



# Full wwPDB NMR Structure Validation Report i

Jun 6, 2023 – 07:54 pm BST

PDB ID : 7AFR  
BMRB ID : 34562  
Title : Ribosome maturation factor RimP (apo)  
Authors : Schedlbauer, A.; Iturrioz, I.; Ochoa-Lizarralde, B.; Diercks, T.; Fucini, P.; Connell, S.  
Deposited on : 2020-09-19

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

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

A user guide is available at

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

with specific help available everywhere you see the 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:

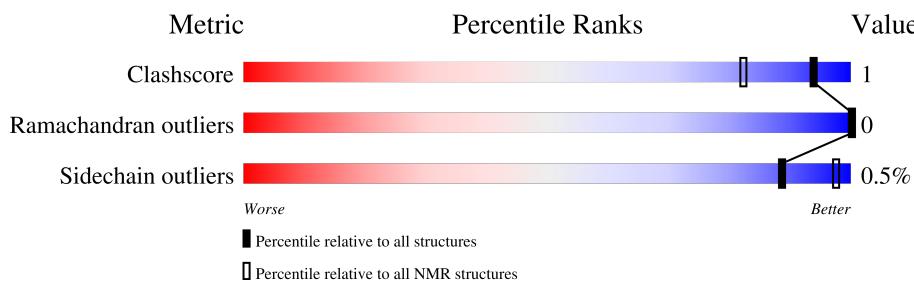
MolProbitiy	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

# 1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 87%.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	X	151	 87% 5% 7%

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 10 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	X:4-X:78 (75)	0.71	10
2	X:84-X:148 (65)	0.65	10

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

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

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2349 atoms, of which 1174 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribosome maturation factor RimP.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	X	151	2349	742	1174	197	231	5	0

There is a discrepancy between the modelled and reference sequences:

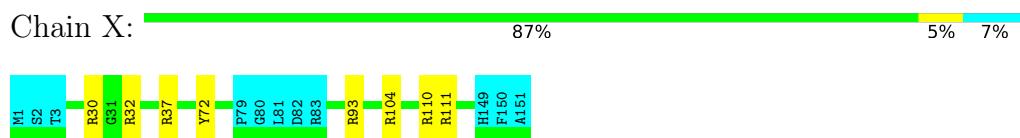
Chain	Residue	Modelled	Actual	Comment	Reference
X	151	ALA	-	expression tag	UNP A0A0J3VRH1

## 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: Ribosome maturation factor RimP

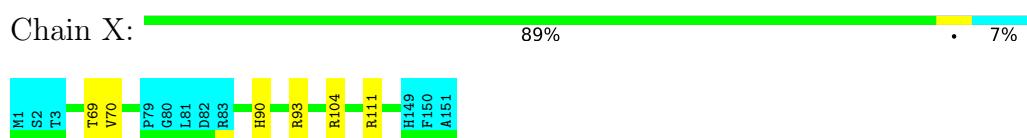


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

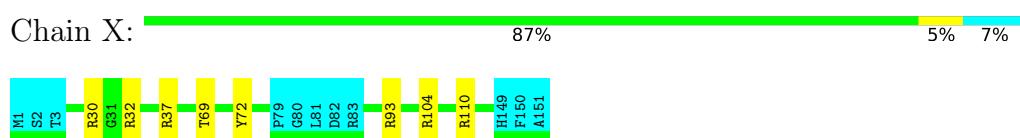
#### 4.2.1 Score per residue for model 1

- Molecule 1: Ribosome maturation factor RimP



#### 4.2.2 Score per residue for model 2

- Molecule 1: Ribosome maturation factor RimP



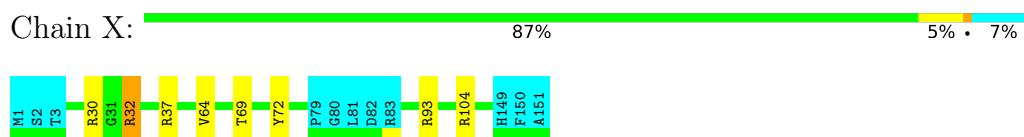
#### 4.2.3 Score per residue for model 3

- Molecule 1: Ribosome maturation factor RimP



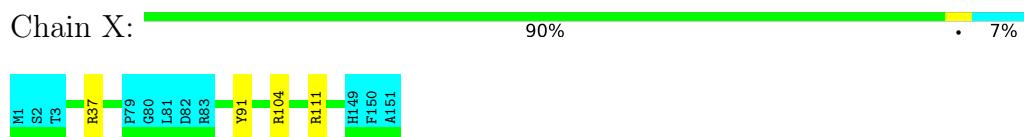
#### 4.2.4 Score per residue for model 4

- Molecule 1: Ribosome maturation factor RimP



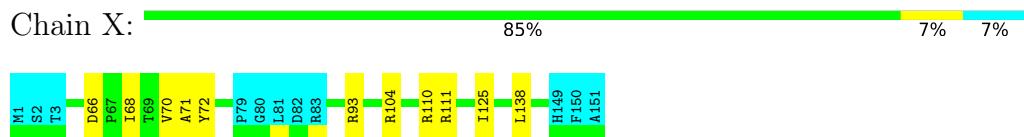
#### 4.2.5 Score per residue for model 5

- Molecule 1: Ribosome maturation factor RimP



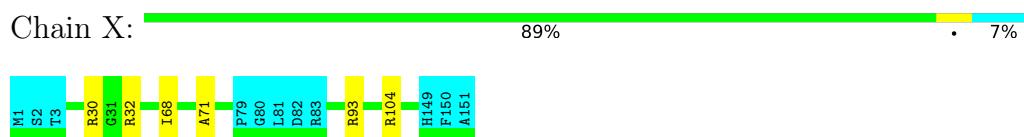
#### 4.2.6 Score per residue for model 6

- Molecule 1: Ribosome maturation factor RimP



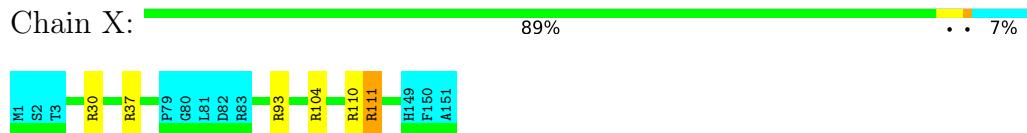
#### 4.2.7 Score per residue for model 7

- Molecule 1: Ribosome maturation factor RimP



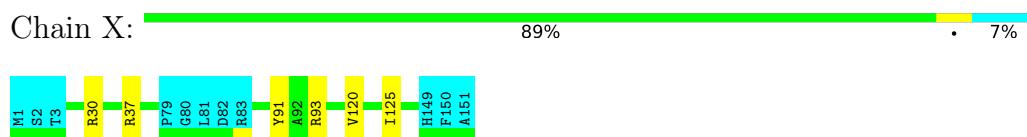
#### 4.2.8 Score per residue for model 8

- Molecule 1: Ribosome maturation factor RimP



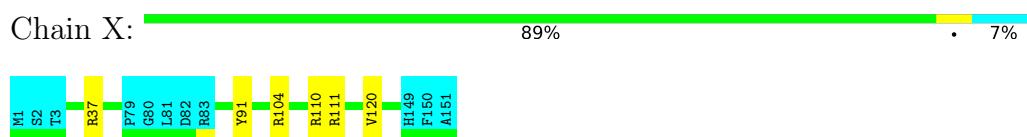
#### 4.2.9 Score per residue for model 9

- Molecule 1: Ribosome maturation factor RimP



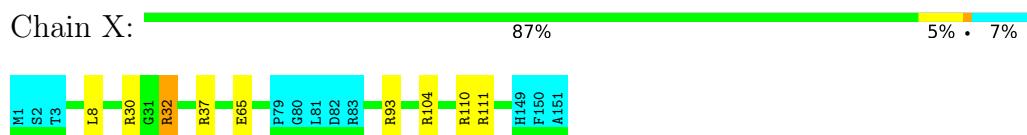
#### 4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Ribosome maturation factor RimP



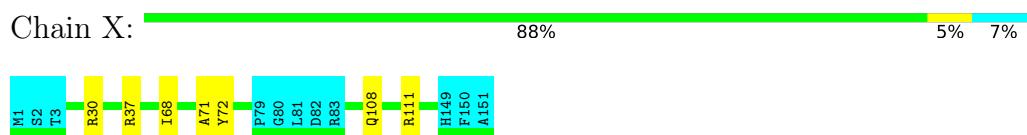
#### 4.2.11 Score per residue for model 11

- Molecule 1: Ribosome maturation factor RimP



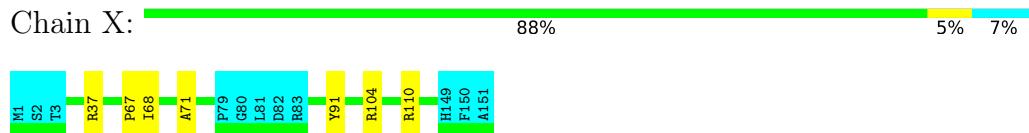
#### 4.2.12 Score per residue for model 12

- Molecule 1: Ribosome maturation factor RimP



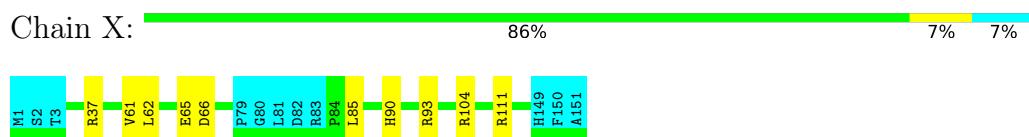
#### 4.2.13 Score per residue for model 13

- Molecule 1: Ribosome maturation factor RimP



#### 4.2.14 Score per residue for model 14

- Molecule 1: Ribosome maturation factor RimP



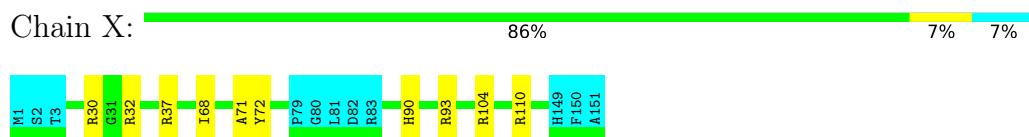
#### 4.2.15 Score per residue for model 15

- Molecule 1: Ribosome maturation factor RimP



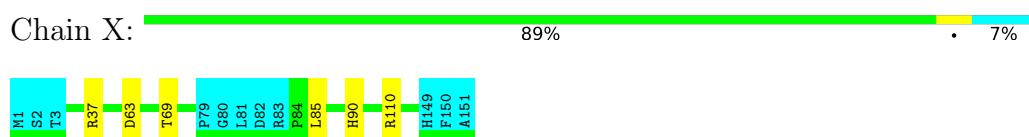
#### 4.2.16 Score per residue for model 16

- Molecule 1: Ribosome maturation factor RimP



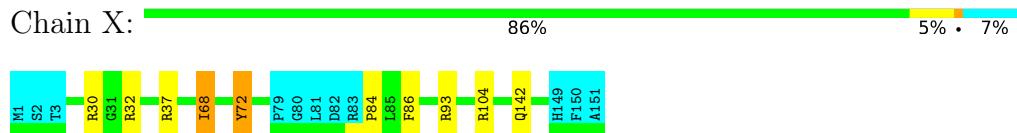
#### 4.2.17 Score per residue for model 17

- Molecule 1: Ribosome maturation factor RimP



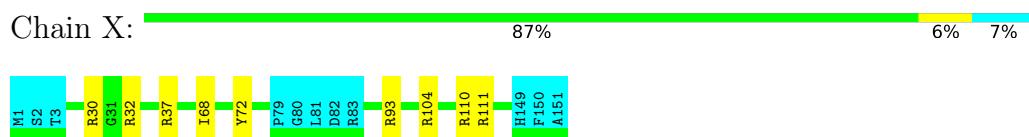
#### 4.2.18 Score per residue for model 18

- Molecule 1: Ribosome maturation factor RimP



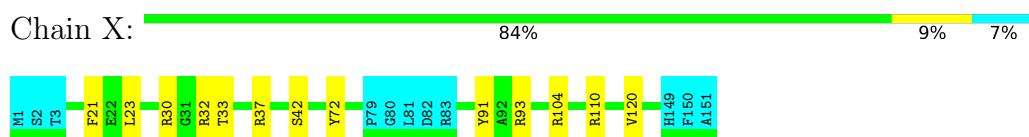
#### 4.2.19 Score per residue for model 19

- Molecule 1: Ribosome maturation factor RimP



#### 4.2.20 Score per residue for model 20

- Molecule 1: Ribosome maturation factor RimP



## 5 Refinement protocol and experimental data overview i

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

Of the 120 calculated structures, 20 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
X-PLOR NIH	structure calculation	
GROMACS	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	1755
Number of shifts mapped to atoms	1755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

## 6 Model quality [\(i\)](#)

### 6.1 Standard geometry [\(i\)](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	X	0.69±0.02	0±0/1105 ( 0.0± 0.0%)	0.98±0.04	5±2/1503 ( 0.3± 0.1%)
All	All	0.69	0/22100 ( 0.0%)	0.98	98/30060 ( 0.3%)

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

Mol	Chain	Chirality	Planarity
1	X	0.0±0.0	0.3±0.5
All	All	0	7

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(°)	Ideal(°)	Models	
								Worst	Total
1	X	30	ARG	NE-CZ-NH2	10.45	125.52	120.30	11	13
1	X	93	ARG	NE-CZ-NH2	9.88	125.24	120.30	20	14
1	X	32	ARG	NE-CZ-NH2	9.59	125.10	120.30	15	8
1	X	110	ARG	NE-CZ-NH2	9.35	124.98	120.30	19	11
1	X	37	ARG	NE-CZ-NH2	8.73	124.66	120.30	16	17
1	X	104	ARG	NE-CZ-NH2	8.53	124.56	120.30	14	14
1	X	111	ARG	NE-CZ-NH2	7.29	123.94	120.30	10	10
1	X	111	ARG	NE-CZ-NH1	-6.66	116.97	120.30	5	1
1	X	72	TYR	CB-CG-CD2	-6.10	117.34	121.00	4	6
1	X	37	ARG	NE-CZ-NH1	-5.45	117.58	120.30	19	2
1	X	110	ARG	NE-CZ-NH1	-5.22	117.69	120.30	20	1
1	X	32	ARG	NE-CZ-NH1	-5.09	117.75	120.30	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	X	32	ARG	Peptide	3
1	X	72	TYR	Sidechain	1
1	X	111	ARG	Sidechain	1
1	X	108	GLN	Peptide	1
1	X	23	LEU	Peptide	1

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	X	1089	1092	1092	3±2
All	All	21780	21840	21840	54

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:66:ASP:OD1	1:X:68:ILE:O	1.10	1.66	6	1
1:X:68:ILE:HG23	1:X:71:ALA:HB3	1.08	1.23	7	1
1:X:68:ILE:CG2	1:X:71:ALA:HB3	1.01	1.86	7	2
1:X:68:ILE:CG2	1:X:71:ALA:CB	0.91	2.48	7	2
1:X:68:ILE:O	1:X:72:TYR:HB2	0.88	1.68	18	1
1:X:68:ILE:HG23	1:X:71:ALA:CB	0.88	1.98	7	1
1:X:61:VAL:O	1:X:65:GLU:HG2	0.87	1.69	14	1
1:X:68:ILE:HG22	1:X:71:ALA:HB3	0.76	1.57	15	1
1:X:69:THR:HG22	1:X:70:VAL:H	0.72	1.43	1	1
1:X:90:HIS:ND1	1:X:93:ARG:NH1	0.71	2.38	16	1
1:X:68:ILE:HD12	1:X:71:ALA:HB3	0.70	1.61	3	1
1:X:68:ILE:O	1:X:68:ILE:HG23	0.69	1.86	16	1
1:X:90:HIS:CE1	1:X:93:ARG:NH1	0.68	2.62	16	1
1:X:68:ILE:O	1:X:72:TYR:HD2	0.65	1.73	15	1
1:X:69:THR:HG22	1:X:70:VAL:N	0.64	2.08	1	1
1:X:68:ILE:HG21	1:X:71:ALA:CB	0.63	2.21	7	1
1:X:68:ILE:O	1:X:68:ILE:HG13	0.60	1.96	19	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:X:68:ILE:HG22	1:X:71:ALA:CB	0.60	2.24	15	1
1:X:104:ARG:HG2	1:X:142:GLN:HB2	0.60	1.72	18	1
1:X:90:HIS:CE1	1:X:93:ARG:HH12	0.59	2.15	16	1
1:X:68:ILE:HG21	1:X:71:ALA:HB2	0.58	1.75	7	1
1:X:91:TYR:HB3	1:X:120:VAL:HG21	0.56	1.75	10	3
1:X:68:ILE:CG1	1:X:71:ALA:HB3	0.56	2.31	16	1
1:X:68:ILE:CG2	1:X:70:VAL:CG1	0.54	2.85	6	1
1:X:63:ASP:O	1:X:69:THR:HG22	0.52	2.04	17	1
1:X:68:ILE:CG2	1:X:71:ALA:HB2	0.52	2.31	7	1
1:X:68:ILE:O	1:X:72:TYR:CD2	0.51	2.60	15	1
1:X:69:THR:HG23	1:X:72:TYR:HB2	0.51	1.82	2	1
1:X:68:ILE:HG12	1:X:71:ALA:CB	0.50	2.36	12	1
1:X:67:PRO:HB2	1:X:68:ILE:HD12	0.50	1.84	13	1
1:X:68:ILE:O	1:X:72:TYR:CB	0.49	2.54	18	1
1:X:68:ILE:O	1:X:68:ILE:CG2	0.49	2.58	16	1
1:X:68:ILE:HG13	1:X:71:ALA:HB3	0.46	1.86	16	1
1:X:120:VAL:HG22	1:X:125:ILE:HG23	0.46	1.88	9	1
1:X:68:ILE:HG23	1:X:68:ILE:O	0.46	2.10	7	1
1:X:68:ILE:HG22	1:X:68:ILE:O	0.46	2.11	15	1
1:X:125:ILE:CD1	1:X:138:LEU:HD23	0.45	2.41	6	1
1:X:68:ILE:HG22	1:X:71:ALA:H	0.45	1.71	13	2
1:X:62:LEU:HD12	1:X:66:ASP:OD1	0.45	2.11	14	1
1:X:68:ILE:CG2	1:X:70:VAL:HG13	0.45	2.42	6	1
1:X:68:ILE:HD11	1:X:72:TYR:CE1	0.44	2.46	3	1
1:X:85:LEU:HD11	1:X:90:HIS:HB3	0.44	1.88	14	2
1:X:21:PHE:CD1	1:X:42:SER:HB3	0.43	2.49	20	1
1:X:61:VAL:O	1:X:65:GLU:CG	0.42	2.58	14	1
1:X:62:LEU:CD1	1:X:66:ASP:OD1	0.42	2.67	14	1
1:X:68:ILE:CG2	1:X:70:VAL:HG12	0.42	2.45	6	1
1:X:84:PRO:HG2	1:X:86:PHE:CE1	0.42	2.50	18	1
1:X:8:LEU:HD13	1:X:65:GLU:HG2	0.41	1.93	11	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	X	140/151 (93%)	137±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	100 100
All	All	2800/3020 (93%)	2738 (98%)	62 (2%)	0 (0%)	100 100

There are no Ramachandran outliers.

