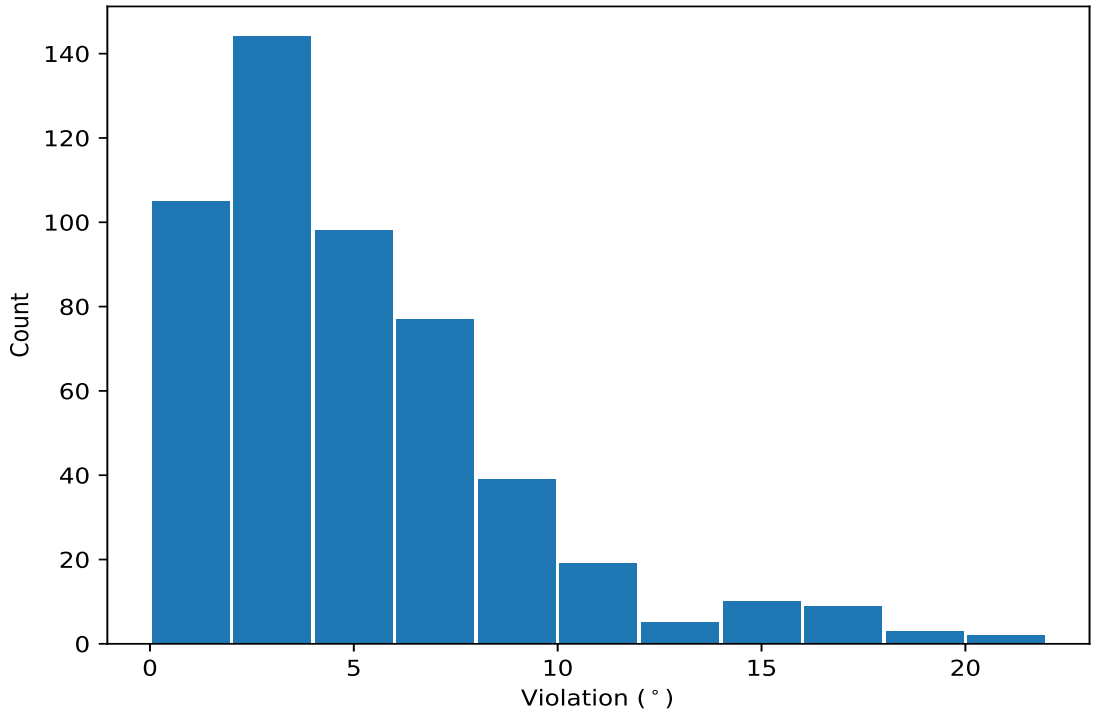
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	3	4.21	2.46	4.53
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	3	4.09	1.87	5.37
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	3	4.0	0.83	3.75
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	3	3.14	0.61	3.19
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	3	3.01	0.28	3.14
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	3	2.43	0.34	2.29
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	3	2.4	0.9	2.51
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	3	2.37	1.17	1.66
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	3	2.3	1.02	1.64
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	3	2.29	0.33	2.35
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	3	1.84	0.95	1.28
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	3	1.68	0.48	1.74
(1,59)	1:48:A:ILE:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	2	8.43	1.93	8.43
(1,118)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:GLU:N	2	7.89	1.41	7.89
(1,218)	1:143:A:SER:N	1:143:A:SER:CA	1:143:A:SER:C	1:144:A:PRO:N	2	2.95	1.0	2.95
(1,25)	1:14:A:ILE:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	2	2.7	0.1	2.7
(1,126)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ASP:N	2	2.66	0.22	2.66
(1,71)	1:54:A:MET:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	2	2.19	0.42	2.19
(1,19)	1:11:A:LYS:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	2	2.15	0.06	2.15
(1,132)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:HIS:N	2	2.11	0.38	2.11
(1,11)	1:7:A:GLN:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	2	1.88	0.75	1.88
(1,17)	1:10:A:THR:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	2	1.84	0.34	1.84
(1,90)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1:65:A:LEU:N	2	1.78	0.46	1.78
(1,148)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:CYS:N	2	1.64	0.36	1.64
(1,219)	1:145:A:GLY:C	1:146:A:CYS:N	1:146:A:CYS:CA	1:146:A:CYS:C	2	1.43	0.19	1.43
(1,87)	1:62:A:GLN:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	2	1.35	0.24	1.35
(1,82)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:TYR:N	2	1.32	0.03	1.32
(1,3)	1:3:A:ILE:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	2	1.06	0.03	1.06

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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 (°)
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	1	21.74
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	3	21.63
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	10	19.92
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	3	18.97
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	4	18.69
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	4	17.65
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	5	16.87
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	1	16.73
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	3	16.43
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	1	16.38
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	2	16.27
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1	16.26
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	4	16.19
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	8	16.14
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	6	15.87
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	8	15.61
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	10	15.24
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	5	15.05
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	7	14.9
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	7	14.83
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	6	14.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:96:A:CYS:C	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	9	14.69
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	9	14.33
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	3	14.06
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	8	13.78
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	7	13.71
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	8	12.82
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	10	12.56
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	2	12.49
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	9	11.88
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	2	11.75
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	1	11.5
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	10	11.4
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	6	11.07
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	2	10.99
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	5	10.92
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	9	10.73
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	9	10.57
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	1	10.51
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	2	10.46
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	4	10.44
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	7	10.38
(1,59)	1:48:A:ILE:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	2	10.37
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	7	10.3
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	3	10.3
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	10	10.27
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	10	10.25
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	4	10.21
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	5	9.94
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	7	9.91
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	6	9.86
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	10	9.84
(1,155)	1:99:A:PRO:C	1:100:A:TRP:N	1:100:A:TRP:CA	1:100:A:TRP:C	8	9.8
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	7	9.65
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	6	9.63