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	121/130 (93%)	120±1 (100±1%)	1±1 (0±1%)	89 97
All	All	2420/2600 (93%)	2409 (100%)	11 (0%)	89 97

All 8 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	X	90	HIS	2
1	X	91	TYR	2
1	X	72	TYR	2
1	X	127	VAL	1
1	X	64	VAL	1
1	X	69	THR	1
1	X	68	ILE	1
1	X	33	THR	1

### 6.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

## 6.7 Other polymers [\(i\)](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping (i)

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

Total number of shifts	1755
Number of shifts mapped to atoms	1755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	-0.03 $\pm$ 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	0.11 $\pm$ 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	147	0.27 $\pm$ 0.14	None needed (< 0.5 ppm)
$^{15}\text{N}$	138	-0.01 $\pm$ 0.24	None needed (< 0.5 ppm)

#### 7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1671 atoms were assigned a chemical shift out of a possible 1910. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	689/700 (98%)	279/284 (98%)	279/280 (100%)	131/136 (96%)
Sidechain	972/1107 (88%)	655/724 (90%)	310/347 (89%)	7/36 (19%)

*Continued on next page...*

*Continued from previous page...*

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	10/103 (10%)	10/51 (20%)	0/49 (0%)	0/3 (0%)
Overall	1671/1910 (87%)	944/1059 (89%)	589/676 (87%)	138/175 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1755 atoms were assigned a chemical shift out of a possible 2054. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	728/754 (97%)	295/306 (96%)	295/302 (98%)	138/146 (95%)
Sidechain	1015/1180 (86%)	684/772 (89%)	324/369 (88%)	7/39 (18%)
Aromatic	12/120 (10%)	12/60 (20%)	0/56 (0%)	0/4 (0%)
Overall	1755/2054 (85%)	991/1138 (87%)	619/727 (85%)	145/189 (77%)

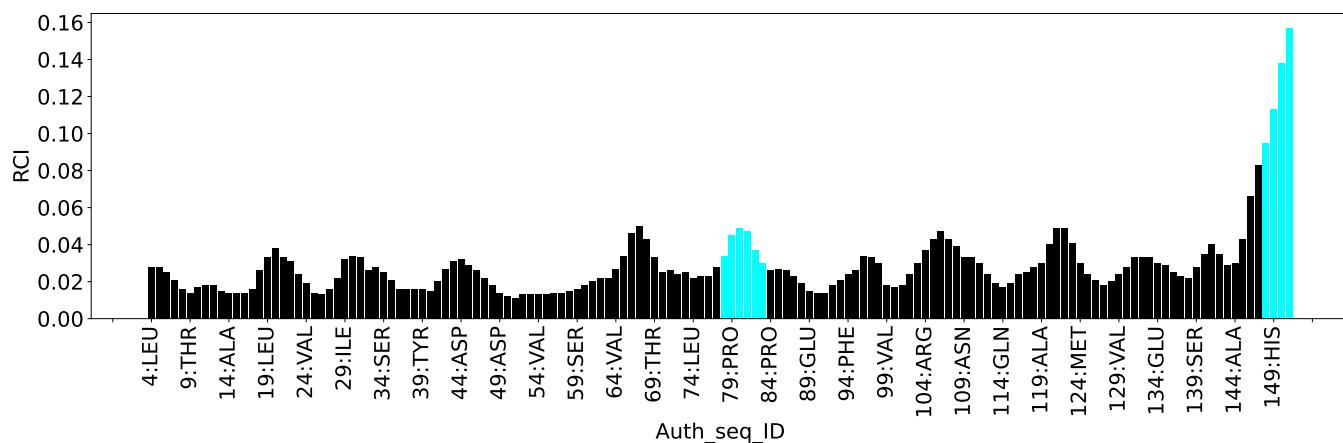
#### 7.1.4 Statistically unusual chemical shifts [\(i\)](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain X:



## 8 NMR restraints analysis i

### 8.1 Conformationally restricting restraints i

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	2559
Intra-residue ( $ i-j =0$ )	752
Sequential ( $ i-j =1$ )	876
Medium range ( $ i-j >1$ and $ i-j <5$ )	396
Long range ( $ i-j \geq 5$ )	395
Inter-chain	0
Hydrogen bond restraints	140
Disulfide bond restraints	0
Total dihedral-angle restraints	264
Number of unmapped restraints	0
Number of restraints per residue	18.7
Number of long range restraints per residue <sup>1</sup>	3.1

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations i

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 i

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)	45.0	0.2
0.2-0.5 (Medium)	59.5	0.5
>0.5 (Large)	31.6	4.78

### 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)	31.6	9.9
10.0-20.0 (Medium)	4.6	19.9
>20.0 (Large)	6.7	159.9

## 9 Distance violation analysis (i)

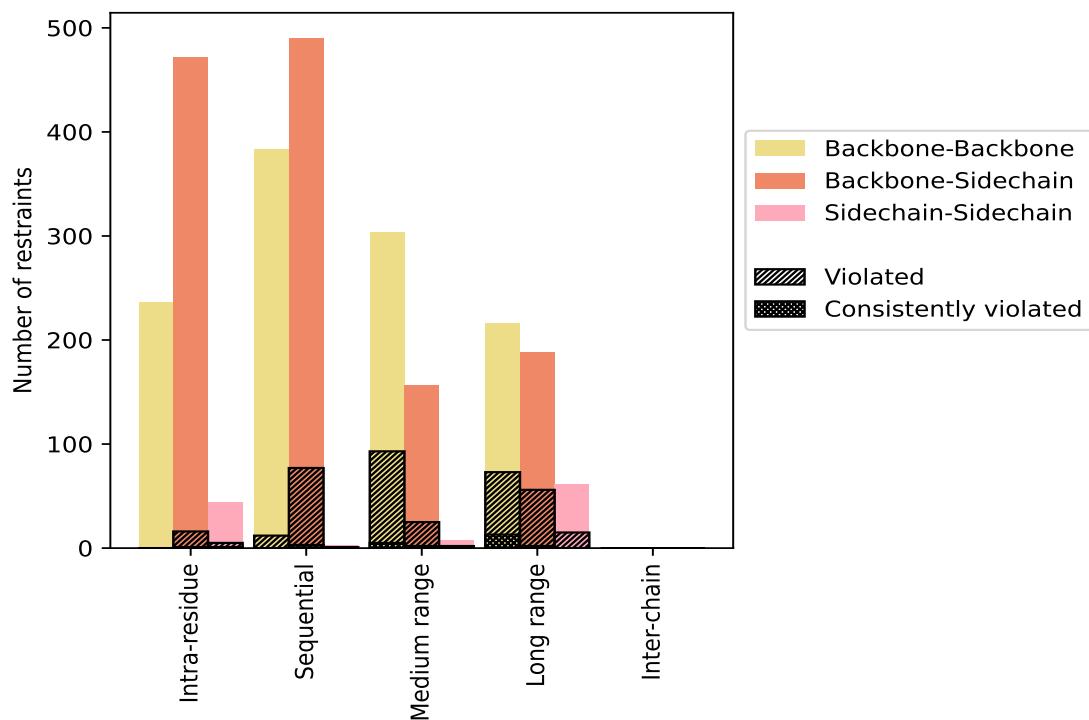
### 9.1 Summary of distance violations (i)

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	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
Intra-residue ( $ i-j =0$ )	752	29.4	21	2.8	0.8	2	0.3	0.1
Backbone-Backbone	236	9.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	472	18.4	16	3.4	0.6	1	0.2	0.0
Sidechain-Sidechain	44	1.7	5	11.4	0.2	1	2.3	0.0
Sequential ( $ i-j =1$ )	876	34.2	90	10.3	3.5	3	0.3	0.1
Backbone-Backbone	383	15.0	12	3.1	0.5	0	0.0	0.0
Backbone-Sidechain	490	19.1	77	15.7	3.0	3	0.6	0.1
Sidechain-Sidechain	3	0.1	1	33.3	0.0	0	0.0	0.0
Medium range ( $ i-j >1 \text{ & }  i-j <5$ )	396	15.5	86	21.7	3.4	5	1.3	0.2
Backbone-Backbone	233	9.1	59	25.3	2.3	3	1.3	0.1
Backbone-Sidechain	156	6.1	25	16.0	1.0	2	1.3	0.1
Sidechain-Sidechain	7	0.3	2	28.6	0.1	0	0.0	0.0
Long range ( $ i-j \geq 5$ )	395	15.4	125	31.6	4.9	9	2.3	0.4
Backbone-Backbone	146	5.7	54	37.0	2.1	7	4.8	0.3
Backbone-Sidechain	188	7.3	56	29.8	2.2	2	1.1	0.1
Sidechain-Sidechain	61	2.4	15	24.6	0.6	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	140	5.5	53	37.9	2.1	8	5.7	0.3
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2559	100.0	375	14.7	14.7	27	1.1	1.1
Backbone-Backbone	1138	44.5	178	15.6	7.0	18	1.6	0.7
Backbone-Sidechain	1306	51.0	174	13.3	6.8	8	0.6	0.3
Sidechain-Sidechain	115	4.5	23	20.0	0.9	1	0.9	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	10	29	54	56	0	149	0.43	2.46	0.36	0.32
2	11	27	57	54	0	149	0.41	2.1	0.31	0.31
3	8	27	45	56	0	136	0.38	1.51	0.29	0.28
4	8	28	53	53	0	142	0.35	2.26	0.28	0.24
5	10	26	43	77	0	156	0.4	1.85	0.3	0.3
6	9	29	35	51	0	124	0.36	2.38	0.32	0.29
7	6	22	41	48	0	117	0.41	1.61	0.31	0.3
8	9	20	45	36	0	110	0.37	1.62	0.27	0.29
9	10	30	49	52	0	141	0.42	1.74	0.33	0.33
10	9	27	62	51	0	149	0.42	2.27	0.37	0.3
11	6	30	50	54	0	140	0.45	4.78	0.57	0.26

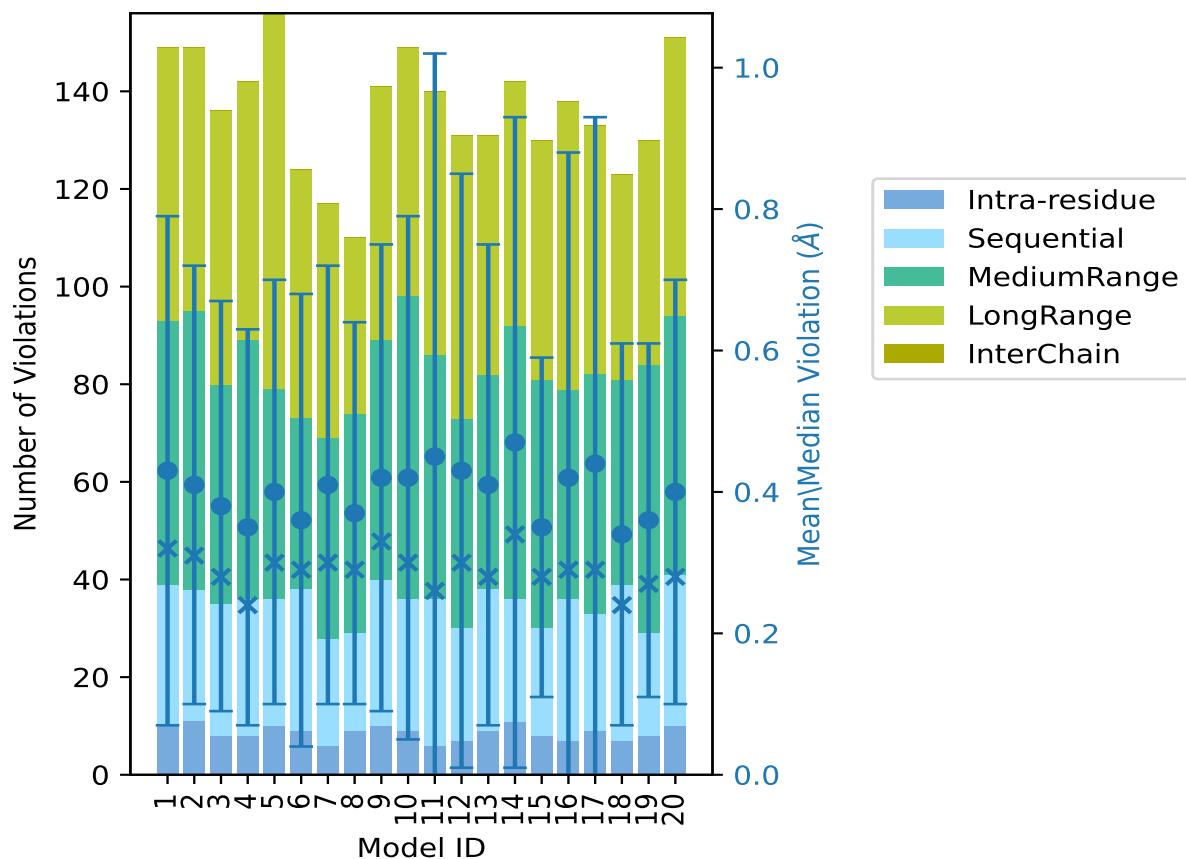
*Continued on next page...*

*Continued from previous page...*

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	7	23	43	58	0	131	0.43	2.76	0.42	0.3
13	9	29	44	49	0	131	0.41	2.27	0.34	0.28
14	11	25	56	50	0	142	0.47	3.02	0.46	0.34
15	8	22	51	49	0	130	0.35	1.3	0.24	0.28
16	7	29	43	59	0	138	0.42	3.13	0.46	0.29
17	9	24	49	51	0	133	0.44	3.3	0.49	0.29
18	7	32	42	42	0	123	0.34	1.58	0.27	0.24
19	8	21	55	46	0	130	0.36	1.63	0.25	0.27
20	10	31	53	57	0	151	0.4	1.77	0.3	0.28

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,  
<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

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



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

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

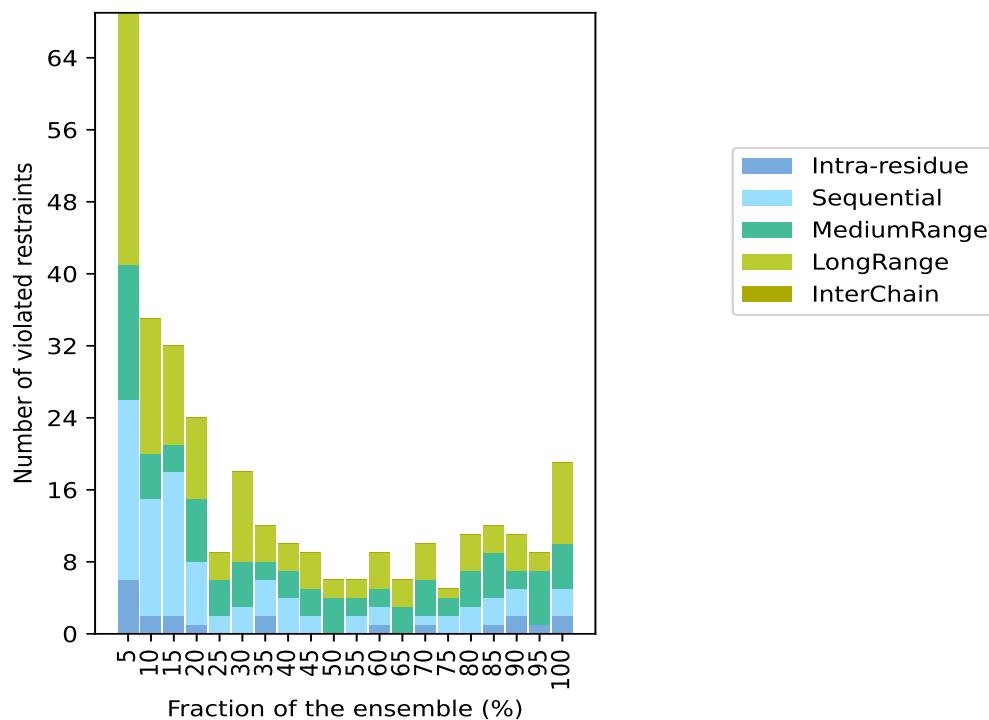
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2097(IR:731, SQ:786, MR:310, LR:270, IC:0) restraints are not violated in the ensemble.

IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Fraction of the ensemble	
						Count <sup>6</sup>	%
6	20	15	28	0	69	1	5.0
2	13	5	15	0	35	2	10.0
2	16	3	11	0	32	3	15.0
1	7	7	9	0	24	4	20.0
0	2	4	3	0	9	5	25.0
0	3	5	10	0	18	6	30.0
2	4	2	4	0	12	7	35.0
0	4	3	3	0	10	8	40.0
0	2	3	4	0	9	9	45.0
0	0	4	2	0	6	10	50.0
0	2	2	2	0	6	11	55.0
1	2	2	4	0	9	12	60.0
0	0	3	3	0	6	13	65.0
1	1	4	4	0	10	14	70.0
0	2	2	1	0	5	15	75.0
0	3	4	4	0	11	16	80.0
1	3	5	3	0	12	17	85.0
2	3	2	4	0	11	18	90.0
1	0	6	2	0	9	19	95.0
2	3	5	9	0	19	20	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

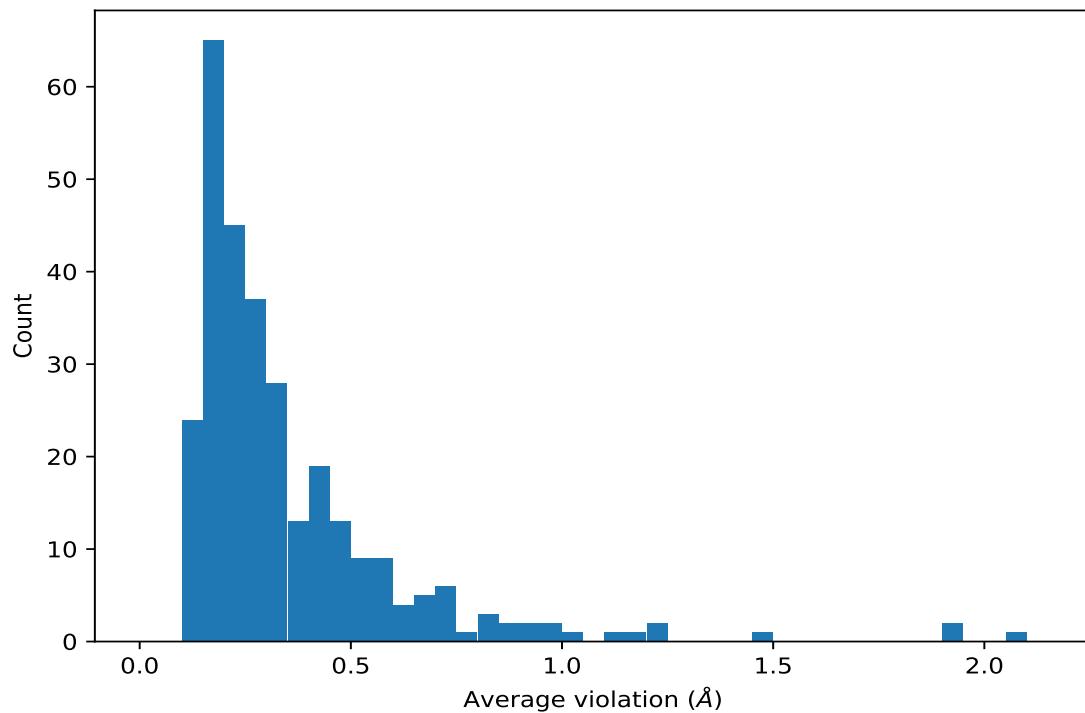
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [\(i\)](#)



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

### 9.4.1 Histogram : Distribution of mean distance violations [\(i\)](#)

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



#### 9.4.2 Table: Most violated distance restraints [\(i\)](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	20	1.49	0.66	1.6
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	20	1.2	0.14	1.21
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	20	1.16	0.16	1.15
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	20	1.12	0.66	0.76
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	20	1.0	0.2	0.96
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	20	0.93	0.48	0.98
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	20	0.81	0.52	0.49
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	20	0.8	0.3	0.88
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	20	0.75	0.22	0.71
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	20	0.7	0.17	0.66
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	20	0.7	0.39	0.62
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	20	0.67	0.2	0.62
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	20	0.66	0.11	0.64
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	20	0.62	0.2	0.66
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	20	0.62	0.09	0.62
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	20	0.57	0.18	0.57

Continued on next page...

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	20	0.56	0.21	0.55
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	20	0.51	0.11	0.48
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	20	0.51	0.16	0.56
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	20	0.44	0.01	0.45
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	20	0.42	0.2	0.44
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	20	0.41	0.18	0.38
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	20	0.41	0.1	0.4
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	20	0.31	0.0	0.31
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	20	0.3	0.13	0.28
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	20	0.24	0.16	0.21
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	20	0.22	0.16	0.2
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	19	0.57	0.25	0.6
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	19	0.43	0.02	0.43
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	19	0.38	0.15	0.37
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	19	0.35	0.12	0.35
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	19	0.32	0.11	0.31
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	19	0.31	0.11	0.29
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	19	0.27	0.12	0.23
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	19	0.26	0.1	0.26
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	19	0.24	0.08	0.23
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	18	1.21	1.33	0.57
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	18	0.48	0.11	0.49
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	18	0.43	0.02	0.43
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	18	0.42	0.01	0.42
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	18	0.41	0.19	0.44
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	18	0.4	0.15	0.38
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	18	0.39	0.12	0.41
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	18	0.32	0.19	0.26
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	18	0.3	0.12	0.3
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	18	0.3	0.12	0.27
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	18	0.21	0.06	0.2
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	18	0.2	0.05	0.18
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	17	0.85	0.32	0.88
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	17	0.67	0.37	0.6
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	17	0.58	0.39	0.48
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	17	0.53	0.41	0.34
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	17	0.52	0.12	0.53
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	17	0.5	0.26	0.44
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	17	0.27	0.1	0.25
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	17	0.27	0.12	0.24
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	17	0.26	0.12	0.24
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	17	0.22	0.08	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	17	0.22	0.07	0.23
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	17	0.2	0.05	0.18
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	16	0.64	0.15	0.66
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	16	0.6	0.48	0.48
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	16	0.58	0.33	0.49
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	16	0.55	0.36	0.38
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	16	0.47	0.36	0.32
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	16	0.42	0.2	0.36
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	16	0.37	0.17	0.33
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	16	0.36	0.16	0.32
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	16	0.3	0.15	0.28
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	16	0.26	0.07	0.25
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	16	0.21	0.09	0.19
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	15	0.3	0.15	0.28
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	15	0.22	0.06	0.19
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	15	0.17	0.04	0.17
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	15	0.16	0.03	0.16
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	15	0.15	0.03	0.15
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	14	0.49	0.2	0.56
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	14	0.42	0.23	0.42
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	14	0.29	0.15	0.26
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	14	0.27	0.09	0.26
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	14	0.26	0.1	0.28
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	14	0.22	0.07	0.22
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	14	0.2	0.05	0.19
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	14	0.18	0.05	0.18
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	14	0.17	0.04	0.16
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	14	0.16	0.03	0.16
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	13	0.53	0.36	0.37
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	13	0.42	0.21	0.42
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	13	0.41	0.28	0.34
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	13	0.39	0.15	0.4
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	13	0.34	0.09	0.34
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	13	0.31	0.14	0.29
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	13	0.19	0.06	0.17
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	12	0.46	0.36	0.32
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	12	0.43	0.26	0.4
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	12	0.38	0.24	0.28
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	12	0.33	0.13	0.32
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	12	0.31	0.08	0.29
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	12	0.25	0.05	0.25
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	12	0.23	0.07	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	12	0.22	0.1	0.2
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	12	0.2	0.07	0.2
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	12	0.19	0.09	0.16
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	12	0.11	0.0	0.11
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	11	0.27	0.12	0.3
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	11	0.25	0.13	0.19
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	11	0.23	0.09	0.2
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	11	0.19	0.07	0.19
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	11	0.18	0.05	0.18
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	11	0.12	0.0	0.12
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	10	0.33	0.12	0.32
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	10	0.3	0.13	0.24
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	10	0.26	0.04	0.26
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	10	0.26	0.12	0.23
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	10	0.25	0.14	0.2
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	10	0.24	0.15	0.18
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	10	0.16	0.04	0.16
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	9	0.87	0.42	0.77
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	9	0.5	0.38	0.31
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	9	0.46	0.14	0.55
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	9	0.36	0.21	0.31
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	9	0.32	0.11	0.33
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	9	0.27	0.12	0.24
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	9	0.22	0.1	0.22
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	9	0.21	0.07	0.2
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	9	0.19	0.06	0.18
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	9	0.14	0.02	0.14
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	8	0.99	0.13	1.0
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	8	0.72	0.59	0.41
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	8	0.49	0.09	0.51
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	8	0.34	0.11	0.32
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	8	0.29	0.11	0.24
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	8	0.27	0.07	0.29
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	8	0.27	0.14	0.24
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	8	0.25	0.1	0.22
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	8	0.22	0.06	0.22
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	8	0.2	0.07	0.18
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	8	0.19	0.03	0.18
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	8	0.17	0.05	0.16
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	8	0.17	0.05	0.16
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	8	0.16	0.04	0.15
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	7	1.92	1.25	2.72