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	4	9.61
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	6	9.56
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	5	9.53
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	5	9.49
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	7	9.46
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	5	9.4
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	5	9.38
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	7	9.36
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	9	9.33
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	8	9.31
(1,118)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:GLU:N	2	9.3
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	5	9.18
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	6	9.15
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	8	9.0
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	8	8.93
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	5	8.87
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	1	8.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1	8.77
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	2	8.66
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	2	8.63
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	4	8.52
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	6	8.5
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	3	8.35
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	3	8.32
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	5	8.3
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	8	8.28
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	3	8.23
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	3	8.18
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	7	8.11
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	6	8.08
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	7	8.07
(1,42)	1:23:A:ASP:N	1:23:A:ASP:CA	1:23:A:ASP:C	1:24:A:ILE:N	3	8.0
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	6	7.98
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	10	7.95
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	8	7.94
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	8	7.89
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	3	7.8
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	9	7.76
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	9	7.74
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	3	7.72
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	1	7.62
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	4	7.61
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	7	7.61
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	5	7.61
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	10	7.59
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	10	7.59
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	4	7.56
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	3	7.52
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	1	7.47
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	3	7.46
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	8	7.46
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	1	7.38
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	5	7.36
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	5	7.3
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	10	7.3
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	2	7.25
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	3	7.23
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	4	7.2
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	9	7.19
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	5	7.16
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	6	7.16
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	5	7.13
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	6	7.08
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	5	7.05
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	4	6.99
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	6	6.95
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	4	6.89
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	9	6.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	8	6.87
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1	6.85
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	7	6.81
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	2	6.77
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	8	6.7
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	2	6.65
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	9	6.65
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	5	6.62
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	4	6.61
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	5	6.6
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	5	6.59
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	10	6.58
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	6	6.58
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	6	6.57
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	8	6.54
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1	6.51
(1,59)	1:48:A:ILE:C	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	7	6.5
(1,141)	1:91:A:ALA:C	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	4	6.49
(1,118)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:GLU:N	10	6.48
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	7	6.45
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1	6.43
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	6	6.41
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	1	6.38
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	8	6.34
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	9	6.29
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	8	6.28
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	9	6.28
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	8	6.27
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	9	6.27
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	10	6.25
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	10	6.21
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	6	6.2
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	7	6.19
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	5	6.18
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	3	6.15
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	3	6.14
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	4	6.07
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	6	6.05
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	5	6.04
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	7	6.03
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	8	6.03
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	9	5.99
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	8	5.98
(1,160)	1:104:A:LEU:N	1:104:A:LEU:CA	1:104:A:LEU:C	1:105:A:GLU:N	9	5.95
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	2	5.9
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	7	5.87
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	10	5.85
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1	5.83
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	7	5.82
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	9	5.77
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	3	5.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	1	5.73
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	3	5.7
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	3	5.66
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	7	5.66
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	2	5.63
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	10	5.63
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	6	5.6
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	6	5.55
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	6	5.55
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	2	5.5
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	8	5.46
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	10	5.45
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	4	5.42
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	1	5.38
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	6	5.37
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	2	5.37
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	4	5.36
(1,172)	1:110:A:LEU:N	1:110:A:LEU:CA	1:110:A:LEU:C	1:111:A:GLY:N	1	5.33
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1	5.33
(1,73)	1:55:A:ASP:C	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	10	5.31
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	3	5.3
(1,67)	1:52:A:SER:C	1:53:A:LYS:N	1:53:A:LYS:CA	1:53:A:LYS:C	4	5.28
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	4	5.26
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	1	5.26
(1,27)	1:15:A:LYS:C	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	2	5.25
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	7	5.23
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	6	5.23
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	7	5.23
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	9	5.22
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	9	5.18
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	8	5.15
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	7	5.12
(1,53)	1:41:A:PHE:C	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1	5.11
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	1	5.08
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	5	5.05
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	9	5.04
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	1	5.03
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	4	5.01
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	5	5.0
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	8	4.99
(1,26)	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	1:16:A:THR:N	7	4.97
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	2	4.96
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	2	4.95
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	1	4.93
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	9	4.89
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	8	4.85
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	4	4.81
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	7	4.79
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	1	4.78
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	7	4.74
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	10	4.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	1	4.69
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	4	4.64
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	4	4.64
(1,52)	1:41:A:PHE:N	1:41:A:PHE:CA	1:41:A:PHE:C	1:42:A:ILE:N	4	4.63
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	7	4.62
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	10	4.62
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	10	4.61
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	2	4.6
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	8	4.55
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	5	4.54
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	4	4.53
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	4.53
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	4	4.53
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	10	4.49
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	2	4.45
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	5	4.43
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	9	4.4
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	2	4.39
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	7	4.37
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	9	4.35
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	2	4.35