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	7	1.92	1.25	2.72
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	7	0.94	0.86	0.29
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	7	0.81	0.87	0.31
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	7	0.47	0.11	0.51
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	7	0.42	0.02	0.43
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	7	0.42	0.02	0.42
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	7	0.28	0.11	0.22
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	7	0.2	0.03	0.2
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	7	0.19	0.04	0.17
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	7	0.18	0.06	0.16
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	7	0.17	0.04	0.17
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	7	0.14	0.03	0.12
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	6	0.46	0.21	0.44
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	6	0.35	0.12	0.34
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	6	0.35	0.2	0.29
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	6	0.34	0.29	0.25
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	6	0.33	0.23	0.24
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	6	0.28	0.12	0.26
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	6	0.26	0.08	0.28
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	6	0.23	0.09	0.2
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	6	0.22	0.1	0.16
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	6	0.21	0.07	0.2
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	6	0.2	0.09	0.17
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	6	0.19	0.05	0.2
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	6	0.19	0.08	0.16
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	6	0.18	0.08	0.16
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	6	0.17	0.05	0.15
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	6	0.16	0.03	0.15
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	6	0.15	0.03	0.16
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	6	0.15	0.04	0.14
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	6	0.13	0.01	0.13
(3,587)	1:X:91:TYR:N	1:X:85:LEU:CD1	5	0.58	0.31	0.79
(5,58)	1:X:121:ASP:C	1:X:124:MET:H	5	0.5	0.06	0.5
(5,3)	1:X:6:GLN:C	1:X:10:GLU:H	5	0.39	0.25	0.37
(1,836)	1:X:99:VAL:H	1:X:117:ILE:HG12	5	0.35	0.07	0.4
(5,2)	1:X:5:GLU:C	1:X:9:THR:H	5	0.29	0.2	0.21
(4,65)	1:X:56:HIS:O	1:X:60:ALA:H	5	0.23	0.12	0.17
(1,248)	1:X:37:ARG:H	1:X:36:LEU:HB3	5	0.2	0.08	0.23
(4,67)	1:X:57:GLN:O	1:X:61:VAL:H	5	0.2	0.08	0.19
(5,63)	1:X:128:THR:C	1:X:116:VAL:H	5	0.18	0.06	0.14
(3,556)	1:X:87:THR:N	1:X:86:PHE:CB	5	0.18	0.03	0.19
(1,51)	1:X:10:GLU:H	1:X:7:LYS:HA	5	0.17	0.03	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(4,21)	1:X:15:PRO:O	1:X:19:LEU:H	5	0.16	0.03	0.15
(3,448)	1:X:65:GLU:N	1:X:11:MET:CE	4	2.07	0.61	1.8
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG21	4	0.74	0.25	0.75
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG22	4	0.74	0.25	0.75
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG23	4	0.74	0.25	0.75
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD1	4	0.45	0.21	0.5
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD2	4	0.45	0.21	0.5
(2,28)	1:X:29:ILE:CG2	1:X:29:ILE:CD1	4	0.43	0.01	0.43
(1,925)	1:X:108:GLN:HB2	1:X:109:ASN:H	4	0.34	0.09	0.31
(2,86)	1:X:91:TYR:CA	1:X:117:ILE:CD1	4	0.32	0.08	0.34
(2,107)	1:X:120:VAL:CG2	1:X:125:ILE:CD1	4	0.26	0.09	0.29
(1,1190)	1:X:141:ILE:HG13	1:X:137:ALA:H	4	0.24	0.05	0.25
(1,640)	1:X:74:LEU:HD21	1:X:39:TYR:H	4	0.24	0.09	0.22
(1,640)	1:X:74:LEU:HD22	1:X:39:TYR:H	4	0.24	0.09	0.22
(1,640)	1:X:74:LEU:HD23	1:X:39:TYR:H	4	0.24	0.09	0.22
(1,453)	1:X:56:HIS:HB3	1:X:55:SER:H	4	0.22	0.05	0.22
(1,5)	1:X:5:GLU:H	1:X:4:LEU:HG	4	0.2	0.04	0.2
(4,68)	1:X:57:GLN:O	1:X:61:VAL:N	4	0.2	0.08	0.18
(5,67)	1:X:136:PHE:C	1:X:125:ILE:H	4	0.19	0.04	0.2
(1,575)	1:X:65:GLU:HB2	1:X:64:VAL:H	4	0.18	0.05	0.18
(3,554)	1:X:85:LEU:CA	1:X:87:THR:N	4	0.18	0.03	0.18
(5,24)	1:X:47:ASN:C	1:X:50:ASP:H	4	0.18	0.07	0.14
(5,9)	1:X:13:THR:C	1:X:17:GLU:H	4	0.17	0.03	0.18
(3,666)	1:X:94:PHE:N	1:X:117:ILE:CG2	4	0.17	0.04	0.18
(2,121)	1:X:138:LEU:CD1	1:X:141:ILE:CD1	4	0.16	0.02	0.16
(1,96)	1:X:19:LEU:H	1:X:16:VAL:HA	4	0.16	0.03	0.16
(1,1007)	1:X:122:GLY:H	1:X:124:MET:H	4	0.16	0.01	0.15
(3,749)	1:X:113:TRP:N	1:X:101:LEU:CD1	4	0.16	0.03	0.16
(5,56)	1:X:116:VAL:C	1:X:128:THR:H	4	0.16	0.03	0.16
(1,204)	1:X:33:THR:H	1:X:32:ARG:HG2	4	0.15	0.02	0.16
(3,189)	1:X:34:SER:N	1:X:33:THR:CB	4	0.13	0.01	0.13
(1,915)	1:X:108:GLN:HE21	1:X:107:VAL:CB	3	0.96	0.08	0.99
(2,85)	1:X:85:LEU:CD2	1:X:117:ILE:CD1	3	0.66	0.15	0.7
(1,1034)	1:X:125:ILE:H	1:X:124:MET:HB3	3	0.57	0.02	0.57
(3,145)	1:X:27:GLU:N	1:X:26:ILE:CD1	3	0.56	0.31	0.73
(5,15)	1:X:29:ILE:C	1:X:35:THR:H	3	0.47	0.05	0.44
(3,479)	1:X:70:VAL:CG1	1:X:70:VAL:N	3	0.46	0.0	0.46
(1,610)	1:X:71:ALA:H	1:X:70:VAL:CB	3	0.45	0.09	0.4
(1,193)	1:X:31:GLY:H	1:X:30:ARG:HG3	3	0.4	0.07	0.38
(3,464)	1:X:66:ASP:N	1:X:64:VAL:CG1	3	0.37	0.1	0.41
(1,221)	1:X:35:THR:H	1:X:34:SER:HB3	3	0.3	0.06	0.26
(1,773)	1:X:94:PHE:HB3	1:X:97:GLU:H	3	0.28	0.07	0.3

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(5,49)	1:X:97:GLU:C	1:X:117:ILE:H	3	0.27	0.21	0.14
(4,54)	1:X:50:ASP:O	1:X:54:VAL:H	3	0.26	0.09	0.27
(3,765)	1:X:115:GLY:N	1:X:129:VAL:CG2	3	0.26	0.08	0.29
(1,595)	1:X:66:ASP:HB2	1:X:72:TYR:H	3	0.25	0.12	0.18
(3,823)	1:X:124:MET:CB	1:X:125:ILE:N	3	0.24	0.0	0.24
(3,159)	1:X:29:ILE:N	1:X:28:PHE:CB	3	0.21	0.06	0.23
(3,484)	1:X:71:ALA:N	1:X:70:VAL:CB	3	0.2	0.07	0.16
(1,315)	1:X:44:ASP:H	1:X:43:GLU:HG2	3	0.19	0.05	0.17
(4,1)	1:X:4:LEU:O	1:X:8:LEU:H	3	0.19	0.08	0.15
(1,658)	1:X:76:VAL:HB	1:X:55:SER:H	3	0.18	0.05	0.16
(4,47)	1:X:47:ASN:O	1:X:50:ASP:H	3	0.17	0.04	0.17
(3,878)	1:X:133:ASP:N	1:X:128:THR:CG2	3	0.17	0.05	0.16
(3,197)	1:X:35:THR:N	1:X:34:SER:CB	3	0.16	0.02	0.15
(3,716)	1:X:104:ARG:N	1:X:105:MET:CB	3	0.16	0.03	0.17
(1,1191)	1:X:141:ILE:H	1:X:138:LEU:HA	3	0.15	0.01	0.15
(5,23)	1:X:41:ASP:C	1:X:23:LEU:H	3	0.15	0.04	0.15
(4,88)	1:X:89:GLU:O	1:X:93:ARG:N	3	0.15	0.04	0.14
(5,62)	1:X:127:VAL:C	1:X:134:GLU:H	3	0.15	0.01	0.15
(5,46)	1:X:115:GLY:C	1:X:99:VAL:H	3	0.14	0.02	0.15
(1,241)	1:X:37:ARG:H	1:X:27:GLU:HB2	3	0.14	0.02	0.13
(3,208)	1:X:36:LEU:N	1:X:37:ARG:CG	3	0.14	0.01	0.13
(3,566)	1:X:88:ALA:N	1:X:89:GLU:CB	3	0.12	0.0	0.12
(3,92)	1:X:19:LEU:N	1:X:18:ALA:CB	3	0.12	0.01	0.12
(3,366)	1:X:56:HIS:N	1:X:57:GLN:CB	3	0.12	0.0	0.12
(1,566)	1:X:64:VAL:HB	1:X:64:VAL:H	3	0.11	0.0	0.11
(3,425)	1:X:62:LEU:N	1:X:61:VAL:CG2	2	0.68	0.56	0.68
(1,506)	1:X:59:SER:HB2	1:X:60:ALA:H	2	0.52	0.04	0.52
(1,701)	1:X:81:LEU:H	1:X:82:ASP:H	2	0.44	0.04	0.44
(1,227)	1:X:35:THR:HG21	1:X:75:GLU:H	2	0.34	0.01	0.34
(1,227)	1:X:35:THR:HG22	1:X:75:GLU:H	2	0.34	0.01	0.34
(1,227)	1:X:35:THR:HG23	1:X:75:GLU:H	2	0.34	0.01	0.34
(4,66)	1:X:56:HIS:O	1:X:60:ALA:N	2	0.3	0.05	0.3
(3,313)	1:X:52:ALA:N	1:X:40:ILE:CD1	2	0.3	0.1	0.3
(4,75)	1:X:71:ALA:O	1:X:34:SER:H	2	0.3	0.02	0.3
(1,175)	1:X:29:ILE:HB	1:X:35:THR:H	2	0.29	0.02	0.29
(4,53)	1:X:50:ASP:O	1:X:54:VAL:N	2	0.29	0.01	0.29
(1,218)	1:X:34:SER:H	1:X:73:ASN:H	2	0.29	0.18	0.29
(3,203)	1:X:36:LEU:N	1:X:35:THR:CG2	2	0.27	0.07	0.27
(1,1043)	1:X:125:ILE:H	1:X:136:PHE:H	2	0.26	0.01	0.26
(3,212)	1:X:37:ARG:N	1:X:27:GLU:CB	2	0.26	0.11	0.26
(1,864)	1:X:101:LEU:H	1:X:114:GLN:HB2	2	0.25	0.09	0.25
(1,351)	1:X:47:ASN:H	1:X:46:ILE:HG13	2	0.22	0.01	0.22

*Continued on next page...*

*Continued from previous page...*

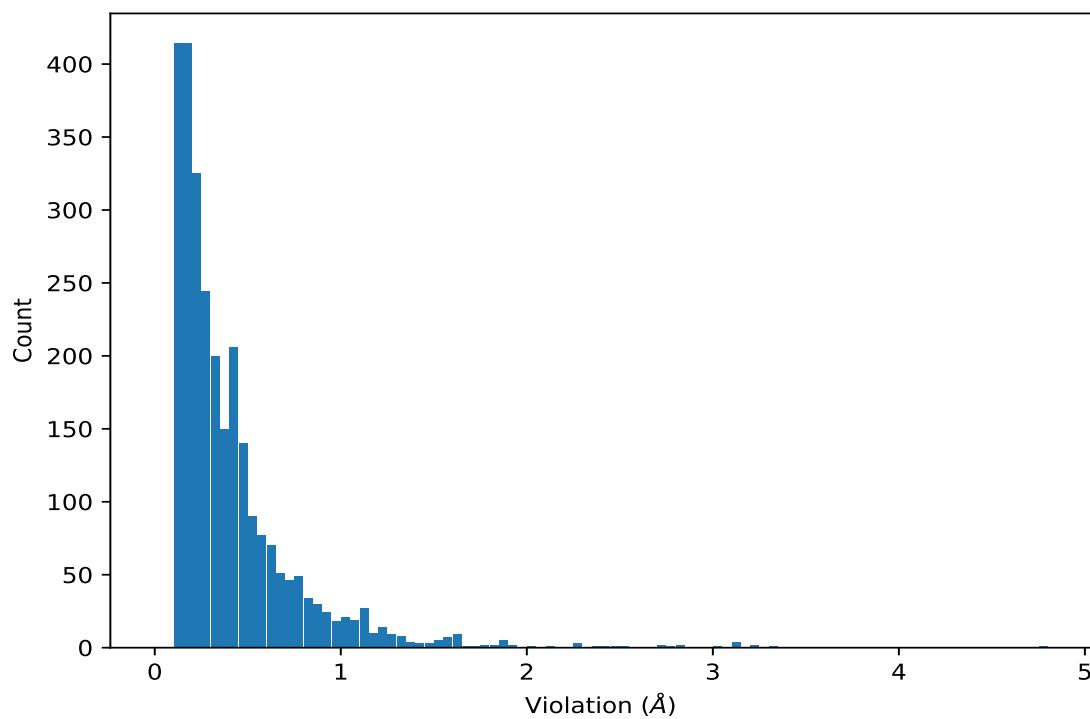
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,661)	1:X:91:TYR:N	1:X:120:VAL:CG1	2	0.22	0.01	0.22
(4,2)	1:X:4:LEU:O	1:X:8:LEU:N	2	0.21	0.08	0.21
(4,76)	1:X:71:ALA:O	1:X:34:SER:N	2	0.21	0.08	0.21
(1,420)	1:X:54:VAL:H	1:X:51:CYS:HA	2	0.2	0.03	0.2
(3,847)	1:X:128:THR:CB	1:X:116:VAL:N	2	0.2	0.02	0.2
(1,1135)	1:X:134:GLU:H	1:X:127:VAL:H	2	0.18	0.02	0.18
(3,371)	1:X:57:GLN:N	1:X:54:VAL:CG2	2	0.18	0.06	0.18
(1,685)	1:X:78:SER:HB2	1:X:78:SER:H	2	0.17	0.0	0.17
(5,19)	1:X:36:LEU:C	1:X:75:GLU:H	2	0.17	0.0	0.17
(4,71)	1:X:59:SER:O	1:X:63:ASP:H	2	0.16	0.04	0.16
(1,146)	1:X:25:GLY:H	1:X:39:TYR:HB2	2	0.16	0.04	0.16
(1,179)	1:X:29:ILE:H	1:X:36:LEU:H	2	0.16	0.04	0.16
(4,115)	1:X:121:ASP:O	1:X:124:MET:H	2	0.16	0.05	0.16
(5,40)	1:X:75:GLU:C	1:X:38:ILE:H	2	0.16	0.05	0.16
(1,531)	1:X:62:LEU:HB2	1:X:61:VAL:H	2	0.15	0.02	0.15
(1,931)	1:X:109:ASN:HD21	1:X:109:ASN:HB3	2	0.15	0.02	0.15
(3,124)	1:X:24:VAL:N	1:X:23:LEU:CD1	2	0.15	0.0	0.15
(1,1018)	1:X:123:GLU:H	1:X:124:MET:HB2	2	0.14	0.0	0.14
(5,6)	1:X:9:THR:C	1:X:13:THR:H	2	0.14	0.01	0.14
(1,392)	1:X:50:ASP:HA	1:X:53:ASP:H	2	0.14	0.02	0.14
(3,239)	1:X:41:ASP:N	1:X:16:VAL:CG1	2	0.14	0.02	0.14
(3,534)	1:X:80:GLY:N	1:X:79:PRO:CB	2	0.14	0.01	0.14
(1,609)	1:X:71:ALA:H	1:X:70:VAL:HA	2	0.12	0.01	0.12
(1,532)	1:X:62:LEU:H	1:X:61:VAL:CB	2	0.12	0.0	0.12
(1,598)	1:X:67:PRO:HA	1:X:68:ILE:H	2	0.12	0.0	0.12
(1,606)	1:X:69:THR:HA	1:X:70:VAL:H	2	0.12	0.0	0.12
(4,117)	1:X:124:MET:O	1:X:121:ASP:H	2	0.12	0.0	0.12
(3,315)	1:X:52:ALA:N	1:X:48:VAL:CA	2	0.11	0.0	0.11

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

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

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	11	4.78
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	17	3.3
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	17	3.23
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	17	3.23
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	16	3.13
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	16	3.13
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	16	3.11
(3,448)	1:X:65:GLU:N	1:X:11:MET:CE	11	3.11
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	14	3.02
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	11	2.82
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	11	2.82
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	12	2.76
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	14	2.72
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	14	2.72
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	11	2.53
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	1	2.46

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	12	2.44
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	6	2.38
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	13	2.27
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	10	2.27
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	4	2.26
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	2	2.1
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	12	2.03
(3,448)	1:X:65:GLU:N	1:X:11:MET:CE	17	1.94
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	10	1.9
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	1	1.88
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	14	1.88
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	14	1.87
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	6	1.86
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	5	1.85
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	17	1.82
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	13	1.8
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	14	1.79
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	20	1.77
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	9	1.74
(3,448)	1:X:65:GLU:N	1:X:11:MET:CE	14	1.65
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	1	1.64
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	10	1.64
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	20	1.64
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	19	1.63
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	16	1.62
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	8	1.62
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	16	1.62
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	7	1.61
(3,448)	1:X:65:GLU:N	1:X:11:MET:CE	16	1.6
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	10	1.59
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	10	1.59
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	17	1.59
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	12	1.58
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	18	1.58
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	9	1.57
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	1	1.56
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	5	1.53
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	17	1.52
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	3	1.51
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	5	1.5
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	5	1.5
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	1	1.47

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	7	1.45
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	3	1.45
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	14	1.44
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	14	1.42
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	10	1.41
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	3	1.39
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	12	1.37
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	9	1.36
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	14	1.36
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	13	1.33
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	10	1.33
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	3	1.32
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	7	1.32
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	2	1.32
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	4	1.31
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	8	1.31
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	15	1.3
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	13	1.28
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	16	1.28
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	17	1.27
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	15	1.26
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	13	1.25
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	10	1.25
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	12	1.25
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	7	1.25
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	9	1.25
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	1	1.24
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	19	1.24
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	6	1.24
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	12	1.24
(3,425)	1:X:62:LEU:N	1:X:61:VAL:CG2	2	1.24
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	10	1.24
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	7	1.24
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	18	1.22
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	11	1.22
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	12	1.21
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	2	1.21
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	19	1.21
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	13	1.21
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	16	1.2
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	11	1.18
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	8	1.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	9	1.18
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	7	1.17
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	6	1.15
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	20	1.15
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	12	1.15
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	16	1.15
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	10	1.15
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	11	1.15
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	7	1.14
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	5	1.14
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	1	1.14
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	14	1.14
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	3	1.14
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	16	1.13
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	11	1.13
(1,939)	1:X:109:ASN:H	1:X:110:ARG:H	9	1.13
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	14	1.13
(1,1188)	1:X:141:ILE:CG2	1:X:102:VAL:H	5	1.13
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	3	1.12
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	17	1.12
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	9	1.12
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	9	1.12
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	16	1.11
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	20	1.11
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	16	1.11
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	20	1.11
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	10	1.11
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	20	1.11
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	18	1.11
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	2	1.1
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	11	1.1
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	14	1.1
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	17	1.1
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	20	1.1
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	7	1.1
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	6	1.09
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	19	1.09
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	3	1.09
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	7	1.08
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	18	1.08
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	2	1.08
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	1	1.08

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	1	1.07
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	15	1.07
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	12	1.07
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	9	1.07
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	20	1.06
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	13	1.06
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	8	1.06
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	14	1.05
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	3	1.05
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG21	1	1.05
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG22	1	1.05
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG23	1	1.05
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	19	1.04
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	19	1.04
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	14	1.04
(1,915)	1:X:108:GLN:HE21	1:X:107:VAL:CB	11	1.04
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	4	1.03
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	5	1.03
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	18	1.03
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	18	1.03
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	17	1.03
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	16	1.02
(1,906)	1:X:106:ALA:HB1	1:X:110:ARG:H	9	1.02
(1,906)	1:X:106:ALA:HB2	1:X:110:ARG:H	9	1.02
(1,906)	1:X:106:ALA:HB3	1:X:110:ARG:H	9	1.02
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	13	1.01
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	2	1.01
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	2	1.01
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	18	1.01
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	12	1.0
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	10	1.0
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	17	1.0
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	2	1.0
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	2	0.99
(1,915)	1:X:108:GLN:HE21	1:X:107:VAL:CB	13	0.99
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	8	0.98
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	6	0.98
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	14	0.98
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	7	0.98
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	12	0.98
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	16	0.98
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	13	0.98

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	8	0.97
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	5	0.96
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	5	0.96
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	2	0.96
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	1	0.96
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	2	0.96
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	8	0.96
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	11	0.96
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	9	0.95
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	15	0.94
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	13	0.93
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	9	0.93
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	13	0.93
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	17	0.93
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	9	0.92
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	10	0.92
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG21	20	0.92
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG22	20	0.92
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG23	20	0.92
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	14	0.92
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	18	0.91
(5,47)	1:X:117:ILE:C	1:X:97:GLU:H	5	0.91
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	5	0.91
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	2	0.91
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	9	0.91
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	19	0.91
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	16	0.91
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	12	0.91
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	17	0.91
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	20	0.9
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	13	0.9
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	20	0.9
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	11	0.9
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	9	0.89
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	16	0.89
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	20	0.89
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	4	0.89
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	20	0.89
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	8	0.88
(5,48)	1:X:147:VAL:C	1:X:98:GLU:H	10	0.88
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	20	0.88
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	4	0.88

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	20	0.88
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	3	0.88
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	5	0.88
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	5	0.88
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	9	0.88
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	7	0.87
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	9	0.87
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	1	0.87
(3,587)	1:X:91:TYR:N	1:X:85:LEU:CD1	12	0.87
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	4	0.87
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	4	0.86
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	11	0.86
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	14	0.86
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	13	0.86
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	11	0.86
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	10	0.86
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	15	0.86
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	3	0.86
(5,3)	1:X:6:GLN:C	1:X:10:GLU:H	2	0.85
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	2	0.85
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	10	0.85
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	5	0.84
(1,915)	1:X:108:GLN:HE21	1:X:107:VAL:CB	6	0.84
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	4	0.84
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	19	0.84
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	2	0.84
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	15	0.83
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	17	0.83
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	4	0.83
(3,145)	1:X:27:GLU:N	1:X:26:ILE:CD1	11	0.83
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	7	0.83
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	1	0.83
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	2	0.83
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	5	0.82
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	15	0.82
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	1	0.82
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	20	0.82
(2,85)	1:X:85:LEU:CD2	1:X:117:ILE:CD1	20	0.82
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	4	0.82
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	11	0.82
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	14	0.81
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	8	0.81