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	1	4.33
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1	4.32
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	3	4.31
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	9	4.28
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	10	4.27
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	5	4.27
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	4	4.27
(1,152)	1:97:A:HIS:N	1:97:A:HIS:CA	1:97:A:HIS:C	1:98:A:LEU:N	2	4.26
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	3	4.25
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1	4.23
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	10	4.23
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	9	4.16
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	9	4.05
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	4	4.04
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	6	4.02
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	7	4.0
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	10	3.98
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	9	3.96
(1,218)	1:143:A:SER:N	1:143:A:SER:CA	1:143:A:SER:C	1:144:A:PRO:N	10	3.95
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	2	3.94
(1,133)	1:87:A:LEU:C	1:88:A:HIS:N	1:88:A:HIS:CA	1:88:A:HIS:C	4	3.89
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	4	3.89
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	5	3.88
(1,213)	1:140:A:LEU:C	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	9	3.85
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1	3.85
(1,128)	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	1:86:A:LEU:N	4	3.85
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	9	3.84
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	10	3.82
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	4	3.77
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	8	3.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	9	3.75
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	6	3.75
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	3	3.75
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	9	3.75
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	2	3.74
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	2	3.73
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	7	3.73
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:GLN:N	2	3.72
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	10	3.67
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	9	3.64
(1,41)	1:22:A:ASN:C	1:23:A:ASP:N	1:23:A:ASP:CA	1:23:A:ASP:C	6	3.64
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	5	3.61
(1,212)	1:140:A:LEU:N	1:140:A:LEU:CA	1:140:A:LEU:C	1:141:A:ASP:N	10	3.6
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	5	3.58
(1,70)	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	1:55:A:ASP:N	7	3.57
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	10	3.56
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	10	3.56
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	1	3.5
(1,89)	1:63:A:GLN:C	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	9	3.48
(1,196)	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	1:133:A:LEU:N	7	3.45
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	1	3.45
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	4	3.45
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	2	3.44
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	3	3.44
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	10	3.42
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	3	3.36
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	6	3.36
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	9	3.34
(1,76)	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	1:58:A:LEU:N	8	3.33
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	7	3.31
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	7	3.31
(1,142)	1:92:A:PHE:N	1:92:A:PHE:CA	1:92:A:PHE:C	1:93:A:SER:N	6	3.29
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	2	3.28
(1,22)	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1:14:A:ILE:N	6	3.28
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	8	3.27
(1,198)	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	1:134:A:GLN:N	3	3.26
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1	3.25
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	8	3.25
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	3	3.23
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	10	3.19
(1,86)	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	1:63:A:GLN:N	8	3.19
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	3	3.17
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	9	3.14
(1,157)	1:101:A:ALA:C	1:102:A:SER:N	1:102:A:SER:CA	1:102:A:SER:C	5	3.12
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	9	3.09
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	8	3.04
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	6	3.04
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	2	3.03
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	10	3.02
(1,104)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:ILE:N	9	3.02
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	4	3.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	9	3.0
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	10	2.97
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	6	2.93
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	8	2.9
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1	2.89
(1,126)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ASP:N	5	2.87
(1,115)	1:78:A:ASN:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	2	2.87
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	10	2.84
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	3	2.83
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	6	2.82
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	6	2.8