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	11	0.81
(3,587)	1:X:91:TYR:N	1:X:85:LEU:CD1	5	0.81
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	8	0.81
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	14	0.81
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	13	0.81
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	9	0.81
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	7	0.8
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	13	0.8
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	17	0.8
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	10	0.8
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	17	0.8
(1,570)	1:X:64:VAL:H	1:X:65:GLU:HB3	14	0.8
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	7	0.8
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	15	0.79
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	12	0.79
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	19	0.79
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	9	0.79
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	4	0.79
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	1	0.79
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	15	0.79
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	14	0.79
(3,587)	1:X:91:TYR:N	1:X:85:LEU:CD1	2	0.79
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	10	0.79
(1,8)	1:X:5:GLU:HG3	1:X:5:GLU:H	14	0.79
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	3	0.79
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	10	0.79
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	20	0.79
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	17	0.79
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	9	0.79
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	11	0.78
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	15	0.78
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	16	0.78
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	9	0.78
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	7	0.78
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	9	0.78
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	2	0.77
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	1	0.77
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	2	0.77
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	15	0.77
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	1	0.77
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	13	0.77
(3,481)	1:X:70:VAL:N	1:X:72:TYR:CB	1	0.77

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	2	0.77
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	4	0.76
(4,32)	1:X:33:THR:O	1:X:31:GLY:N	3	0.76
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	18	0.76
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	12	0.76
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	20	0.75
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	18	0.75
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	2	0.75
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	10	0.75
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	14	0.75
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	9	0.75
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	7	0.75
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	12	0.75
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	15	0.75
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	7	0.75
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	11	0.75
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	16	0.75
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	14	0.75
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	4	0.75
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	5	0.75
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	3	0.74
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	18	0.74
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	5	0.74
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	3	0.74
(4,94)	1:X:117:ILE:O	1:X:97:GLU:H	5	0.74
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	12	0.74
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	20	0.74
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	6	0.74
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	2	0.74
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	20	0.74
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	6	0.74
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	9	0.73
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	12	0.73
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	3	0.73
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	16	0.73
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	5	0.73
(3,145)	1:X:27:GLU:N	1:X:26:ILE:CD1	3	0.73
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	11	0.72
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	20	0.72
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	1	0.72
(1,942)	1:X:110:ARG:HG3	1:X:109:ASN:H	9	0.72
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	4	0.72

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	5	0.72
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	3	0.72
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	13	0.72
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	20	0.72
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	14	0.72
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	17	0.71
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	6	0.71
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	12	0.71
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	8	0.71
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	11	0.71
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	17	0.71
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	16	0.71
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	13	0.71
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	5	0.71
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	1	0.71
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	10	0.7
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	16	0.7
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	7	0.7
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	9	0.7
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	19	0.7
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	1	0.7
(2,85)	1:X:85:LEU:CD2	1:X:117:ILE:CD1	14	0.7
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	9	0.7
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	12	0.7
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	15	0.69
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	17	0.69
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	20	0.69
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	4	0.69
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	7	0.69
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	13	0.69
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	14	0.68
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	17	0.68
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	3	0.68
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	12	0.68
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	2	0.68
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	12	0.68
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	18	0.68
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	6	0.68
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	13	0.68
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	20	0.68
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	16	0.67
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	3	0.67

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	4	0.67
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	20	0.67
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	7	0.67
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	3	0.67
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	12	0.67
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	5	0.67
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	17	0.67
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	1	0.66
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	17	0.66
(5,2)	1:X:5:GLU:C	1:X:9:THR:H	2	0.66
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	20	0.66
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	11	0.66
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	15	0.66
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	13	0.66
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	11	0.66
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	3	0.66
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	14	0.66
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	19	0.66
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	16	0.66
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	20	0.66
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	1	0.65
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	6	0.65
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	17	0.65
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	18	0.65
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	5	0.65
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	10	0.65
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	2	0.65
(2,81)	1:X:85:LEU:CD2	1:X:99:VAL:CG1	5	0.65
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	17	0.65
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD1	2	0.65
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD2	2	0.65
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	3	0.65
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	17	0.65
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	8	0.64
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	18	0.64
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	14	0.64
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	12	0.64
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	20	0.64
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	16	0.64
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	17	0.64
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	19	0.64
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	7	0.64

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	11	0.64
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	4	0.64
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	18	0.64
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	9	0.64
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	8	0.64
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	17	0.64
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	12	0.63
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	9	0.63
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	20	0.63
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	15	0.63
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	3	0.63
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	15	0.63
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	1	0.63
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	2	0.63
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	5	0.63
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	1	0.63
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	4	0.63
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	4	0.62
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	1	0.62
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	10	0.62
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	7	0.62
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	1	0.62
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	5	0.62
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	4	0.62
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD1	9	0.62
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD2	9	0.62
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	1	0.62
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	6	0.62
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	14	0.62
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	15	0.61
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	14	0.61
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	1	0.61
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	9	0.61
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	8	0.61
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	13	0.61
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	13	0.61
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	10	0.61
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	10	0.61
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	19	0.61
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	5	0.61
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	18	0.61
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	15	0.61

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	11	0.61
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	18	0.61
(5,58)	1:X:121:ASP:C	1:X:124:MET:H	10	0.6
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	1	0.6
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	8	0.6
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	19	0.6
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	2	0.6
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	7	0.6
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	9	0.6
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	3	0.6
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	12	0.6
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	2	0.6
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	18	0.6
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	15	0.6
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	17	0.6
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	15	0.6
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	12	0.6
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	5	0.6
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	20	0.6
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	2	0.59
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	5	0.59
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	11	0.59
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	17	0.59
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	11	0.59
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	1	0.59
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	1	0.59
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	1	0.59
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	11	0.59
(1,917)	1:X:108:GLN:H	1:X:107:VAL:HB	18	0.59
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	20	0.59
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	2	0.59
(1,1034)	1:X:125:ILE:H	1:X:124:MET:HB3	4	0.59
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	1	0.58
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	7	0.58
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	14	0.58
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	8	0.58
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	19	0.58
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	14	0.58
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	16	0.58
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	6	0.58
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	19	0.58
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	4	0.58

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	5	0.58
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	20	0.58
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	1	0.58
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	9	0.58
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	10	0.58
(2,46)	1:X:38:ILE:CD1	1:X:76:VAL:CG1	16	0.58
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	6	0.58
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	16	0.58
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	19	0.58
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG21	13	0.58
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG22	13	0.58
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG23	13	0.58
(1,610)	1:X:71:ALA:H	1:X:70:VAL:CB	1	0.58
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	17	0.58
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	4	0.58
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	13	0.58
(5,49)	1:X:97:GLU:C	1:X:117:ILE:H	10	0.57
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	19	0.57
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	17	0.57
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	19	0.57
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	8	0.57
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	8	0.57
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	5	0.57
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	4	0.57
(1,1034)	1:X:125:ILE:H	1:X:124:MET:HB3	1	0.57
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	2	0.56
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	19	0.56
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	10	0.56
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	20	0.56
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	4	0.56
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	6	0.56
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	20	0.56
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	20	0.56
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	11	0.56
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	20	0.56
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	2	0.56
(1,506)	1:X:59:SER:HB2	1:X:60:ALA:H	16	0.56
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	12	0.56
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	6	0.56
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	13	0.56
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	3	0.56
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	10	0.56

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	11	0.56
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	7	0.55
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	11	0.55
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	5	0.55
(5,15)	1:X:29:ILE:C	1:X:35:THR:H	5	0.55
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	3	0.55
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	10	0.55
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	3	0.55
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	9	0.55
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	8	0.55
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	1	0.55
(1,1034)	1:X:125:ILE:H	1:X:124:MET:HB3	2	0.55
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	6	0.54
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	19	0.54
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	10	0.54
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	19	0.54
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	10	0.54
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	15	0.54
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	2	0.54
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	4	0.54
(4,4)	1:X:5:GLU:O	1:X:9:THR:H	2	0.54
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	15	0.54
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	14	0.54
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	20	0.54
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	13	0.54
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	7	0.54
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	19	0.54
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	15	0.54
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	6	0.54
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	1	0.54
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	5	0.54
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	3	0.53
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	4	0.53
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	15	0.53
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	9	0.53
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	2	0.53
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	14	0.53
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	7	0.53
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	15	0.53
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	1	0.53
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	8	0.53
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	11	0.53

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:X:40:ILE:CD1	1:X:54:VAL:H	5	0.53
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	7	0.53
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	10	0.53
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	10	0.53
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	10	0.53
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	9	0.52
(5,58)	1:X:121:ASP:C	1:X:124:MET:H	14	0.52
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	20	0.52
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	10	0.52
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	14	0.52
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	11	0.52
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	17	0.52
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	15	0.52
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	2	0.52
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	6	0.52
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	9	0.52
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	13	0.52
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	18	0.52
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	9	0.52
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	16	0.52
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	9	0.52
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	5	0.52
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	10	0.52
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	3	0.52
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	8	0.51
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	19	0.51
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	5	0.51
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	3	0.51
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	12	0.51
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	6	0.51
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	15	0.51
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	15	0.51
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	2	0.51
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	3	0.51
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	9	0.51
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	14	0.51
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	1	0.51
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	3	0.51
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	2	0.51
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	13	0.51
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	6	0.51
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	2	0.51

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	7	0.51
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	19	0.51
(5,58)	1:X:121:ASP:C	1:X:124:MET:H	20	0.5
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	7	0.5
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	4	0.5
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	10	0.5
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	17	0.5
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	7	0.5
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	14	0.5
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	16	0.5
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	19	0.5
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	4	0.5
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	1	0.5
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	10	0.5
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	3	0.5
(1,193)	1:X:31:GLY:H	1:X:30:ARG:HG3	5	0.5
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	2	0.5
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	16	0.5
(5,8)	1:X:12:ILE:C	1:X:16:VAL:H	16	0.49
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	10	0.49
(5,58)	1:X:121:ASP:C	1:X:124:MET:H	9	0.49
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	14	0.49
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	1	0.49
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	4	0.49
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	5	0.49
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	8	0.49
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	9	0.49
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	19	0.49
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	8	0.49
(4,5)	1:X:6:GLN:O	1:X:10:GLU:H	2	0.49
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	19	0.49
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	4	0.49
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	6	0.49
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	18	0.49
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	12	0.49
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	20	0.49
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	7	0.49
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	5	0.49
(1,925)	1:X:108:GLN:HB2	1:X:109:ASN:H	9	0.49
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	9	0.49
(1,701)	1:X:81:LEU:H	1:X:82:ASP:H	13	0.49
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	5	0.49

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	9	0.49
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	20	0.49
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	2	0.49
(1,506)	1:X:59:SER:HB2	1:X:60:ALA:H	14	0.49
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	16	0.49
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	17	0.49
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	4	0.48
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	13	0.48
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	6	0.48
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	9	0.48
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	15	0.48
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	1	0.48
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	15	0.48
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	11	0.48
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	19	0.48
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	7	0.48
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	3	0.48
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	4	0.48
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	14	0.48
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	5	0.48
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	8	0.48
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	14	0.48
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	13	0.48
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	1	0.48
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	12	0.48
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	11	0.47
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	2	0.47
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	5	0.47
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	3	0.47
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	8	0.47
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	9	0.47
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	20	0.47
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	16	0.47
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	13	0.47
(2,85)	1:X:85:LEU:CD2	1:X:117:ILE:CD1	17	0.47
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	2	0.47
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	6	0.47
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	13	0.47
(1,218)	1:X:34:SER:H	1:X:73:ASN:H	14	0.47
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	5	0.47
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	11	0.46
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	17	0.46

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	2	0.46
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	17	0.46
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	7	0.46
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	12	0.46
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	15	0.46
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	7	0.46
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	16	0.46
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	4	0.46
(3,479)	1:X:70:VAL:CG1	1:X:70:VAL:N	1	0.46
(3,479)	1:X:70:VAL:CG1	1:X:70:VAL:N	2	0.46
(3,479)	1:X:70:VAL:CG1	1:X:70:VAL:N	13	0.46
(3,464)	1:X:66:ASP:N	1:X:64:VAL:CG1	20	0.46
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	10	0.46
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	11	0.46
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	2	0.46
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	8	0.46
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	16	0.46
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	18	0.46
(2,30)	1:X:33:THR:CG2	1:X:71:ALA:CB	5	0.46
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	6	0.46
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	14	0.46
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	10	0.46
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	16	0.46
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	18	0.46
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	4	0.46
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	7	0.46
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	13	0.46
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	14	0.46
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	4	0.46
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	20	0.46
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	8	0.46
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	18	0.46
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	2	0.45
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	1	0.45
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	12	0.45
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	16	0.45
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	3	0.45
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	20	0.45
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	16	0.45
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	7	0.45
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	8	0.45
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	2	0.45

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	9	0.45
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	18	0.45
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	12	0.45
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	6	0.45
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	11	0.45
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	7	0.45
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	9	0.45
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	19	0.45
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	6	0.45
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	19	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	3	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	4	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	5	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	6	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	7	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	10	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	11	0.45
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	19	0.45
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	17	0.45
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	16	0.45
(2,49)	1:X:40:ILE:CG2	1:X:40:ILE:CD1	5	0.45
(2,28)	1:X:29:ILE:CG2	1:X:29:ILE:CD1	8	0.45
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	1	0.45
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	10	0.45
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	11	0.45
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	7	0.45
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	15	0.45
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	18	0.45
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	10	0.45
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	19	0.45
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	2	0.45
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	16	0.45
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	4	0.44
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	1	0.44
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	16	0.44
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	15	0.44
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	16	0.44
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	8	0.44
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	12	0.44
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	19	0.44
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	4	0.44
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	15	0.44

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,15)	1:X:29:ILE:C	1:X:35:THR:H	14	0.44
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	2	0.44
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	18	0.44
(4,65)	1:X:56:HIS:O	1:X:60:ALA:H	3	0.44
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	9	0.44
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	19	0.44
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	9	0.44
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	10	0.44
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	5	0.44
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	12	0.44
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	13	0.44
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	20	0.44
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	3	0.44
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	5	0.44
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	10	0.44
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	17	0.44
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	1	0.44
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	9	0.44
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	2	0.44
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	13	0.44
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	16	0.44
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	17	0.44
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	5	0.44
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	9	0.44
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	2	0.44
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	6	0.44
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	16	0.44
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	9	0.44
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	12	0.44
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	13	0.44
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	14	0.44
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	17	0.44
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	15	0.44
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	11	0.44
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	8	0.44
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	19	0.44
(1,689)	1:X:79:PRO:HB3	1:X:80:GLY:H	18	0.44
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	5	0.44
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	13	0.44
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	6	0.43
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	18	0.43
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	17	0.43

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	10	0.43
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	18	0.43
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	10	0.43
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	8	0.43
(5,15)	1:X:29:ILE:C	1:X:35:THR:H	1	0.43
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	20	0.43
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	20	0.43
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	6	0.43
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	14	0.43
(4,6)	1:X:6:GLN:O	1:X:10:GLU:N	2	0.43
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	16	0.43
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	17	0.43
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	7	0.43
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	11	0.43
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	3	0.43
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	10	0.43
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	11	0.43
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	17	0.43
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	19	0.43
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	9	0.43
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	13	0.43
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	15	0.43
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	19	0.43
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	4	0.43
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	5	0.43
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	8	0.43
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	11	0.43
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	6	0.43
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	13	0.43
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	15	0.43
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	4	0.43
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	9	0.43
(3,415)	1:X:61:VAL:N	1:X:61:VAL:CG1	2	0.43
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	1	0.43
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	1	0.43
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	12	0.43
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	2	0.43
(2,28)	1:X:29:ILE:CG2	1:X:29:ILE:CD1	2	0.43
(2,28)	1:X:29:ILE:CG2	1:X:29:ILE:CD1	18	0.43
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	6	0.43
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	3	0.43
(1,62)	1:X:9:THR:HB	1:X:10:GLU:H	2	0.43

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	13	0.43
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	16	0.43
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	6	0.43
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	20	0.43
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	13	0.42
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	14	0.42
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	11	0.42
(4,97)	1:X:97:GLU:O	1:X:117:ILE:N	10	0.42
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	20	0.42
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	19	0.42
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	12	0.42
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	8	0.42
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	12	0.42
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	3	0.42
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	4	0.42
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	15	0.42
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	16	0.42
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	1	0.42
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	2	0.42
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	7	0.42
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	12	0.42
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	14	0.42
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	16	0.42
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	5	0.42
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	14	0.42
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	20	0.42
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	3	0.42
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	19	0.42
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	5	0.42
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	6	0.42
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	15	0.42
(2,86)	1:X:91:TYR:CA	1:X:117:ILE:CD1	9	0.42
(1,843)	1:X:100:THR:HA	1:X:115:GLY:H	18	0.42
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	6	0.42
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	12	0.42
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	17	0.42
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG21	2	0.42
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG22	2	0.42
(1,611)	1:X:71:ALA:H	1:X:70:VAL:HG23	2	0.42
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	9	0.42
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	3	0.42
(5,54)	1:X:102:VAL:C	1:X:143:LYS:H	7	0.41

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	10	0.41
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	20	0.41
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	11	0.41
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	1	0.41
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	14	0.41
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	13	0.41
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	8	0.41
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	17	0.41
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	20	0.41
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	6	0.41
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	10	0.41
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	12	0.41
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	15	0.41
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	20	0.41
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	7	0.41
(3,464)	1:X:66:ASP:N	1:X:64:VAL:CG1	13	0.41
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	19	0.41
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	2	0.41
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	8	0.41
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	5	0.41
(3,188)	1:X:33:THR:N	1:X:33:THR:CG2	20	0.41
(2,28)	1:X:29:ILE:CG2	1:X:29:ILE:CD1	6	0.41
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	9	0.41
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	12	0.41
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	18	0.41
(1,836)	1:X:99:VAL:H	1:X:117:ILE:HG12	11	0.41
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	14	0.41
(1,595)	1:X:66:ASP:HB2	1:X:72:TYR:H	20	0.41
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	1	0.41
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	18	0.41
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	15	0.41
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	5	0.41
(5,58)	1:X:121:ASP:C	1:X:124:MET:H	11	0.4
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	9	0.4
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	6	0.4
(5,3)	1:X:6:GLN:C	1:X:10:GLU:H	19	0.4
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	9	0.4
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	14	0.4
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	9	0.4
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	12	0.4
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	17	0.4
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	14	0.4

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	17	0.4
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	8	0.4
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	1	0.4
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	3	0.4
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	14	0.4
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	8	0.4
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	19	0.4
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	12	0.4
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	3	0.4
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	1	0.4
(3,574)	1:X:89:GLU:N	1:X:89:GLU:CG	3	0.4
(3,507)	1:X:75:GLU:N	1:X:75:GLU:CG	16	0.4
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	1	0.4
(3,45)	1:X:11:MET:N	1:X:11:MET:CG	18	0.4
(3,313)	1:X:52:ALA:N	1:X:40:ILE:CD1	5	0.4
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	10	0.4
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	11	0.4
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	8	0.4
(1,836)	1:X:99:VAL:H	1:X:117:ILE:HG12	4	0.4
(1,836)	1:X:99:VAL:H	1:X:117:ILE:HG12	5	0.4
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	10	0.4
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	12	0.4
(1,701)	1:X:81:LEU:H	1:X:82:ASP:H	7	0.4
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	16	0.4
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	4	0.4
(1,610)	1:X:71:ALA:H	1:X:70:VAL:CB	5	0.4
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	13	0.4
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	4	0.4
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	3	0.39
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	13	0.39
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	12	0.39
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	16	0.39
(4,3)	1:X:5:GLU:O	1:X:9:THR:N	2	0.39
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	20	0.39
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	9	0.39
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	15	0.39
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	14	0.39
(3,721)	1:X:105:MET:N	1:X:105:MET:CG	6	0.39
(3,712)	1:X:104:ARG:N	1:X:104:ARG:CG	4	0.39
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	7	0.39
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	6	0.39
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	16	0.39

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	2	0.39
(3,5)	1:X:5:GLU:N	1:X:5:GLU:CG	14	0.39
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	19	0.39
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	1	0.39
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	1	0.39
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	3	0.39
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD1	12	0.39
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD2	12	0.39
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	1	0.39
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	14	0.39
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	20	0.39
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	3	0.39
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	11	0.39
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	11	0.39
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	19	0.39
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	6	0.39
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	9	0.39
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	4	0.39
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	11	0.39
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	13	0.39
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	4	0.38
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	14	0.38
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	18	0.38
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	19	0.38
(4,98)	1:X:97:GLU:O	1:X:117:ILE:H	10	0.38
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	18	0.38
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	18	0.38
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	6	0.38
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	13	0.38
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	9	0.38
(3,474)	1:X:68:ILE:N	1:X:68:ILE:CG2	17	0.38
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	11	0.38
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	18	0.38
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	15	0.38
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	6	0.38
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	4	0.38
(1,640)	1:X:74:LEU:HD21	1:X:39:TYR:H	1	0.38
(1,640)	1:X:74:LEU:HD22	1:X:39:TYR:H	1	0.38
(1,640)	1:X:74:LEU:HD23	1:X:39:TYR:H	1	0.38
(1,610)	1:X:71:ALA:H	1:X:70:VAL:CB	20	0.38
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	19	0.38
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	4	0.38

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	5	0.38
(1,221)	1:X:35:THR:H	1:X:34:SER:HB3	5	0.38
(1,193)	1:X:31:GLY:H	1:X:30:ARG:HG3	1	0.38
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	13	0.37
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	6	0.37
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	19	0.37
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	5	0.37
(5,3)	1:X:6:GLN:C	1:X:10:GLU:H	9	0.37
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	5	0.37
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	7	0.37
(4,96)	1:X:147:VAL:O	1:X:98:GLU:H	10	0.37
(4,93)	1:X:117:ILE:O	1:X:97:GLU:N	5	0.37
(4,54)	1:X:50:ASP:O	1:X:54:VAL:H	10	0.37
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	10	0.37
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	19	0.37
(4,33)	1:X:34:SER:O	1:X:73:ASN:H	14	0.37
(4,31)	1:X:33:THR:O	1:X:31:GLY:H	18	0.37
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	3	0.37
(3,955)	1:X:147:VAL:N	1:X:146:LEU:CD1	9	0.37
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	2	0.37
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	16	0.37
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	6	0.37
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	7	0.37
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	15	0.37
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	18	0.37
(3,212)	1:X:37:ARG:N	1:X:27:GLU:CB	2	0.37
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	20	0.37
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	10	0.37
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	20	0.37
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	6	0.37
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	16	0.37
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	11	0.37
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	15	0.37
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	17	0.37
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	18	0.37
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	14	0.37
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	1	0.37
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	14	0.36
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	9	0.36
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	12	0.36
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	13	0.36
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	11	0.36

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	16	0.36
(4,85)	1:X:88:ALA:O	1:X:92:ALA:H	1	0.36
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	14	0.36
(4,66)	1:X:56:HIS:O	1:X:60:ALA:N	3	0.36
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	1	0.36
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	18	0.36
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	16	0.36
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	13	0.36
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	15	0.36
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	14	0.36
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	6	0.36
(1,998)	1:X:121:ASP:H	1:X:125:ILE:CD1	16	0.36
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	9	0.36
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	12	0.36
(1,773)	1:X:94:PHE:HB3	1:X:97:GLU:H	19	0.36
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	10	0.36
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	19	0.36
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	4	0.36
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	6	0.36
(1,292)	1:X:40:ILE:CD1	1:X:51:CYS:H	5	0.36
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	16	0.36
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	13	0.35
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	9	0.35
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	1	0.35
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	1	0.35
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	13	0.35
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	20	0.35
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	14	0.35
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	17	0.35
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	7	0.35
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	10	0.35
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	8	0.35
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	6	0.35
(2,86)	1:X:91:TYR:CA	1:X:117:ILE:CD1	14	0.35
(2,107)	1:X:120:VAL:CG2	1:X:125:ILE:CD1	7	0.35
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	2	0.35
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	15	0.35
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	1	0.35
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	11	0.35
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	3	0.35
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	19	0.35
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	20	0.35

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	4	0.35
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	11	0.35
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	10	0.35
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	1	0.35
(1,227)	1:X:35:THR:HG21	1:X:75:GLU:H	14	0.35
(1,227)	1:X:35:THR:HG22	1:X:75:GLU:H	14	0.35
(1,227)	1:X:35:THR:HG23	1:X:75:GLU:H	14	0.35
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	14	0.35
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	2	0.35
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	17	0.35
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	4	0.34
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	18	0.34
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	3	0.34
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	17	0.34
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	18	0.34
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	2	0.34
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	10	0.34
(4,67)	1:X:57:GLN:O	1:X:61:VAL:H	7	0.34
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	3	0.34
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	19	0.34
(3,954)	1:X:147:VAL:N	1:X:146:LEU:CD2	11	0.34
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	17	0.34
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	13	0.34
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	14	0.34
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	5	0.34
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	7	0.34
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	8	0.34
(3,203)	1:X:36:LEU:N	1:X:35:THR:CG2	14	0.34
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	4	0.34
(1,864)	1:X:101:LEU:H	1:X:114:GLN:HB2	6	0.34
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	14	0.34
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	1	0.34
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	4	0.34
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	14	0.34
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	11	0.34
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	1	0.34
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	17	0.34
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	14	0.34
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	4	0.34
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	6	0.34
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	4	0.34
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	2	0.33

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	11	0.33
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	8	0.33
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	17	0.33
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	19	0.33
(4,68)	1:X:57:GLN:O	1:X:61:VAL:N	7	0.33
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	8	0.33
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	10	0.33
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	5	0.33
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	5	0.33
(3,894)	1:X:136:PHE:N	1:X:126:THR:CG2	20	0.33
(3,765)	1:X:115:GLY:N	1:X:129:VAL:CG2	17	0.33
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	5	0.33
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	3	0.33
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	5	0.33
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	5	0.33
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	17	0.33
(3,468)	1:X:66:ASP:N	1:X:67:PRO:CG	14	0.33
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	12	0.33
(2,86)	1:X:91:TYR:CA	1:X:117:ILE:CD1	20	0.33
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	4	0.33
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	3	0.33
(1,925)	1:X:108:GLN:HB2	1:X:109:ASN:H	6	0.33
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	16	0.33
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	20	0.33
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	9	0.33
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	19	0.33
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	8	0.33
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	10	0.33
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	16	0.33
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	15	0.33
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	8	0.33
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	7	0.33
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	11	0.33
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	18	0.32
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	18	0.32
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	7	0.32
(5,2)	1:X:5:GLU:C	1:X:9:THR:H	1	0.32
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	6	0.32
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	3	0.32
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	1	0.32
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	12	0.32
(4,75)	1:X:71:ALA:O	1:X:34:SER:H	5	0.32

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	14	0.32
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	9	0.32
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	12	0.32
(4,30)	1:X:29:ILE:O	1:X:35:THR:H	5	0.32
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	6	0.32
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	5	0.32
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	13	0.32
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	12	0.32
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	4	0.32
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	6	0.32
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	9	0.32
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	20	0.32
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	1	0.32
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	15	0.32
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	8	0.32
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	15	0.32
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	2	0.32
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	10	0.32
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	8	0.32
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	16	0.32
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	3	0.32
(1,227)	1:X:35:THR:HG21	1:X:75:GLU:H	1	0.32
(1,227)	1:X:35:THR:HG22	1:X:75:GLU:H	1	0.32
(1,227)	1:X:35:THR:HG23	1:X:75:GLU:H	1	0.32
(1,193)	1:X:31:GLY:H	1:X:30:ARG:HG3	14	0.32
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	17	0.32
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	7	0.31
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	13	0.31
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	6	0.31
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	20	0.31
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	18	0.31
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	8	0.31
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	4	0.31
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	8	0.31
(4,86)	1:X:88:ALA:O	1:X:92:ALA:N	1	0.31
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	2	0.31
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	20	0.31
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	19	0.31
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	15	0.31
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	20	0.31
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	10	0.31
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	14	0.31

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	5	0.31
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	5	0.31
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	10	0.31
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	18	0.31
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	3	0.31
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	12	0.31
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	16	0.31
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	18	0.31
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	2	0.31
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	7	0.31
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	18	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	1	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	2	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	3	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	4	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	5	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	6	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	7	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	8	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	9	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	10	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	11	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	12	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	13	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	14	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	15	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	16	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	17	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	18	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	19	0.31
(1,960)	1:X:114:GLN:HE22	1:X:114:GLN:HE21	20	0.31
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	17	0.31
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	6	0.31
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	1	0.31
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	16	0.31
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	11	0.31
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	2	0.31
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	12	0.31
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	12	0.31
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	9	0.31
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	12	0.31
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	11	0.31

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:X:29:ILE:HB	1:X:35:THR:H	19	0.31
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	12	0.31
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	15	0.31
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	12	0.31
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	1	0.3
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	5	0.3
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	8	0.3
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	10	0.3
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	10	0.3
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	1	0.3
(5,24)	1:X:47:ASN:C	1:X:50:ASP:H	3	0.3
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	7	0.3
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	11	0.3
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	7	0.3
(4,53)	1:X:50:ASP:O	1:X:54:VAL:N	10	0.3
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	1	0.3
(4,1)	1:X:4:LEU:O	1:X:8:LEU:H	15	0.3
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	3	0.3
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	7	0.3
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	16	0.3
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	10	0.3
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	6	0.3
(3,484)	1:X:71:ALA:N	1:X:70:VAL:CB	1	0.3
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	19	0.3
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	12	0.3
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	5	0.3
(2,107)	1:X:120:VAL:CG2	1:X:125:ILE:CD1	12	0.3
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	15	0.3
(1,773)	1:X:94:PHE:HB3	1:X:97:GLU:H	4	0.3
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	8	0.3
(1,590)	1:X:66:ASP:H	1:X:65:GLU:HB3	14	0.3
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	8	0.3
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	7	0.3
(1,248)	1:X:37:ARG:H	1:X:36:LEU:HB3	12	0.3
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	10	0.3
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	7	0.3
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	19	0.3
(1,1190)	1:X:141:ILE:HG13	1:X:137:ALA:H	14	0.3
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	18	0.3
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	16	0.3
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	14	0.3
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	7	0.3

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	11	0.29
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	15	0.29
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	15	0.29
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	20	0.29
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	13	0.29
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	16	0.29
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	8	0.29
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	6	0.29
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	9	0.29
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	18	0.29
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	3	0.29
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	19	0.29
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	15	0.29
(4,76)	1:X:71:ALA:O	1:X:34:SER:N	5	0.29
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	1	0.29
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	15	0.29
(4,2)	1:X:4:LEU:O	1:X:8:LEU:N	15	0.29
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	10	0.29
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	13	0.29
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	5	0.29
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	17	0.29
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	18	0.29
(3,765)	1:X:115:GLY:N	1:X:129:VAL:CG2	20	0.29
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	3	0.29
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	17	0.29
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	6	0.29
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	15	0.29
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	8	0.29
(3,587)	1:X:91:TYR:N	1:X:85:LEU:CD1	16	0.29
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	17	0.29
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	15	0.29
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	18	0.29
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	8	0.29
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	4	0.29
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	17	0.29
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	16	0.29
(2,92)	1:X:101:LEU:CD2	1:X:141:ILE:CG2	5	0.29
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	19	0.29
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	17	0.29
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	20	0.29
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	20	0.29
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	13	0.29

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	3	0.29
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	15	0.29
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	13	0.29
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	19	0.29
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	8	0.29
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	12	0.29
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	12	0.29
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	3	0.29
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	6	0.29
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	16	0.29
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	20	0.28
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	5	0.28
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	20	0.28
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	5	0.28
(4,53)	1:X:50:ASP:O	1:X:54:VAL:N	15	0.28
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	1	0.28
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	4	0.28
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	12	0.28
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	20	0.28
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	19	0.28
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	13	0.28
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	8	0.28
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	18	0.28
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	3	0.28
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	5	0.28
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	2	0.28
(2,107)	1:X:120:VAL:CG2	1:X:125:ILE:CD1	10	0.28
(2,106)	1:X:117:ILE:CD1	1:X:125:ILE:CG2	5	0.28
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	20	0.28
(1,925)	1:X:108:GLN:HB2	1:X:109:ASN:H	11	0.28
(1,925)	1:X:108:GLN:HB2	1:X:109:ASN:H	13	0.28
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	15	0.28
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	18	0.28
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	20	0.28
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	20	0.28
(1,618)	1:X:71:ALA:HB1	1:X:72:TYR:H	11	0.28
(1,618)	1:X:71:ALA:HB2	1:X:72:TYR:H	11	0.28
(1,618)	1:X:71:ALA:HB3	1:X:72:TYR:H	11	0.28
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	2	0.28
(1,453)	1:X:56:HIS:HB3	1:X:55:SER:H	3	0.28
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	13	0.28
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	14	0.28

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	5	0.28
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	16	0.28
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	7	0.28
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	14	0.28
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	3	0.28
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	6	0.28
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	7	0.28
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	20	0.28
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	18	0.27
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	2	0.27
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	7	0.27
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	13	0.27
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	5	0.27
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	1	0.27
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	3	0.27
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	14	0.27
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	19	0.27
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	10	0.27
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	11	0.27
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	12	0.27
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	13	0.27
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	6	0.27
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	3	0.27
(4,75)	1:X:71:ALA:O	1:X:34:SER:H	1	0.27
(4,65)	1:X:56:HIS:O	1:X:60:ALA:H	11	0.27
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	14	0.27
(4,54)	1:X:50:ASP:O	1:X:54:VAL:H	15	0.27
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	20	0.27
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	8	0.27
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	2	0.27
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	6	0.27
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	19	0.27
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	8	0.27
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	19	0.27
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	8	0.27
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	2	0.27
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	10	0.27
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	17	0.27
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	19	0.27
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	2	0.27
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	9	0.27
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	5	0.27

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:X:99:VAL:H	1:X:117:ILE:HG12	2	0.27
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	17	0.27
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	5	0.27
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	10	0.27
(1,52)	1:X:10:GLU:H	1:X:7:LYS:H	2	0.27
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	5	0.27
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	13	0.27
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	17	0.27
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	2	0.27
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	1	0.27
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	20	0.27
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	19	0.27
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	19	0.27
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	16	0.27
(1,175)	1:X:29:ILE:HB	1:X:35:THR:H	18	0.27
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	4	0.27
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	12	0.27
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	14	0.27
(1,1043)	1:X:125:ILE:H	1:X:136:PHE:H	1	0.27
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	7	0.26
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	3	0.26
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	16	0.26
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	20	0.26
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	1	0.26
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	13	0.26
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	15	0.26
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	16	0.26
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	1	0.26
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	16	0.26
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	13	0.26
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	20	0.26
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	15	0.26
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	20	0.26
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	4	0.26
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	12	0.26
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	4	0.26
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	19	0.26
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	5	0.26
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	9	0.26
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	3	0.26
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	1	0.26
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	13	0.26

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	14	0.26
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	17	0.26
(3,159)	1:X:29:ILE:N	1:X:28:PHE:CB	12	0.26
(1,899)	1:X:106:ALA:HA	1:X:103:LEU:H	12	0.26
(1,836)	1:X:99:VAL:H	1:X:117:ILE:HG12	3	0.26
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	19	0.26
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	9	0.26
(1,679)	1:X:77:SER:HB3	1:X:78:SER:H	19	0.26
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	8	0.26
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	5	0.26
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	4	0.26
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	2	0.26
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	17	0.26
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	11	0.26
(1,5)	1:X:5:GLU:H	1:X:4:LEU:HG	19	0.26
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	15	0.26
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	19	0.26
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	20	0.26
(1,248)	1:X:37:ARG:H	1:X:36:LEU:HB3	11	0.26
(1,221)	1:X:35:THR:H	1:X:34:SER:HB3	13	0.26
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	12	0.26
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	6	0.26
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	6	0.26
(1,1190)	1:X:141:ILE:HG13	1:X:137:ALA:H	17	0.26
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	15	0.26
(1,1043)	1:X:125:ILE:H	1:X:136:PHE:H	4	0.26
(5,63)	1:X:128:THR:C	1:X:116:VAL:H	11	0.25
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	12	0.25
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	8	0.25
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	15	0.25
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	11	0.25
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	20	0.25
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	19	0.25
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	3	0.25
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	7	0.25
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	17	0.25
(4,66)	1:X:56:HIS:O	1:X:60:ALA:N	11	0.25
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	3	0.25
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	4	0.25
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	7	0.25
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	20	0.25
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	3	0.25

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	9	0.25
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	7	0.25
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	17	0.25
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	8	0.25
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	12	0.25
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	19	0.25
(2,4)	1:X:8:LEU:CD1	1:X:11:MET:CE	13	0.25
(2,4)	1:X:8:LEU:CD2	1:X:11:MET:CE	13	0.25
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	13	0.25
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	7	0.25
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	2	0.25
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	4	0.25
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	11	0.25
(1,658)	1:X:76:VAL:HB	1:X:55:SER:H	16	0.25
(1,636)	1:X:73:ASN:HB3	1:X:74:LEU:H	19	0.25
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	1	0.25
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	3	0.25
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	15	0.25
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	1	0.25
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	12	0.25
(1,315)	1:X:44:ASP:H	1:X:43:GLU:HG2	3	0.25
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	2	0.25
(1,221)	1:X:35:THR:H	1:X:34:SER:HB3	17	0.25
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	11	0.25
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	9	0.25
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	17	0.25
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	1	0.25
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	6	0.25
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	18	0.25
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	7	0.25
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	13	0.25
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	2	0.25
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	14	0.25
(1,1045)	1:X:125:ILE:H	1:X:138:LEU:H	9	0.25
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	5	0.24
(5,67)	1:X:136:PHE:C	1:X:125:ILE:H	4	0.24
(5,63)	1:X:128:THR:C	1:X:116:VAL:H	5	0.24
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	1	0.24
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	14	0.24
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	3	0.24
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	20	0.24
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	13	0.24

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	7	0.24
(5,3)	1:X:6:GLN:C	1:X:10:GLU:H	10	0.24
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	13	0.24
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	11	0.24
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	5	0.24
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	15	0.24
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	15	0.24
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	17	0.24
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	7	0.24
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	10	0.24
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	4	0.24
(4,24)	1:X:23:LEU:O	1:X:41:ASP:H	13	0.24
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	8	0.24
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	5	0.24
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	17	0.24
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	8	0.24
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	10	0.24
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	2	0.24
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	12	0.24
(3,823)	1:X:124:MET:CB	1:X:125:ILE:N	1	0.24
(3,823)	1:X:124:MET:CB	1:X:125:ILE:N	2	0.24
(3,823)	1:X:124:MET:CB	1:X:125:ILE:N	4	0.24
(3,814)	1:X:124:MET:N	1:X:121:ASP:CB	16	0.24
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	18	0.24
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	4	0.24
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	18	0.24
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	19	0.24
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	3	0.24
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	11	0.24
(3,371)	1:X:57:GLN:N	1:X:54:VAL:CG2	3	0.24
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	2	0.24
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	14	0.24
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	15	0.24
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	8	0.24
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	13	0.24
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	11	0.24
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	17	0.24
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	13	0.24
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	8	0.24
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	12	0.24
(1,575)	1:X:65:GLU:HB2	1:X:64:VAL:H	4	0.24
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	17	0.24

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	1	0.24
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	2	0.24
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	3	0.24
(1,289)	1:X:40:ILE:H	1:X:39:TYR:HB3	6	0.24
(1,148)	1:X:25:GLY:H	1:X:40:ILE:HG13	5	0.24
(1,1190)	1:X:141:ILE:HG13	1:X:137:ALA:H	20	0.24
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	9	0.24
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	4	0.24
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	1	0.24
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	2	0.24
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	10	0.23
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	1	0.23
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	3	0.23
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	5	0.23
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	7	0.23
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	12	0.23
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	4	0.23
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	6	0.23
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	19	0.23
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	4	0.23
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	17	0.23
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	16	0.23
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	7	0.23
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	13	0.23
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	20	0.23
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	14	0.23
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	10	0.23
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	3	0.23
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	19	0.23
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	20	0.23
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	3	0.23
(3,878)	1:X:133:ASP:N	1:X:128:THR:CG2	10	0.23
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	12	0.23
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	18	0.23
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	10	0.23
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	15	0.23
(3,555)	1:X:87:THR:N	1:X:85:LEU:CD1	13	0.23
(3,464)	1:X:66:ASP:N	1:X:64:VAL:CG1	17	0.23
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	18	0.23
(3,159)	1:X:29:ILE:N	1:X:28:PHE:CB	11	0.23
(2,59)	1:X:54:VAL:CG2	1:X:40:ILE:CD1	14	0.23
(1,912)	1:X:107:VAL:H	1:X:110:ARG:H	9	0.23

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	10	0.23
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	7	0.23
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	6	0.23
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	20	0.23
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	18	0.23
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	20	0.23
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	16	0.23
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	9	0.23
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	17	0.23
(1,51)	1:X:10:GLU:H	1:X:7:LYS:HA	12	0.23
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	5	0.23
(1,453)	1:X:56:HIS:HB3	1:X:55:SER:H	2	0.23
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	5	0.23
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	17	0.23
(1,420)	1:X:54:VAL:H	1:X:51:CYS:HA	3	0.23
(1,248)	1:X:37:ARG:H	1:X:36:LEU:HB3	16	0.23
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	2	0.23
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	19	0.23
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	6	0.23
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	15	0.23
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	19	0.23
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	9	0.23
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	13	0.23
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	12	0.22
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	4	0.22
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	8	0.22
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	12	0.22
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	10	0.22
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	13	0.22
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	13	0.22
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	2	0.22
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	20	0.22
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	7	0.22
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	20	0.22
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	13	0.22
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	17	0.22
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	4	0.22
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	4	0.22
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	13	0.22
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	9	0.22
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	9	0.22
(4,47)	1:X:47:ASN:O	1:X:50:ASP:H	3	0.22

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	19	0.22
(3,847)	1:X:128:THR:CB	1:X:116:VAL:N	11	0.22
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	2	0.22
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	2	0.22
(3,746)	1:X:112:LYS:N	1:X:111:ARG:CB	9	0.22
(3,666)	1:X:94:PHE:N	1:X:117:ILE:CG2	11	0.22
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	20	0.22
(3,661)	1:X:91:TYR:N	1:X:120:VAL:CG1	15	0.22
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	8	0.22
(3,595)	1:X:92:ALA:N	1:X:85:LEU:CD1	8	0.22
(3,556)	1:X:87:THR:N	1:X:86:PHE:CB	13	0.22
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	18	0.22
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	8	0.22
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	12	0.22
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	16	0.22
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	19	0.22
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	10	0.22
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	13	0.22
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	4	0.22
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	15	0.22
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	16	0.22
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	11	0.22
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	19	0.22
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	6	0.22
(1,640)	1:X:74:LEU:HD21	1:X:39:TYR:H	14	0.22
(1,640)	1:X:74:LEU:HD22	1:X:39:TYR:H	14	0.22
(1,640)	1:X:74:LEU:HD23	1:X:39:TYR:H	14	0.22
(1,575)	1:X:65:GLU:HB2	1:X:64:VAL:H	8	0.22
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	5	0.22
(1,5)	1:X:5:GLU:H	1:X:4:LEU:HG	15	0.22
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	4	0.22
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	20	0.22
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	5	0.22
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	19	0.22
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	14	0.22
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	20	0.22
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	2	0.22
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	19	0.22
(1,351)	1:X:47:ASN:H	1:X:46:ILE:HG13	20	0.22
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	16	0.22
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	4	0.22
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	11	0.22

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	11	0.22
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	3	0.22
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	13	0.22
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	10	0.22
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	7	0.22
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	6	0.22
(5,9)	1:X:13:THR:C	1:X:17:GLU:H	13	0.21
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	9	0.21
(5,67)	1:X:136:PHE:C	1:X:125:ILE:H	1	0.21
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	3	0.21
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	18	0.21
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	11	0.21
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	10	0.21
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	3	0.21
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	2	0.21
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	7	0.21
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	12	0.21
(5,2)	1:X:5:GLU:C	1:X:9:THR:H	12	0.21
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	7	0.21
(5,16)	1:X:33:THR:C	1:X:31:GLY:H	18	0.21
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	19	0.21
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	15	0.21
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	5	0.21
(4,60)	1:X:53:ASP:O	1:X:57:GLN:N	10	0.21
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	8	0.21
(4,21)	1:X:15:PRO:O	1:X:19:LEU:H	7	0.21
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	11	0.21
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	17	0.21
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	11	0.21
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	15	0.21
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	8	0.21
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	10	0.21
(3,940)	1:X:144:ALA:N	1:X:143:LYS:CG	5	0.21
(3,887)	1:X:135:VAL:CG2	1:X:125:ILE:N	4	0.21
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	1	0.21
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	4	0.21
(3,661)	1:X:91:TYR:N	1:X:120:VAL:CG1	16	0.21
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	8	0.21
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	9	0.21
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	10	0.21
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	15	0.21
(3,462)	1:X:66:ASP:N	1:X:11:MET:CE	10	0.21