(1,25)	1:14:A:ILE:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	5	2.8
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	1	2.78
(1,178)	1:122:A:GLU:N	1:122:A:GLU:CA	1:122:A:GLU:C	1:123:A:VAL:N	1	2.77
(1,184)	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	1:126:A:LEU:N	1	2.75
(1,37)	1:20:A:ARG:C	1:21:A:ILE:N	1:21:A:ILE:CA	1:21:A:ILE:C	2	2.73
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	6	2.7
(1,88)	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1:64:A:ILE:N	6	2.69
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	7	2.67
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	3	2.66
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	2	2.65
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	2	2.64
(1,11)	1:7:A:GLN:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	10	2.63
(1,74)	1:56:A:GLN:N	1:56:A:GLN:CA	1:56:A:GLN:C	1:57:A:THR:N	8	2.62
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	10	2.62
(1,71)	1:54:A:MET:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	9	2.61
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	3	2.61
(1,25)	1:14:A:ILE:C	1:15:A:LYS:N	1:15:A:LYS:CA	1:15:A:LYS:C	9	2.59
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	2	2.58
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	3	2.56
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	6	2.56
(1,111)	1:76:A:ILE:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	5	2.55
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	1	2.54
(1,69)	1:53:A:LYS:C	1:54:A:MET:N	1:54:A:MET:CA	1:54:A:MET:C	8	2.53
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	6	2.52
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	8	2.51
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	4	2.5
(1,132)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:HIS:N	10	2.49
(1,126)	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	1:85:A:ASP:N	8	2.44
(1,124)	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	1:84:A:ARG:N	5	2.44
(1,60)	1:49:A:LEU:N	1:49:A:LEU:CA	1:49:A:LEU:C	1:50:A:THR:N	7	2.44
(1,179)	1:122:A:GLU:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	7	2.42
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	6	2.4
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	9	2.4
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	4	2.39
(1,167)	1:107:A:LEU:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	3	2.37
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	10	2.37
(1,102)	1:72:A:ASN:N	1:72:A:ASN:CA	1:72:A:ASN:C	1:73:A:VAL:N	10	2.36
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	1	2.35
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	7	2.32
(1,72)	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	1:56:A:GLN:N	4	2.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	8	2.3
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	5	2.29
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	7	2.29
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	6	2.27
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	7	2.26
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	2	2.25
(1,117)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	2.24
(1,90)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1:65:A:LEU:N	4	2.24
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	5	2.24
(1,19)	1:11:A:LYS:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	10	2.21
(1,85)	1:61:A:TYR:C	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	7	2.19
(1,17)	1:10:A:THR:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	7	2.17
(1,83)	1:60:A:VAL:C	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	5	2.16
(1,84)	1:61:A:TYR:N	1:61:A:TYR:CA	1:61:A:TYR:C	1:62:A:GLN:N	2	2.14
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	5	2.12
(1,165)	1:106:A:THR:C	1:107:A:LEU:N	1:107:A:LEU:CA	1:107:A:LEU:C	3	2.11
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	10	2.1
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1	2.1
(1,19)	1:11:A:LYS:C	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	6	2.09
(1,207)	1:137:A:LEU:C	1:138:A:TRP:N	1:138:A:TRP:CA	1:138:A:TRP:C	5	2.08
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	2	2.07
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	7	2.06
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	9	2.06
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	4	2.03
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	9	2.03
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	5	2.01
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	3	2.01
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	7	2.01
(1,148)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:CYS:N	7	1.99
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	3	1.98
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	4	1.97
(1,218)	1:143:A:SER:N	1:143:A:SER:CA	1:143:A:SER:C	1:144:A:PRO:N	7	1.95
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	10	1.93
(1,15)	1:9:A:ASP:C	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	6	1.93
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	5	1.91
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	6	1.88
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	3	1.88
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	2	1.87
(1,187)	1:126:A:LEU:C	1:127:A:SER:N	1:127:A:SER:CA	1:127:A:SER:C	8	1.86
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	7	1.86
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	10	1.85
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	4	1.85
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	9	1.85
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	7	1.85
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	4	1.82
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	8	1.81
(1,43)	1:23:A:ASP:C	1:24:A:ILE:N	1:24:A:ILE:CA	1:24:A:ILE:C	10	1.78
(1,71)	1:54:A:MET:C	1:55:A:ASP:N	1:55:A:ASP:CA	1:55:A:ASP:C	5	1.77
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	7	1.77