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	10	0.21
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	20	0.21
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	20	0.21
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	19	0.21
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	12	0.21
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	2	0.21
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	15	0.21
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	20	0.21
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	5	0.21
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	12	0.21
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	11	0.21
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	18	0.21
(1,640)	1:X:74:LEU:HD21	1:X:39:TYR:H	11	0.21
(1,640)	1:X:74:LEU:HD22	1:X:39:TYR:H	11	0.21
(1,640)	1:X:74:LEU:HD23	1:X:39:TYR:H	11	0.21
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	11	0.21
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	12	0.21
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	15	0.21
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	10	0.21
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	16	0.21
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	17	0.21
(1,453)	1:X:56:HIS:HB3	1:X:55:SER:H	7	0.21
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	18	0.21
(1,351)	1:X:47:ASN:H	1:X:46:ILE:HG13	16	0.21
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	16	0.21
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	3	0.21
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	20	0.21
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	4	0.21
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	3	0.21
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	20	0.21
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	5	0.21
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	16	0.21
(5,9)	1:X:13:THR:C	1:X:17:GLU:H	10	0.2
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	18	0.2
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	3	0.2
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	5	0.2
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	14	0.2
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	1	0.2
(5,40)	1:X:75:GLU:C	1:X:38:ILE:H	9	0.2
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	15	0.2
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	9	0.2
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	2	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	15	0.2
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	2	0.2
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	7	0.2
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	3	0.2
(5,23)	1:X:41:ASP:C	1:X:23:LEU:H	12	0.2
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	2	0.2
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	5	0.2
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	17	0.2
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	4	0.2
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	3	0.2
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	18	0.2
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	1	0.2
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	18	0.2
(4,88)	1:X:89:GLU:O	1:X:93:ARG:N	19	0.2
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	1	0.2
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	4	0.2
(4,71)	1:X:59:SER:O	1:X:63:ASP:H	4	0.2
(4,67)	1:X:57:GLN:O	1:X:61:VAL:H	9	0.2
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	10	0.2
(4,23)	1:X:23:LEU:O	1:X:41:ASP:N	13	0.2
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	5	0.2
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	11	0.2
(4,115)	1:X:121:ASP:O	1:X:124:MET:H	10	0.2
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	6	0.2
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	11	0.2
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	15	0.2
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	20	0.2
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	14	0.2
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	10	0.2
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	14	0.2
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	6	0.2
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	1	0.2
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	7	0.2
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	16	0.2
(3,666)	1:X:94:PHE:N	1:X:117:ILE:CG2	3	0.2
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	12	0.2
(3,554)	1:X:85:LEU:CA	1:X:87:THR:N	8	0.2
(3,554)	1:X:85:LEU:CA	1:X:87:THR:N	9	0.2
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	19	0.2
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	3	0.2
(3,313)	1:X:52:ALA:N	1:X:40:ILE:CD1	16	0.2
(3,203)	1:X:36:LEU:N	1:X:35:THR:CG2	1	0.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:X:91:TYR:CA	1:X:117:ILE:CD1	1	0.2
(2,37)	1:X:38:ILE:CG2	1:X:26:ILE:CD1	3	0.2
(2,121)	1:X:138:LEU:CD1	1:X:141:ILE:CD1	6	0.2
(1,916)	1:X:108:GLN:H	1:X:107:VAL:CB	18	0.2
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	11	0.2
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	15	0.2
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	10	0.2
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	13	0.2
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	20	0.2
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	10	0.2
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	17	0.2
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	1	0.2
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	2	0.2
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	10	0.2
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	5	0.2
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	12	0.2
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	4	0.2
(1,146)	1:X:25:GLY:H	1:X:39:TYR:HB2	7	0.2
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	7	0.2
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	10	0.2
(1,1135)	1:X:134:GLU:H	1:X:127:VAL:H	16	0.2
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	14	0.2
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	4	0.2
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	20	0.19
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	4	0.19
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	12	0.19
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	16	0.19
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	14	0.19
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	15	0.19
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	15	0.19
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	4	0.19
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	10	0.19
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	14	0.19
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	19	0.19
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	15	0.19
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	4	0.19
(5,26)	1:X:49:ASP:C	1:X:53:ASP:H	4	0.19
(5,25)	1:X:48:VAL:C	1:X:52:ALA:H	8	0.19
(4,68)	1:X:57:GLN:O	1:X:61:VAL:N	9	0.19
(4,67)	1:X:57:GLN:O	1:X:61:VAL:H	8	0.19
(4,21)	1:X:15:PRO:O	1:X:19:LEU:H	2	0.19
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	2	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	16	0.19
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	2	0.19
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	4	0.19
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	17	0.19
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	14	0.19
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	20	0.19
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	11	0.19
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	16	0.19
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	1	0.19
(3,716)	1:X:104:ARG:N	1:X:105:MET:CB	7	0.19
(3,690)	1:X:101:LEU:CG	1:X:115:GLY:N	13	0.19
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	18	0.19
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	13	0.19
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	2	0.19
(3,556)	1:X:87:THR:N	1:X:86:PHE:CB	6	0.19
(3,556)	1:X:87:THR:N	1:X:86:PHE:CB	12	0.19
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	10	0.19
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	1	0.19
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	14	0.19
(3,356)	1:X:55:SER:N	1:X:76:VAL:CG1	16	0.19
(3,243)	1:X:41:ASP:N	1:X:22:GLU:CG	17	0.19
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	11	0.19
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	11	0.19
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	15	0.19
(1,96)	1:X:19:LEU:H	1:X:16:VAL:HA	9	0.19
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	8	0.19
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	17	0.19
(1,773)	1:X:94:PHE:HB3	1:X:97:GLU:H	11	0.19
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	2	0.19
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	8	0.19
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	16	0.19
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	4	0.19
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	18	0.19
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	1	0.19
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	4	0.19
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	12	0.19
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	7	0.19
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	18	0.19
(1,295)	1:X:41:ASP:H	1:X:21:PHE:HA	3	0.19
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	13	0.19
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	6	0.19
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	19	0.19

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,179)	1:X:29:ILE:H	1:X:36:LEU:H	7	0.19
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	15	0.19
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	5	0.19
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	17	0.19
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	19	0.18
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	3	0.18
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	9	0.18
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	10	0.18
(5,67)	1:X:136:PHE:C	1:X:125:ILE:H	12	0.18
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	2	0.18
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	7	0.18
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	11	0.18
(5,56)	1:X:116:VAL:C	1:X:128:THR:H	5	0.18
(5,56)	1:X:116:VAL:C	1:X:128:THR:H	11	0.18
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	6	0.18
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	9	0.18
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	19	0.18
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	8	0.18
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	15	0.18
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	18	0.18
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	16	0.18
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	6	0.18
(5,41)	1:X:77:SER:C	1:X:40:ILE:H	14	0.18
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	5	0.18
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	9	0.18
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	20	0.18
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	9	0.18
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	14	0.18
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	8	0.18
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	10	0.18
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	2	0.18
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	15	0.18
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	4	0.18
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	5	0.18
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	12	0.18
(5,1)	1:X:4:LEU:C	1:X:8:LEU:H	17	0.18
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	10	0.18
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	16	0.18
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	6	0.18
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	4	0.18
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	18	0.18
(3,749)	1:X:113:TRP:N	1:X:101:LEU:CD1	1	0.18

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	7	0.18
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	3	0.18
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	14	0.18
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	13	0.18
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	14	0.18
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	6	0.18
(3,197)	1:X:35:THR:N	1:X:34:SER:CB	5	0.18
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	18	0.18
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	5	0.18
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	19	0.18
(1,96)	1:X:19:LEU:H	1:X:16:VAL:HA	6	0.18
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	14	0.18
(1,774)	1:X:94:PHE:HA	1:X:97:GLU:H	11	0.18
(1,759)	1:X:93:ARG:H	1:X:90:HIS:HA	12	0.18
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	11	0.18
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	20	0.18
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	11	0.18
(1,595)	1:X:66:ASP:HB2	1:X:72:TYR:H	19	0.18
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	6	0.18
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	6	0.18
(1,585)	1:X:66:ASP:H	1:X:63:ASP:HA	18	0.18
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	13	0.18
(1,5)	1:X:5:GLU:H	1:X:4:LEU:HG	10	0.18
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	7	0.18
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	9	0.18
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	5	0.18
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	9	0.18
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	4	0.18
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	18	0.18
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	9	0.18
(1,219)	1:X:35:THR:H	1:X:28:PHE:HA	10	0.18
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	3	0.18
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	13	0.18
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	19	0.18
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	20	0.18
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	11	0.18
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	9	0.18
(1,1007)	1:X:122:GLY:H	1:X:124:MET:H	10	0.18
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	2	0.17
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	4	0.17
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	1	0.17
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	15	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	10	0.17
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	6	0.17
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	14	0.17
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	19	0.17
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	11	0.17
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	5	0.17
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	11	0.17
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	19	0.17
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	4	0.17
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	7	0.17
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	18	0.17
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	1	0.17
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	20	0.17
(5,34)	1:X:57:GLN:C	1:X:61:VAL:H	14	0.17
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	4	0.17
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	6	0.17
(5,28)	1:X:51:CYS:C	1:X:55:SER:H	10	0.17
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	1	0.17
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	8	0.17
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	17	0.17
(5,19)	1:X:36:LEU:C	1:X:75:GLU:H	9	0.17
(5,19)	1:X:36:LEU:C	1:X:75:GLU:H	12	0.17
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	4	0.17
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	19	0.17
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	11	0.17
(4,74)	1:X:60:ALA:O	1:X:64:VAL:N	16	0.17
(4,65)	1:X:56:HIS:O	1:X:60:ALA:H	5	0.17
(4,47)	1:X:47:ASN:O	1:X:50:ASP:H	5	0.17
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	2	0.17
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	19	0.17
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	1	0.17
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	7	0.17
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	12	0.17
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	7	0.17
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	5	0.17
(3,847)	1:X:128:THR:CB	1:X:116:VAL:N	3	0.17
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	9	0.17
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	11	0.17
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	7	0.17
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	12	0.17
(3,749)	1:X:113:TRP:N	1:X:101:LEU:CD1	8	0.17
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	4	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,716)	1:X:104:ARG:N	1:X:105:MET:CB	9	0.17
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	2	0.17
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	9	0.17
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	2	0.17
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	13	0.17
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	17	0.17
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	6	0.17
(3,435)	1:X:63:ASP:N	1:X:62:LEU:CD1	13	0.17
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	15	0.17
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	16	0.17
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	15	0.17
(3,175)	1:X:31:GLY:N	1:X:30:ARG:CD	13	0.17
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	4	0.17
(2,121)	1:X:138:LEU:CD1	1:X:141:ILE:CD1	15	0.17
(1,717)	1:X:87:THR:H	1:X:86:PHE:HB2	19	0.17
(1,685)	1:X:78:SER:HB2	1:X:78:SER:H	3	0.17
(1,685)	1:X:78:SER:HB2	1:X:78:SER:H	14	0.17
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	16	0.17
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	20	0.17
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	3	0.17
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	2	0.17
(1,51)	1:X:10:GLU:H	1:X:7:LYS:HA	13	0.17
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	18	0.17
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	1	0.17
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	7	0.17
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	15	0.17
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	17	0.17
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	4	0.17
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	7	0.17
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	11	0.17
(1,420)	1:X:54:VAL:H	1:X:51:CYS:HA	2	0.17
(1,335)	1:X:46:ILE:H	1:X:45:GLY:H	16	0.17
(1,315)	1:X:44:ASP:H	1:X:43:GLU:HG2	11	0.17
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	10	0.17
(1,241)	1:X:37:ARG:H	1:X:27:GLU:HB2	2	0.17
(1,204)	1:X:33:THR:H	1:X:32:ARG:HG2	9	0.17
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	4	0.17
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	17	0.17
(1,1191)	1:X:141:ILE:H	1:X:138:LEU:HA	11	0.17
(1,1135)	1:X:134:GLU:H	1:X:127:VAL:H	11	0.17
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	9	0.17
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	1	0.17

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	11	0.16
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	17	0.16
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	6	0.16
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	17	0.16
(5,62)	1:X:127:VAL:C	1:X:134:GLU:H	18	0.16
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	3	0.16
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	17	0.16
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	2	0.16
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	17	0.16
(5,46)	1:X:115:GLY:C	1:X:99:VAL:H	5	0.16
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	6	0.16
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	7	0.16
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	8	0.16
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	17	0.16
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	17	0.16
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	6	0.16
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	4	0.16
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	2	0.16
(4,68)	1:X:57:GLN:O	1:X:61:VAL:N	8	0.16
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	12	0.16
(4,43)	1:X:39:TYR:O	1:X:25:GLY:H	13	0.16
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	13	0.16
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	17	0.16
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	16	0.16
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	7	0.16
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	17	0.16
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	19	0.16
(3,878)	1:X:133:ASP:N	1:X:128:THR:CG2	17	0.16
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	4	0.16
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	10	0.16
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	14	0.16
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	17	0.16
(3,749)	1:X:113:TRP:N	1:X:101:LEU:CD1	19	0.16
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	20	0.16
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	4	0.16
(3,610)	1:X:94:PHE:N	1:X:85:LEU:CD1	14	0.16
(3,556)	1:X:87:THR:N	1:X:86:PHE:CB	20	0.16
(3,554)	1:X:85:LEU:CA	1:X:87:THR:N	4	0.16
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	11	0.16
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	20	0.16
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	1	0.16
(3,484)	1:X:71:ALA:N	1:X:70:VAL:CB	5	0.16

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,304)	1:X:51:CYS:N	1:X:40:ILE:CD1	5	0.16
(3,266)	1:X:45:GLY:N	1:X:43:GLU:CG	15	0.16
(3,239)	1:X:41:ASP:N	1:X:16:VAL:CG1	8	0.16
(3,130)	1:X:25:GLY:N	1:X:23:LEU:CG	1	0.16
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	5	0.16
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	18	0.16
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	13	0.16
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	19	0.16
(1,931)	1:X:109:ASN:HD21	1:X:109:ASN:HB3	20	0.16
(1,864)	1:X:101:LEU:H	1:X:114:GLN:HB2	10	0.16
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	13	0.16
(1,658)	1:X:76:VAL:HB	1:X:55:SER:H	4	0.16
(1,624)	1:X:73:ASN:H	1:X:36:LEU:HB2	18	0.16
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	2	0.16
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	6	0.16
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	15	0.16
(1,531)	1:X:62:LEU:HB2	1:X:61:VAL:H	11	0.16
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	2	0.16
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	12	0.16
(1,51)	1:X:10:GLU:H	1:X:7:LYS:HA	2	0.16
(1,51)	1:X:10:GLU:H	1:X:7:LYS:HA	3	0.16
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	11	0.16
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	18	0.16
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	11	0.16
(1,392)	1:X:50:ASP:HA	1:X:53:ASP:H	19	0.16
(1,246)	1:X:37:ARG:H	1:X:29:ILE:H	1	0.16
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	14	0.16
(1,204)	1:X:33:THR:H	1:X:32:ARG:HG2	4	0.16
(1,177)	1:X:29:ILE:HA	1:X:35:THR:H	5	0.16
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	8	0.16
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	17	0.16
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	9	0.16
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	11	0.16
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	16	0.16
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	6	0.16
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	7	0.16
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	19	0.16
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	20	0.16
(1,1048)	1:X:125:ILE:H	1:X:138:LEU:HG	19	0.16
(1,1030)	1:X:124:MET:HG3	1:X:138:LEU:H	10	0.16
(5,9)	1:X:13:THR:C	1:X:17:GLU:H	20	0.15
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	3	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	1	0.15
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	20	0.15
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	11	0.15
(5,62)	1:X:127:VAL:C	1:X:134:GLU:H	10	0.15
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	12	0.15
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	20	0.15
(5,6)	1:X:9:THR:C	1:X:13:THR:H	19	0.15
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	17	0.15
(5,52)	1:X:100:THR:C	1:X:145:ASN:H	6	0.15
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	11	0.15
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	18	0.15
(5,46)	1:X:115:GLY:C	1:X:99:VAL:H	4	0.15
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	5	0.15
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	18	0.15
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	1	0.15
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	2	0.15
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	5	0.15
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	15	0.15
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	8	0.15
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	17	0.15
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	20	0.15
(5,23)	1:X:41:ASP:C	1:X:23:LEU:H	6	0.15
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	14	0.15
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	12	0.15
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	5	0.15
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	14	0.15
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	14	0.15
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	8	0.15
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	18	0.15
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	17	0.15
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	1	0.15
(4,73)	1:X:60:ALA:O	1:X:64:VAL:H	16	0.15
(4,72)	1:X:59:SER:O	1:X:63:ASP:N	4	0.15
(4,21)	1:X:15:PRO:O	1:X:19:LEU:H	11	0.15
(4,21)	1:X:15:PRO:O	1:X:19:LEU:H	18	0.15
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	19	0.15
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	1	0.15
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	12	0.15
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	17	0.15
(4,1)	1:X:4:LEU:O	1:X:8:LEU:H	6	0.15
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	20	0.15
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	20	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,921)	1:X:141:ILE:N	1:X:101:LEU:CD2	11	0.15
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	1	0.15
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	7	0.15
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	9	0.15
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	12	0.15
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	2	0.15
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	9	0.15
(3,765)	1:X:115:GLY:N	1:X:129:VAL:CG2	5	0.15
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	16	0.15
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	2	0.15
(3,666)	1:X:94:PHE:N	1:X:117:ILE:CG2	4	0.15
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	4	0.15
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	7	0.15
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	3	0.15
(3,563)	1:X:88:ALA:N	1:X:87:THR:CG2	13	0.15
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	17	0.15
(3,484)	1:X:71:ALA:N	1:X:70:VAL:CB	20	0.15
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	9	0.15
(3,212)	1:X:37:ARG:N	1:X:27:GLU:CB	1	0.15
(3,209)	1:X:36:LEU:N	1:X:74:LEU:CD2	20	0.15
(3,208)	1:X:36:LEU:N	1:X:37:ARG:CG	3	0.15
(3,197)	1:X:35:THR:N	1:X:34:SER:CB	13	0.15
(3,189)	1:X:34:SER:N	1:X:33:THR:CB	3	0.15
(3,124)	1:X:24:VAL:N	1:X:23:LEU:CD1	15	0.15
(2,29)	1:X:29:ILE:CD1	1:X:35:THR:CG2	15	0.15
(2,23)	1:X:16:VAL:CG2	1:X:54:VAL:CG2	5	0.15
(2,121)	1:X:138:LEU:CD1	1:X:141:ILE:CD1	5	0.15
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	15	0.15
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	16	0.15
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	16	0.15
(1,972)	1:X:116:VAL:HB	1:X:128:THR:H	13	0.15
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	11	0.15
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	15	0.15
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	20	0.15
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	4	0.15
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	9	0.15
(1,595)	1:X:66:ASP:HB2	1:X:72:TYR:H	3	0.15
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	5	0.15
(1,575)	1:X:65:GLU:HB2	1:X:64:VAL:H	19	0.15
(1,511)	1:X:59:SER:H	1:X:62:LEU:HB3	3	0.15
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	14	0.15
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	16	0.15

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,493)	1:X:58:VAL:CB	1:X:60:ALA:H	13	0.15
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	6	0.15
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	13	0.15
(1,453)	1:X:56:HIS:HB3	1:X:55:SER:H	18	0.15
(1,204)	1:X:33:THR:H	1:X:32:ARG:HG2	11	0.15
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	1	0.15
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	10	0.15
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	7	0.15
(1,1191)	1:X:141:ILE:H	1:X:138:LEU:HA	14	0.15
(1,1190)	1:X:141:ILE:HG13	1:X:137:ALA:H	4	0.15
(1,1109)	1:X:130:GLU:HB2	1:X:132:LYS:H	12	0.15
(1,1087)	1:X:128:THR:HA	1:X:134:GLU:H	9	0.15
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	6	0.15
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	8	0.15
(1,1028)	1:X:124:MET:H	1:X:138:LEU:HG	15	0.15
(1,1007)	1:X:122:GLY:H	1:X:124:MET:H	9	0.15
(1,1007)	1:X:122:GLY:H	1:X:124:MET:H	14	0.15
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	6	0.14
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	6	0.14
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	5	0.14
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	19	0.14
(5,63)	1:X:128:THR:C	1:X:116:VAL:H	13	0.14
(5,63)	1:X:128:THR:C	1:X:116:VAL:H	19	0.14
(5,59)	1:X:124:MET:C	1:X:121:ASP:H	13	0.14
(5,56)	1:X:116:VAL:C	1:X:128:THR:H	15	0.14
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	3	0.14
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	6	0.14
(5,49)	1:X:97:GLU:C	1:X:117:ILE:H	17	0.14
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	11	0.14
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	12	0.14
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	11	0.14
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	18	0.14
(5,39)	1:X:73:ASN:C	1:X:36:LEU:H	19	0.14
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	3	0.14
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	8	0.14
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	16	0.14
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	8	0.14
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	10	0.14
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	18	0.14
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	2	0.14
(5,24)	1:X:47:ASN:C	1:X:50:ASP:H	11	0.14
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	9	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	1	0.14
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	3	0.14
(5,12)	1:X:23:LEU:C	1:X:41:ASP:H	8	0.14
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	1	0.14
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	9	0.14
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	10	0.14
(4,88)	1:X:89:GLU:O	1:X:93:ARG:N	10	0.14
(4,67)	1:X:57:GLN:O	1:X:61:VAL:H	4	0.14
(4,65)	1:X:56:HIS:O	1:X:60:ALA:H	9	0.14
(4,59)	1:X:53:ASP:O	1:X:57:GLN:H	2	0.14
(4,54)	1:X:50:ASP:O	1:X:54:VAL:H	5	0.14
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	14	0.14
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	6	0.14
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	14	0.14
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	13	0.14
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	10	0.14
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	15	0.14
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	20	0.14
(3,906)	1:X:137:ALA:N	1:X:141:ILE:CD1	16	0.14
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	5	0.14
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	3	0.14
(3,632)	1:X:97:GLU:N	1:X:94:PHE:CA	7	0.14
(3,554)	1:X:85:LEU:CA	1:X:87:THR:N	10	0.14
(3,545)	1:X:81:LEU:CD1	1:X:82:ASP:N	10	0.14
(3,534)	1:X:80:GLY:N	1:X:79:PRO:CB	11	0.14
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	12	0.14
(3,476)	1:X:68:ILE:N	1:X:68:ILE:CD1	5	0.14
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	20	0.14
(3,197)	1:X:35:THR:N	1:X:34:SER:CB	17	0.14
(3,189)	1:X:34:SER:N	1:X:33:THR:CB	5	0.14
(3,124)	1:X:24:VAL:N	1:X:23:LEU:CD1	1	0.14
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	1	0.14
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	4	0.14
(2,121)	1:X:138:LEU:CD1	1:X:141:ILE:CD1	9	0.14
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	16	0.14
(1,96)	1:X:19:LEU:H	1:X:16:VAL:HA	2	0.14
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	1	0.14
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	5	0.14
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	20	0.14
(1,896)	1:X:105:MET:HA	1:X:106:ALA:H	18	0.14
(1,818)	1:X:146:LEU:H	1:X:85:LEU:H	16	0.14
(1,80)	1:X:14:ALA:H	1:X:11:MET:HA	15	0.14

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	8	0.14
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	18	0.14
(1,671)	1:X:77:SER:H	1:X:39:TYR:HA	16	0.14
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	3	0.14
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	7	0.14
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	16	0.14
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	19	0.14
(1,59)	1:X:12:ILE:H	1:X:9:THR:HA	4	0.14
(1,58)	1:X:12:ILE:H	1:X:9:THR:H	14	0.14
(1,51)	1:X:10:GLU:H	1:X:7:LYS:HA	10	0.14
(1,5)	1:X:5:GLU:H	1:X:4:LEU:HG	1	0.14
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	10	0.14
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	14	0.14
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	15	0.14
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	20	0.14
(1,315)	1:X:44:ASP:H	1:X:43:GLU:HG2	15	0.14
(1,296)	1:X:41:ASP:H	1:X:22:GLU:HB3	6	0.14
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	4	0.14
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	15	0.14
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	19	0.14
(1,173)	1:X:29:ILE:H	1:X:35:THR:H	3	0.14
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	18	0.14
(1,1191)	1:X:141:ILE:H	1:X:138:LEU:HA	17	0.14
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	16	0.14
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	2	0.14
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	3	0.14
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	15	0.14
(1,1031)	1:X:124:MET:HA	1:X:138:LEU:H	18	0.14
(1,1018)	1:X:123:GLU:H	1:X:124:MET:HB2	10	0.14
(1,1018)	1:X:123:GLU:H	1:X:124:MET:HB2	20	0.14
(1,1007)	1:X:122:GLY:H	1:X:124:MET:H	20	0.14
(5,9)	1:X:13:THR:C	1:X:17:GLU:H	15	0.13
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	14	0.13
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	16	0.13
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	8	0.13
(5,68)	1:X:137:ALA:C	1:X:140:ASN:H	20	0.13
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	15	0.13
(5,62)	1:X:127:VAL:C	1:X:134:GLU:H	5	0.13
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	20	0.13
(5,6)	1:X:9:THR:C	1:X:13:THR:H	13	0.13
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	15	0.13
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	20	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	12	0.13
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	11	0.13
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	14	0.13
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	14	0.13
(5,27)	1:X:50:ASP:C	1:X:54:VAL:H	13	0.13
(5,24)	1:X:47:ASN:C	1:X:50:ASP:H	5	0.13
(5,24)	1:X:47:ASN:C	1:X:50:ASP:H	12	0.13
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	15	0.13
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	8	0.13
(5,20)	1:X:37:ARG:C	1:X:27:GLU:H	10	0.13
(5,2)	1:X:5:GLU:C	1:X:9:THR:H	16	0.13
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	9	0.13
(5,18)	1:X:35:THR:C	1:X:29:ILE:H	15	0.13
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	9	0.13
(5,10)	1:X:14:ALA:C	1:X:18:ALA:H	7	0.13
(4,89)	1:X:90:HIS:O	1:X:94:PHE:H	7	0.13
(4,87)	1:X:89:GLU:O	1:X:93:ARG:H	17	0.13
(4,82)	1:X:77:SER:O	1:X:40:ILE:N	9	0.13
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	18	0.13
(4,76)	1:X:71:ALA:O	1:X:34:SER:N	1	0.13
(4,71)	1:X:59:SER:O	1:X:63:ASP:H	20	0.13
(4,51)	1:X:49:ASP:O	1:X:53:ASP:N	20	0.13
(4,47)	1:X:47:ASN:O	1:X:50:ASP:H	11	0.13
(4,2)	1:X:4:LEU:O	1:X:8:LEU:N	19	0.13
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	16	0.13
(4,108)	1:X:102:VAL:O	1:X:143:LYS:N	18	0.13
(3,930)	1:X:142:GLN:N	1:X:141:ILE:CG2	18	0.13
(3,92)	1:X:19:LEU:N	1:X:18:ALA:CB	20	0.13
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	6	0.13
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	16	0.13
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	17	0.13
(3,797)	1:X:121:ASP:N	1:X:120:VAL:CB	9	0.13
(3,778)	1:X:118:LYS:N	1:X:117:ILE:CG2	20	0.13
(3,663)	1:X:91:TYR:N	1:X:125:ILE:CD1	11	0.13
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	8	0.13
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	17	0.13
(3,651)	1:X:115:GLY:N	1:X:99:VAL:CG2	5	0.13
(3,587)	1:X:91:TYR:N	1:X:85:LEU:CD1	14	0.13
(3,566)	1:X:88:ALA:N	1:X:89:GLU:CB	9	0.13
(3,544)	1:X:81:LEU:CB	1:X:82:ASP:N	2	0.13
(3,534)	1:X:80:GLY:N	1:X:79:PRO:CB	14	0.13
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	8	0.13

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,452)	1:X:65:GLU:N	1:X:64:VAL:CB	20	0.13
(3,386)	1:X:58:VAL:N	1:X:60:ALA:CB	6	0.13
(3,208)	1:X:36:LEU:N	1:X:37:ARG:CG	13	0.13
(3,208)	1:X:36:LEU:N	1:X:37:ARG:CG	14	0.13
(3,159)	1:X:29:ILE:N	1:X:28:PHE:CB	13	0.13
(3,145)	1:X:27:GLU:N	1:X:26:ILE:CD1	12	0.13
(2,22)	1:X:16:VAL:CG1	1:X:54:VAL:CG2	12	0.13
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	19	0.13
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	17	0.13
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	6	0.13
(1,989)	1:X:120:VAL:HA	1:X:124:MET:H	17	0.13
(1,947)	1:X:112:LYS:HA	1:X:103:LEU:H	13	0.13
(1,931)	1:X:109:ASN:HD21	1:X:109:ASN:HB3	9	0.13
(1,680)	1:X:78:SER:HA	1:X:40:ILE:H	2	0.13
(1,640)	1:X:74:LEU:HD21	1:X:39:TYR:H	16	0.13
(1,640)	1:X:74:LEU:HD22	1:X:39:TYR:H	16	0.13
(1,640)	1:X:74:LEU:HD23	1:X:39:TYR:H	16	0.13
(1,609)	1:X:71:ALA:H	1:X:70:VAL:HA	16	0.13
(1,602)	1:X:68:ILE:HG12	1:X:68:ILE:H	18	0.13
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	18	0.13
(1,575)	1:X:65:GLU:HB2	1:X:64:VAL:H	18	0.13
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	10	0.13
(1,531)	1:X:62:LEU:HB2	1:X:61:VAL:H	18	0.13
(1,496)	1:X:58:VAL:HA	1:X:61:VAL:H	6	0.13
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	7	0.13
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	15	0.13
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	14	0.13
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	15	0.13
(1,364)	1:X:48:VAL:HA	1:X:51:CYS:H	4	0.13
(1,241)	1:X:37:ARG:H	1:X:27:GLU:HB2	12	0.13
(1,237)	1:X:36:LEU:CG	1:X:74:LEU:H	18	0.13
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	20	0.13
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	19	0.13
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	16	0.13
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	15	0.13
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	5	0.13
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	13	0.13
(1,123)	1:X:23:LEU:CG	1:X:24:VAL:H	14	0.13
(1,1136)	1:X:134:GLU:H	1:X:127:VAL:HB	16	0.13
(5,69)	1:X:143:LYS:C	1:X:102:VAL:H	12	0.12
(5,67)	1:X:136:PHE:C	1:X:125:ILE:H	2	0.12
(5,63)	1:X:128:THR:C	1:X:116:VAL:H	2	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	1	0.12
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	12	0.12
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	16	0.12
(5,56)	1:X:116:VAL:C	1:X:128:THR:H	6	0.12
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	14	0.12
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	19	0.12
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	16	0.12
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	13	0.12
(5,42)	1:X:87:THR:C	1:X:91:TYR:H	9	0.12
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	4	0.12
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	9	0.12
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	12	0.12
(5,38)	1:X:71:ALA:C	1:X:34:SER:H	19	0.12
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	3	0.12
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	10	0.12
(5,36)	1:X:59:SER:C	1:X:63:ASP:H	12	0.12
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	2	0.12
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	18	0.12
(5,33)	1:X:56:HIS:C	1:X:60:ALA:H	12	0.12
(5,31)	1:X:54:VAL:C	1:X:58:VAL:H	2	0.12
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	6	0.12
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	16	0.12
(5,17)	1:X:34:SER:C	1:X:73:ASN:H	16	0.12
(4,81)	1:X:77:SER:O	1:X:40:ILE:H	11	0.12
(4,67)	1:X:57:GLN:O	1:X:61:VAL:H	3	0.12
(4,52)	1:X:49:ASP:O	1:X:53:ASP:H	11	0.12
(4,44)	1:X:39:TYR:O	1:X:25:GLY:N	13	0.12
(4,29)	1:X:29:ILE:O	1:X:35:THR:N	5	0.12
(4,21)	1:X:15:PRO:O	1:X:19:LEU:H	20	0.12
(4,16)	1:X:12:ILE:O	1:X:16:VAL:H	16	0.12
(4,15)	1:X:12:ILE:O	1:X:16:VAL:N	9	0.12
(4,117)	1:X:124:MET:O	1:X:121:ASP:H	1	0.12
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	14	0.12
(3,92)	1:X:19:LEU:N	1:X:18:ALA:CB	11	0.12
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	18	0.12
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	8	0.12
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	4	0.12
(3,717)	1:X:105:MET:N	1:X:104:ARG:CD	20	0.12
(3,665)	1:X:92:ALA:N	1:X:125:ILE:CD1	2	0.12
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	7	0.12
(3,652)	1:X:117:ILE:CD1	1:X:96:GLY:N	12	0.12
(3,566)	1:X:88:ALA:N	1:X:89:GLU:CB	6	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,566)	1:X:88:ALA:N	1:X:89:GLU:CB	18	0.12
(3,556)	1:X:87:THR:N	1:X:86:PHE:CB	5	0.12
(3,531)	1:X:79:PRO:CD	1:X:40:ILE:N	14	0.12
(3,502)	1:X:75:GLU:N	1:X:74:LEU:CG	6	0.12
(3,482)	1:X:71:ALA:N	1:X:70:VAL:CG2	16	0.12
(3,425)	1:X:62:LEU:N	1:X:61:VAL:CG2	13	0.12
(3,371)	1:X:57:GLN:N	1:X:54:VAL:CG2	12	0.12
(3,366)	1:X:56:HIS:N	1:X:57:GLN:CB	8	0.12
(3,366)	1:X:56:HIS:N	1:X:57:GLN:CB	10	0.12
(3,289)	1:X:49:ASP:N	1:X:46:ILE:CG2	10	0.12
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	3	0.12
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	12	0.12
(3,241)	1:X:41:ASP:N	1:X:21:PHE:CB	16	0.12
(3,189)	1:X:34:SER:N	1:X:33:THR:CB	1	0.12
(3,189)	1:X:34:SER:N	1:X:33:THR:CB	10	0.12
(3,151)	1:X:27:GLU:N	1:X:37:ARG:CB	1	0.12
(2,6)	1:X:8:LEU:CG	1:X:26:ILE:CD1	8	0.12
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD1	5	0.12
(2,15)	1:X:12:ILE:CD1	1:X:62:LEU:CD2	5	0.12
(2,107)	1:X:120:VAL:CG2	1:X:125:ILE:CD1	11	0.12
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	8	0.12
(1,997)	1:X:121:ASP:H	1:X:124:MET:H	17	0.12
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	2	0.12
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	4	0.12
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	17	0.12
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	16	0.12
(1,822)	1:X:85:LEU:H	1:X:145:ASN:HA	6	0.12
(1,811)	1:X:117:ILE:HB	1:X:96:GLY:H	18	0.12
(1,787)	1:X:95:VAL:HB	1:X:97:GLU:H	7	0.12
(1,674)	1:X:77:SER:H	1:X:76:VAL:CB	2	0.12
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	6	0.12
(1,658)	1:X:76:VAL:HB	1:X:55:SER:H	12	0.12
(1,606)	1:X:69:THR:HA	1:X:70:VAL:H	20	0.12
(1,598)	1:X:67:PRO:HA	1:X:68:ILE:H	2	0.12
(1,596)	1:X:67:PRO:HD2	1:X:66:ASP:H	8	0.12
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	14	0.12
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	4	0.12
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	5	0.12
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	7	0.12
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	9	0.12
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	12	0.12
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	15	0.12

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	16	0.12
(1,532)	1:X:62:LEU:H	1:X:61:VAL:CB	4	0.12
(1,523)	1:X:61:VAL:HA	1:X:64:VAL:H	14	0.12
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	8	0.12
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	2	0.12
(1,411)	1:X:52:ALA:HA	1:X:55:SER:H	4	0.12
(1,324)	1:X:45:GLY:H	1:X:42:SER:H	6	0.12
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	1	0.12
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	3	0.12
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	5	0.12
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	8	0.12
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	16	0.12
(1,204)	1:X:33:THR:H	1:X:32:ARG:HG2	12	0.12
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	14	0.12
(1,179)	1:X:29:ILE:H	1:X:36:LEU:H	9	0.12
(1,167)	1:X:29:ILE:H	1:X:28:PHE:CZ	3	0.12
(1,146)	1:X:25:GLY:H	1:X:39:TYR:HB2	8	0.12
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	1	0.12
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	7	0.12
(1,126)	1:X:23:LEU:H	1:X:25:GLY:H	20	0.12
(1,1162)	1:X:137:ALA:HA	1:X:125:ILE:H	5	0.12
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	10	0.12
(1,1079)	1:X:127:VAL:H	1:X:136:PHE:H	18	0.12
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	18	0.12
(1,1020)	1:X:123:GLU:HA	1:X:138:LEU:H	6	0.12
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	5	0.11
(5,70)	1:X:145:ASN:C	1:X:100:THR:H	20	0.11
(5,7)	1:X:10:GLU:C	1:X:14:ALA:H	6	0.11
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	3	0.11
(5,66)	1:X:134:GLU:C	1:X:127:VAL:H	10	0.11
(5,61)	1:X:126:THR:C	1:X:118:LYS:H	17	0.11
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	2	0.11
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	16	0.11
(5,60)	1:X:125:ILE:C	1:X:136:PHE:H	18	0.11
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	6	0.11
(5,57)	1:X:119:ALA:C	1:X:126:THR:H	10	0.11
(5,53)	1:X:101:LEU:C	1:X:113:TRP:H	10	0.11
(5,51)	1:X:99:VAL:C	1:X:115:GLY:H	15	0.11
(5,5)	1:X:8:LEU:C	1:X:12:ILE:H	18	0.11
(5,49)	1:X:97:GLU:C	1:X:117:ILE:H	3	0.11
(5,46)	1:X:115:GLY:C	1:X:99:VAL:H	11	0.11
(5,45)	1:X:90:HIS:C	1:X:94:PHE:H	17	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,44)	1:X:89:GLU:C	1:X:93:ARG:H	4	0.11
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	4	0.11
(5,43)	1:X:88:ALA:C	1:X:92:ALA:H	15	0.11
(5,40)	1:X:75:GLU:C	1:X:38:ILE:H	10	0.11
(5,4)	1:X:7:LYS:C	1:X:11:MET:H	16	0.11
(5,37)	1:X:60:ALA:C	1:X:64:VAL:H	2	0.11
(5,35)	1:X:58:VAL:C	1:X:62:LEU:H	7	0.11
(5,30)	1:X:53:ASP:C	1:X:57:GLN:H	4	0.11
(5,3)	1:X:6:GLN:C	1:X:10:GLU:H	18	0.11
(5,29)	1:X:52:ALA:C	1:X:56:HIS:H	9	0.11
(5,23)	1:X:41:ASP:C	1:X:23:LEU:H	11	0.11
(5,22)	1:X:39:TYR:C	1:X:25:GLY:H	19	0.11
(5,21)	1:X:38:ILE:C	1:X:77:SER:H	16	0.11
(5,2)	1:X:5:GLU:C	1:X:9:THR:H	6	0.11
(5,11)	1:X:15:PRO:C	1:X:19:LEU:H	15	0.11
(4,95)	1:X:147:VAL:O	1:X:98:GLU:N	10	0.11
(4,88)	1:X:89:GLU:O	1:X:93:ARG:N	3	0.11
(4,68)	1:X:57:GLN:O	1:X:61:VAL:N	4	0.11
(4,65)	1:X:56:HIS:O	1:X:60:ALA:H	18	0.11
(4,118)	1:X:124:MET:O	1:X:121:ASP:N	1	0.11
(4,117)	1:X:124:MET:O	1:X:121:ASP:H	10	0.11
(4,115)	1:X:121:ASP:O	1:X:124:MET:H	14	0.11
(4,107)	1:X:102:VAL:O	1:X:143:LYS:H	18	0.11
(4,1)	1:X:4:LEU:O	1:X:8:LEU:H	19	0.11
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	1	0.11
(3,922)	1:X:141:ILE:N	1:X:140:ASN:CB	2	0.11
(3,92)	1:X:19:LEU:N	1:X:18:ALA:CB	1	0.11
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	8	0.11
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	10	0.11
(3,909)	1:X:138:LEU:N	1:X:137:ALA:CB	11	0.11
(3,878)	1:X:133:ASP:N	1:X:128:THR:CG2	13	0.11
(3,813)	1:X:124:MET:N	1:X:120:VAL:CG2	19	0.11
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	2	0.11
(3,806)	1:X:122:GLY:N	1:X:121:ASP:CB	13	0.11
(3,804)	1:X:121:ASP:N	1:X:125:ILE:CD1	3	0.11
(3,760)	1:X:115:GLY:N	1:X:100:THR:CG2	18	0.11
(3,749)	1:X:113:TRP:N	1:X:101:LEU:CD1	5	0.11
(3,716)	1:X:104:ARG:N	1:X:105:MET:CB	3	0.11
(3,667)	1:X:95:VAL:N	1:X:117:ILE:CG2	4	0.11
(3,666)	1:X:94:PHE:N	1:X:117:ILE:CG2	19	0.11
(3,664)	1:X:92:ALA:N	1:X:120:VAL:CG1	12	0.11
(3,583)	1:X:90:HIS:N	1:X:89:GLU:CB	18	0.11

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,366)	1:X:56:HIS:N	1:X:57:GLN:CB	17	0.11
(3,333)	1:X:54:VAL:N	1:X:40:ILE:CD1	15	0.11
(3,315)	1:X:52:ALA:N	1:X:48:VAL:CA	4	0.11
(3,315)	1:X:52:ALA:N	1:X:48:VAL:CA	15	0.11
(3,272)	1:X:46:ILE:N	1:X:44:ASP:CB	4	0.11
(3,239)	1:X:41:ASP:N	1:X:16:VAL:CG1	13	0.11
(2,64)	1:X:61:VAL:CG1	1:X:15:PRO:CD	17	0.11
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	3	0.11
(1,992)	1:X:121:ASP:H	1:X:120:VAL:CB	12	0.11
(1,96)	1:X:19:LEU:H	1:X:16:VAL:HA	7	0.11
(1,930)	1:X:109:ASN:HD21	1:X:109:ASN:HB2	5	0.11
(1,929)	1:X:109:ASN:H	1:X:107:VAL:H	13	0.11
(1,924)	1:X:108:GLN:HA	1:X:109:ASN:H	9	0.11
(1,662)	1:X:76:VAL:H	1:X:75:GLU:HG3	9	0.11
(1,609)	1:X:71:ALA:H	1:X:70:VAL:HA	2	0.11
(1,606)	1:X:69:THR:HA	1:X:70:VAL:H	10	0.11
(1,598)	1:X:67:PRO:HA	1:X:68:ILE:H	6	0.11
(1,574)	1:X:65:GLU:H	1:X:64:VAL:CB	13	0.11
(1,566)	1:X:64:VAL:HB	1:X:64:VAL:H	1	0.11
(1,566)	1:X:64:VAL:HB	1:X:64:VAL:H	10	0.11
(1,566)	1:X:64:VAL:HB	1:X:64:VAL:H	20	0.11
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	3	0.11
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	6	0.11
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	8	0.11
(1,560)	1:X:63:ASP:HA	1:X:64:VAL:H	19	0.11
(1,532)	1:X:62:LEU:H	1:X:61:VAL:CB	18	0.11
(1,494)	1:X:58:VAL:HB	1:X:60:ALA:H	17	0.11
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	11	0.11
(1,477)	1:X:58:VAL:HB	1:X:56:HIS:H	14	0.11
(1,466)	1:X:57:GLN:H	1:X:57:GLN:HG3	9	0.11
(1,441)	1:X:55:SER:H	1:X:53:ASP:HB3	3	0.11
(1,400)	1:X:52:ALA:H	1:X:48:VAL:CB	17	0.11
(1,392)	1:X:50:ASP:HA	1:X:53:ASP:H	5	0.11
(1,283)	1:X:39:TYR:H	1:X:27:GLU:H	9	0.11
(1,25)	1:X:6:GLN:HA	1:X:7:LYS:H	3	0.11
(1,248)	1:X:37:ARG:H	1:X:36:LEU:HB3	4	0.11
(1,248)	1:X:37:ARG:H	1:X:36:LEU:HB3	5	0.11
(1,241)	1:X:37:ARG:H	1:X:27:GLU:HB2	9	0.11
(1,218)	1:X:34:SER:H	1:X:73:ASN:H	1	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	1	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	2	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	6	0.11

*Continued on next page...*

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	10	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	14	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	17	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	18	0.11
(1,206)	1:X:33:THR:H	1:X:32:ARG:HA	19	0.11
(1,2)	1:X:4:LEU:CG	1:X:5:GLU:H	17	0.11
(1,197)	1:X:31:GLY:H	1:X:30:ARG:HD2	12	0.11
(1,183)	1:X:30:ARG:H	1:X:29:ILE:CG2	9	0.11
(1,1077)	1:X:127:VAL:H	1:X:135:VAL:HA	19	0.11
(1,1058)	1:X:126:THR:H	1:X:125:ILE:CD1	16	0.11
(1,1016)	1:X:123:GLU:H	1:X:124:MET:HA	9	0.11