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	2	1.75
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	7	1.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	6	1.74
(1,132)	1:87:A:LEU:N	1:87:A:LEU:CA	1:87:A:LEU:C	1:88:A:HIS:N	4	1.73
(1,20)	1:12:A:THR:N	1:12:A:THR:CA	1:12:A:THR:C	1:13:A:LEU:N	10	1.73
(1,30)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	1	1.72
(1,58)	1:48:A:ILE:N	1:48:A:ILE:CA	1:48:A:ILE:C	1:49:A:LEU:N	7	1.71
(1,36)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ILE:N	7	1.68
(1,123)	1:82:A:ASN:C	1:83:A:LEU:N	1:83:A:LEU:CA	1:83:A:LEU:C	5	1.67
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	3	1.67
(1,116)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	7	1.67
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1	1.66
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	9	1.64
(1,4)	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	1:5:A:LYS:N	4	1.64
(1,219)	1:145:A:GLY:C	1:146:A:CYS:N	1:146:A:CYS:CA	1:146:A:CYS:C	7	1.62
(1,99)	1:70:A:SER:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	8	1.61
(1,79)	1:58:A:LEU:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	5	1.61
(1,66)	1:52:A:SER:N	1:52:A:SER:CA	1:52:A:SER:C	1:53:A:LYS:N	1	1.6
(1,96)	1:67:A:SER:N	1:67:A:SER:CA	1:67:A:SER:C	1:68:A:MET:N	8	1.59
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	8	1.59
(1,87)	1:62:A:GLN:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	1	1.58
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	6	1.56
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	10	1.55
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	5	1.55
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	1	1.55
(1,103)	1:72:A:ASN:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	2	1.55
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	9	1.54
(1,78)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:ALA:N	3	1.53
(1,17)	1:10:A:THR:C	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	8	1.5
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	3	1.49
(1,164)	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	1:107:A:LEU:N	2	1.45
(1,186)	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	1:127:A:SER:N	4	1.44
(1,81)	1:59:A:ALA:C	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	10	1.44
(1,75)	1:56:A:GLN:C	1:57:A:THR:N	1:57:A:THR:CA	1:57:A:THR:C	10	1.43
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	1	1.42
(1,193)	1:129:A:LEU:C	1:130:A:GLN:N	1:130:A:GLN:CA	1:130:A:GLN:C	5	1.42
(1,34)	1:19:A:THR:N	1:19:A:THR:CA	1:19:A:THR:C	1:20:A:ARG:N	6	1.4
(1,23)	1:13:A:LEU:C	1:14:A:ILE:N	1:14:A:ILE:CA	1:14:A:ILE:C	3	1.39
(1,216)	1:142:A:LEU:N	1:142:A:LEU:CA	1:142:A:LEU:C	1:143:A:SER:N	3	1.36
(1,180)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:VAL:N	1	1.35
(1,82)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:TYR:N	1	1.35
(1,61)	1:49:A:LEU:C	1:50:A:THR:N	1:50:A:THR:CA	1:50:A:THR:C	2	1.35
(1,16)	1:10:A:THR:N	1:10:A:THR:CA	1:10:A:THR:C	1:11:A:LYS:N	7	1.35
(1,5)	1:4:A:GLN:C	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	9	1.35
(1,90)	1:64:A:ILE:N	1:64:A:ILE:CA	1:64:A:ILE:C	1:65:A:LEU:N	8	1.32
(1,97)	1:69:A:PRO:C	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	3	1.3
(1,82)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:TYR:N	10	1.29
(1,12)	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	1:9:A:ASP:N	1	1.29
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	4	1.28
(1,148)	1:95:A:SER:N	1:95:A:SER:CA	1:95:A:SER:C	1:96:A:CYS:N	1	1.28
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	7	1.28
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	10	1.27
(1,125)	1:83:A:LEU:C	1:84:A:ARG:N	1:84:A:ARG:CA	1:84:A:ARG:C	9	1.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,219)	1:145:A:GLY:C	1:146:A:CYS:N	1:146:A:CYS:CA	1:146:A:CYS:C	1	1.24
(1,112)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	2	1.24
(1,181)	1:123:A:VAL:C	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	7	1.22
(1,50)	1:27:A:THR:N	1:27:A:THR:CA	1:27:A:THR:C	1:28:A:GLN:N	7	1.21
(1,195)	1:131:A:GLY:C	1:132:A:SER:N	1:132:A:SER:CA	1:132:A:SER:C	4	1.17
(1,183)	1:124:A:VAL:C	1:125:A:ALA:N	1:125:A:ALA:CA	1:125:A:ALA:C	10	1.16
(1,54)	1:42:A:ILE:N	1:42:A:ILE:CA	1:42:A:ILE:C	1:43:A:PRO:N	1	1.16
(1,29)	1:16:A:THR:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	7	1.16
(1,40)	1:22:A:ASN:N	1:22:A:ASN:CA	1:22:A:ASN:C	1:23:A:ASP:N	9	1.14
(1,11)	1:7:A:GLN:C	1:8:A:ASP:N	1:8:A:ASP:CA	1:8:A:ASP:C	9	1.14
(1,199)	1:133:A:LEU:C	1:134:A:GLN:N	1:134:A:GLN:CA	1:134:A:GLN:C	1	1.12
(1,204)	1:136:A:MET:N	1:136:A:MET:CA	1:136:A:MET:C	1:137:A:LEU:N	9	1.11
(1,87)	1:62:A:GLN:C	1:63:A:GLN:N	1:63:A:GLN:CA	1:63:A:GLN:C	3	1.11
(1,18)	1:11:A:LYS:N	1:11:A:LYS:CA	1:11:A:LYS:C	1:12:A:THR:N	4	1.11
(1,92)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:THR:N	5	1.1
(1,28)	1:16:A:THR:N	1:16:A:THR:CA	1:16:A:THR:C	1:17:A:ILE:N	7	1.09
(1,3)	1:3:A:ILE:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	10	1.09
(1,176)	1:121:A:THR:N	1:121:A:THR:CA	1:121:A:THR:C	1:122:A:GLU:N	10	1.08
(1,10)	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	1:8:A:ASP:N	7	1.08
(1,9)	1:6:A:VAL:C	1:7:A:GLN:N	1:7:A:GLN:CA	1:7:A:GLN:C	6	1.08
(1,119)	1:80:A:LEU:C	1:81:A:GLU:N	1:81:A:GLU:CA	1:81:A:GLU:C	4	1.07
(1,197)	1:132:A:SER:C	1:133:A:LEU:N	1:133:A:LEU:CA	1:133:A:LEU:C	7	1.06
(1,185)	1:125:A:ALA:C	1:126:A:LEU:N	1:126:A:LEU:CA	1:126:A:LEU:C	10	1.06
(1,154)	1:98:A:LEU:N	1:98:A:LEU:CA	1:98:A:LEU:C	1:99:A:PRO:N	8	1.06
(1,105)	1:73:A:VAL:C	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	6	1.06
(1,21)	1:12:A:THR:C	1:13:A:LEU:N	1:13:A:LEU:CA	1:13:A:LEU:C	1	1.06
(1,163)	1:105:A:GLU:C	1:106:A:THR:N	1:106:A:THR:CA	1:106:A:THR:C	5	1.05
(1,121)	1:81:A:GLU:C	1:82:A:ASN:N	1:82:A:ASN:CA	1:82:A:ASN:C	6	1.05
(1,182)	1:124:A:VAL:N	1:124:A:VAL:CA	1:124:A:VAL:C	1:125:A:ALA:N	2	1.04
(1,3)	1:3:A:ILE:C	1:4:A:GLN:N	1:4:A:GLN:CA	1:4:A:GLN:C	3	1.03
(1,127)	1:84:A:ARG:C	1:85:A:ASP:N	1:85:A:ASP:CA	1:85:A:ASP:C	1	1.02