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

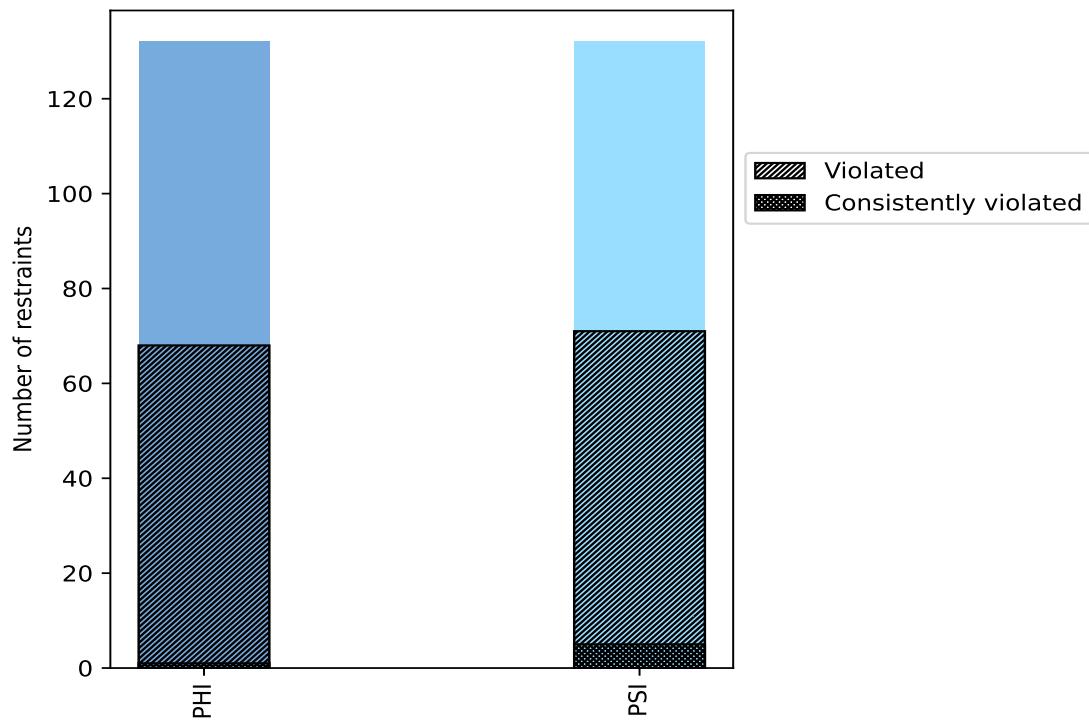
### 10.1 Summary of dihedral-angle violations [\(i\)](#)

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

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PHI	132	50.0	68	51.5	25.8	1	0.8	0.4
PSI	132	50.0	71	53.8	26.9	5	3.8	1.9
Total	264	100.0	139	52.7	52.7	6	2.3	2.3

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

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



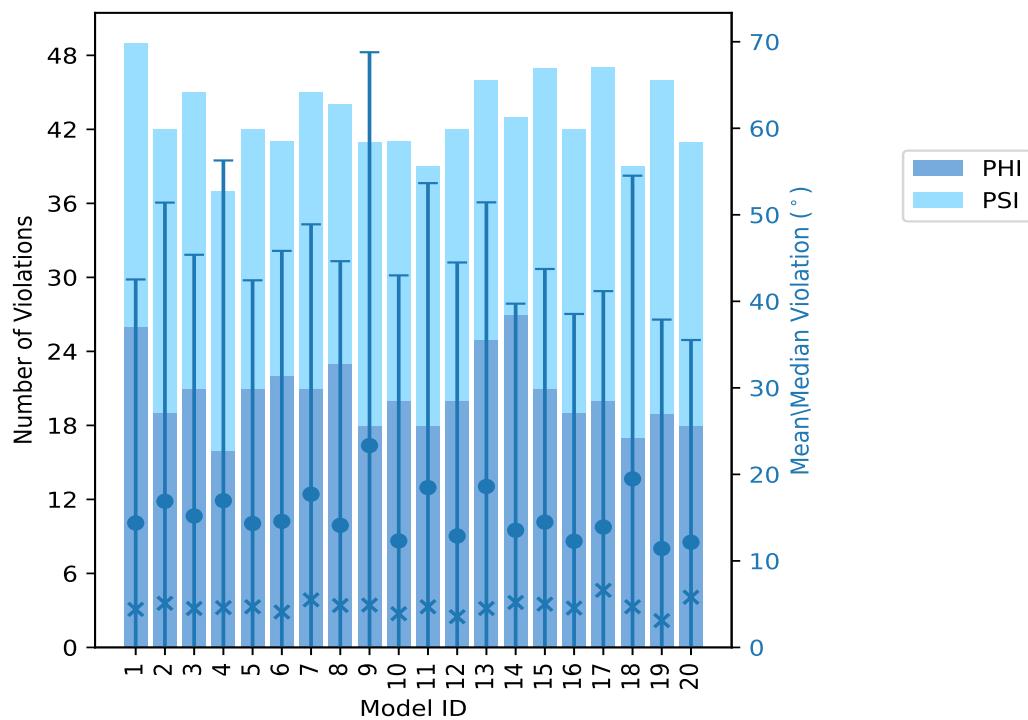
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	26	23	49	14.38	119.4	28.15	4.4
2	19	23	42	16.89	154.8	34.52	5.1
3	21	24	45	15.19	158.6	30.19	4.5
4	16	21	37	16.96	159.5	39.32	4.6
5	21	21	42	14.32	135.9	28.11	4.7
6	22	19	41	14.57	157.5	31.26	4.1
7	21	24	45	17.71	158.2	31.19	5.5
8	23	21	44	14.11	158.6	30.53	4.85
9	18	23	41	23.33	159.9	45.46	4.9
10	20	21	41	12.31	159.1	30.69	3.9
11	18	21	39	18.47	157.0	35.19	4.7
12	20	22	42	12.88	158.2	31.61	3.55
13	25	21	46	18.6	156.9	32.84	4.5
14	27	16	43	13.54	159.2	26.19	5.2
15	21	26	47	14.48	159.1	29.26	5.0
16	19	23	42	12.27	158.3	26.27	4.55
17	20	27	47	13.91	157.6	27.27	6.6
18	17	22	39	19.48	159.1	35.04	4.7
19	19	27	46	11.43	159.9	26.46	3.1
20	18	23	41	12.16	146.0	23.37	5.8

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



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

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

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

PHI	PSI	Total	Fraction of the ensemble	
			Count <sup>1</sup>	%
17	21	38	1	5.0
10	7	17	2	10.0
5	8	13	3	15.0
4	1	5	4	20.0
3	4	7	5	25.0
4	4	8	6	30.0
4	4	8	7	35.0
3	3	6	8	40.0
2	3	5	9	45.0
2	2	4	10	50.0
2	0	2	11	55.0

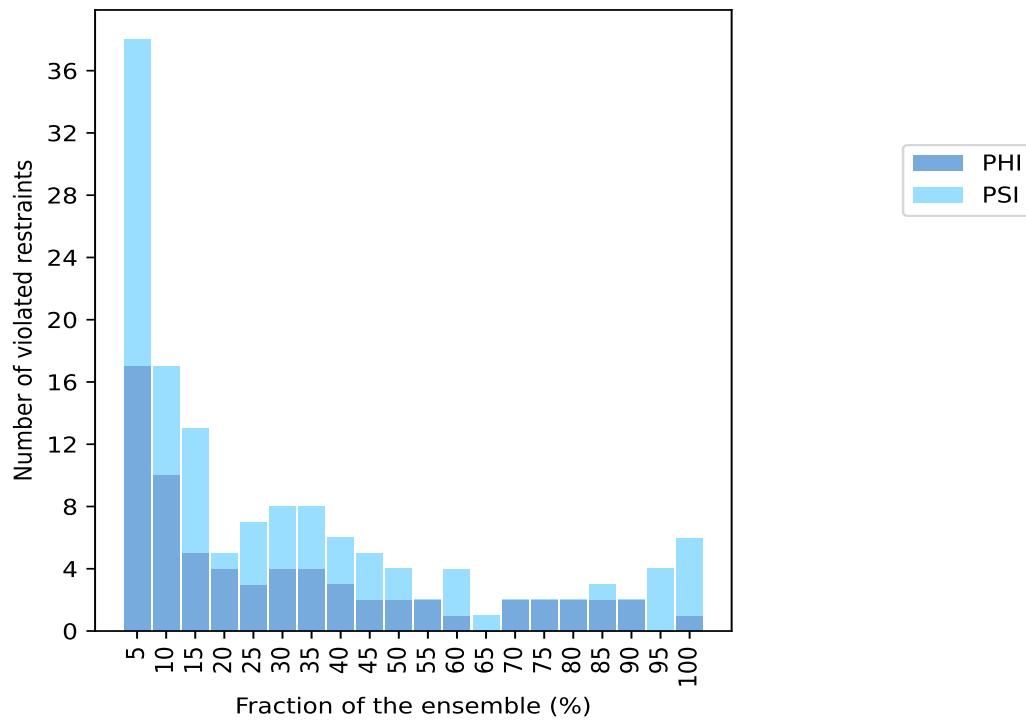
*Continued on next page...*

*Continued from previous page...*

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
1	3	4	12	60.0
0	1	1	13	65.0
2	0	2	14	70.0
2	0	2	15	75.0
2	0	2	16	80.0
2	1	3	17	85.0
2	0	2	18	90.0
0	4	4	19	95.0
1	5	6	20	100.0

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

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

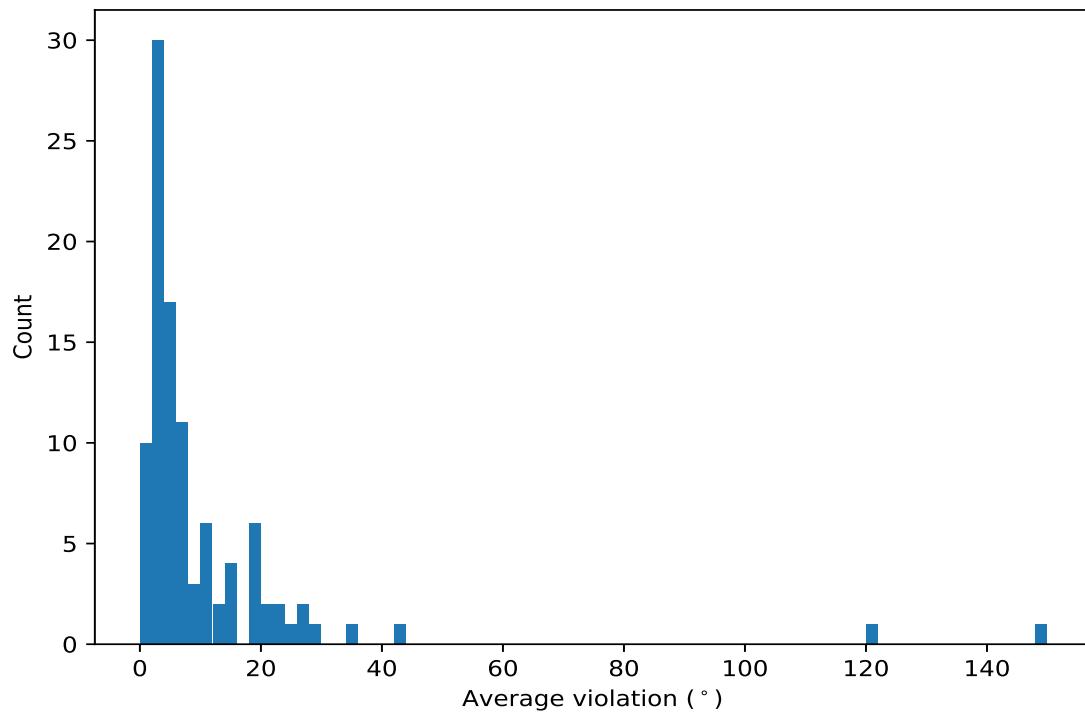


## 10.4 Most violated dihedral-angle restraints in the ensemble [\(i\)](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	20	149.36	24.97	158.25
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	20	22.39	13.53	25.3
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	20	20.65	7.8	19.65
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	20	18.54	13.62	18.6
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	20	18.09	27.0	9.5
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	20	10.35	4.96	10.25
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	19	120.32	22.56	131.8
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	19	4.59	1.82	4.3
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	19	4.56	1.39	4.4
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	19	3.94	2.07	3.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	18	5.69	2.27	5.65
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	18	4.92	2.68	5.65
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	17	13.0	32.77	3.9
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	17	5.1	3.72	4.3
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	17	3.79	1.92	3.2
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	16	5.69	6.47	3.45
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	16	5.26	2.59	5.7
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	15	10.39	1.05	10.3
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	15	6.48	4.42	4.3
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	14	29.39	46.14	9.15

Continued on next page...

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	14	6.67	10.49	4.05
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	13	2.52	0.77	2.3
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	12	27.34	28.88	18.0
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	12	19.37	14.95	20.65
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	12	5.64	2.26	5.6
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	12	5.12	3.47	4.55
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	11	3.46	1.46	2.7
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	11	1.98	0.71	1.8
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	10	15.04	8.06	16.45
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	10	3.16	1.75	2.9
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	10	2.85	1.26	2.45
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	10	2.65	0.52	2.75
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	9	24.57	43.08	2.5
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	9	18.71	12.11	18.6
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	9	15.03	17.25	3.4
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	9	6.73	4.43	4.9
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	9	2.43	2.5	1.4
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	8	23.51	32.68	10.95
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	8	15.56	11.76	14.5
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	8	6.71	5.99	3.5
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	8	6.08	2.88	4.5
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	8	5.62	3.33	4.8
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	8	2.65	0.9	2.6
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	7	35.81	41.55	8.5
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	7	13.6	12.5	9.7
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	7	8.84	2.52	9.2
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	7	8.51	5.97	9.2
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	7	6.17	6.73	4.3
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	7	5.7	2.15	4.7
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	7	3.66	2.07	3.1
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	7	3.0	0.96	2.7
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	6	42.73	50.72	8.15
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	6	19.33	8.47	21.75
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	6	7.93	10.74	3.35
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	6	4.88	3.18	4.55
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	6	4.08	2.73	3.8
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	6	4.02	2.98	2.55
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	6	3.43	0.97	3.25
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	6	1.58	0.57	1.3
(1,124)	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	1:X:73:ASN:N	5	26.64	21.42	33.2
(1,125)	1:X:72:TYR:C	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	5	21.56	16.48	17.2
(1,109)	1:X:63:ASP:C	1:X:64:VAL:N	1:X:64:VAL:CA	1:X:64:VAL:C	5	3.72	0.84	3.8
(1,214)	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	1:X:122:GLY:N	5	3.34	0.95	3.2
(1,14)	1:X:11:MET:N	1:X:11:MET:CA	1:X:11:MET:C	1:X:12:ILE:N	5	2.7	1.12	2.9
(1,92)	1:X:55:SER:N	1:X:55:SER:CA	1:X:55:SER:C	1:X:56:HIS:N	5	2.58	1.07	3.0
(1,203)	1:X:115:GLY:C	1:X:116:VAL:N	1:X:116:VAL:CA	1:X:116:VAL:C	5	1.92	0.57	1.6
(1,47)	1:X:29:ILE:C	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	4	11.82	9.1	10.9
(1,71)	1:X:43:GLU:C	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	4	11.35	7.82	11.45
(1,161)	1:X:92:ALA:C	1:X:93:ARG:N	1:X:93:ARG:CA	1:X:93:ARG:C	4	4.1	3.25	2.45
(1,168)	1:X:96:GLY:N	1:X:96:GLY:CA	1:X:96:GLY:C	1:X:97:GLU:N	4	1.95	0.42	2.0
(1,181)	1:X:102:VAL:C	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	4	1.7	0.29	1.7

*Continued on next page...*

*Continued from previous page...*

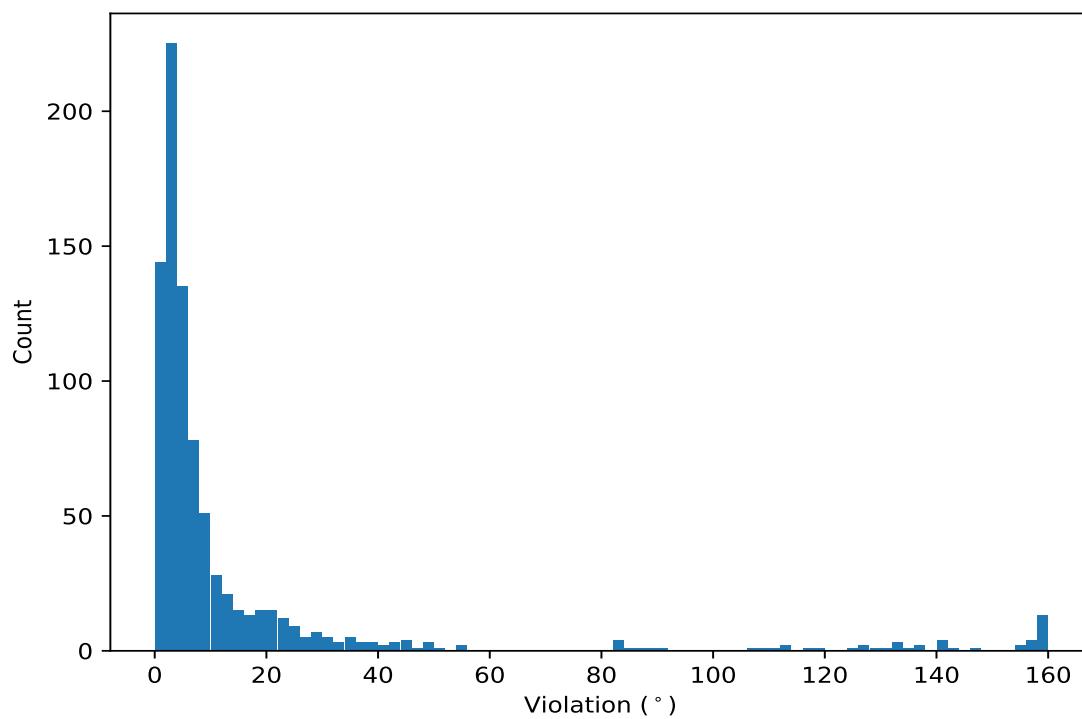
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,217)	1:X:124:MET:C	1:X:125:ILE:N	1:X:125:ILE:CA	1:X:125:ILE:C	3	19.03	6.49	22.8
(1,72)	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	1:X:45:GLY:N	3	11.1	5.71	13.6
(1,52)	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	1:X:35:THR:N	3	10.4	2.2	9.6
(1,53)	1:X:34:SER:C	1:X:35:THR:N	1:X:35:THR:CA	1:X:35:THR:C	3	7.0	4.49	6.8
(1,146)	1:X:84:PRO:N	1:X:84:PRO:CA	1:X:84:PRO:C	1:X:85:LEU:N	3	6.23	3.15	5.5
(1,236)	1:X:134:GLU:N	1:X:134:GLU:CA	1:X:134:GLU:C	1:X:135:VAL:N	3	3.0	0.86	3.4
(1,78)	1:X:48:VAL:N	1:X:48:VAL:CA	1:X:48:VAL:C	1:X:49:ASP:N	3	2.7	0.78	2.8
(1,67)	1:X:41:ASP:C	1:X:42:SER:N	1:X:42:SER:CA	1:X:42:SER:C	3	2.6	1.14	2.0
(1,221)	1:X:126:THR:C	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	3	2.43	0.81	2.9
(1,244)	1:X:138:LEU:N	1:X:138:LEU:CA	1:X:138:LEU:C	1:X:139:SER:N	3	2.4	1.42	1.5
(1,56)	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	1:X:37:ARG:N	3	1.93	0.74	1.8
(1,45)	1:X:28:PHE:C	1:X:29:ILE:N	1:X:29:ILE:CA	1:X:29:ILE:C	3	1.9	0.29	2.0
(1,86)	1:X:52:ALA:N	1:X:52:ALA:CA	1:X:52:ALA:C	1:X:53:ASP:N	3	1.8	0.78	1.3
(1,171)	1:X:97:GLU:C	1:X:98:GLU:N	1:X:98:GLU:CA	1:X:98:GLU:C	2	14.1	2.3	14.1
(1,1)	1:X:4:LEU:C	1:X:5:GLU:N	1:X:5:GLU:CA	1:X:5:GLU:C	2	9.6	5.7	9.6
(1,262)	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	1:X:148:PRO:N	2	6.75	2.15	6.75
(1,192)	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	1:X:111:ARG:N	2	6.3	3.6	6.3
(1,219)	1:X:125:ILE:C	1:X:126:THR:N	1:X:126:THR:CA	1:X:126:THR:C	2	5.45	1.95	5.45
(1,131)	1:X:75:GLU:C	1:X:76:VAL:N	1:X:76:VAL:CA	1:X:76:VAL:C	2	4.2	0.9	4.2
(1,147)	1:X:84:PRO:C	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	2	3.95	0.65	3.95
(1,196)	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	1:X:113:TRP:N	2	3.65	1.05	3.65
(1,55)	1:X:35:THR:C	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	2	2.95	1.85	2.95
(1,133)	1:X:76:VAL:C	1:X:77:SER:N	1:X:77:SER:CA	1:X:77:SER:C	2	2.85	0.05	2.85
(1,199)	1:X:113:TRP:C	1:X:114:GLN:N	1:X:114:GLN:CA	1:X:114:GLN:C	2	2.7	0.8	2.7
(1,66)	1:X:41:ASP:N	1:X:41:ASP:CA	1:X:41:ASP:C	1:X:42:SER:N	2	2.6	1.4	2.6
(1,231)	1:X:131:GLY:C	1:X:132:LYS:N	1:X:132:LYS:CA	1:X:132:LYS:C	2	2.6	0.1	2.6
(1,34)	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	1:X:22:GLU:N	2	2.25	0.95	2.25
(1,246)	1:X:139:SER:N	1:X:139:SER:CA	1:X:139:SER:C	1:X:140:ASN:N	2	2.2	0.8	2.2
(1,130)	1:X:75:GLU:N	1:X:75:GLU:CA	1:X:75:GLU:C	1:X:76:VAL:N	2	1.75	0.05	1.75
(1,207)	1:X:117:ILE:C	1:X:118:LYS:N	1:X:118:LYS:CA	1:X:118:LYS:C	2	1.45	0.05	1.45

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,188)	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	1:X:109:ASN:N	9	159.9
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	19	159.9
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	4	159.5
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	9	159.2
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	14	159.2
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	10	159.1
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	15	159.1
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	18	159.1
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	3	158.6
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	8	158.6
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	16	158.3
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	7	158.2
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	12	158.2
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	17	157.6
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	6	157.5
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	11	157.0
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	13	156.9
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	2	154.8
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	4	154.7
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	20	146.0
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	18	143.7

Continued on next page...

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	9	141.6
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	8	141.6
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	2	141.4
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	12	141.2
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	13	137.7
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	3	136.4
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	5	135.9
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	9	132.9
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	6	132.8
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	10	132.0
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	5	131.8
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	4	128.4
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	11	127.8
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	7	127.4
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	9	124.4
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	1	119.4
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	11	117.2
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	17	113.6
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	2	112.6
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1	111.6
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	15	108.1
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	1	106.3
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	13	90.3
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	15	88.0
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	19	86.4
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	18	84.3
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	1	83.1
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	16	82.7
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	7	82.1
(1,118)	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1:X:69:THR:N	14	82.0
(1,124)	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	1:X:73:ASN:N	7	54.8
(1,116)	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1:X:68:ILE:N	20	54.2
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	13	51.2
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	19	49.2
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	2	48.1
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	18	48.0
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	6	46.8
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	13	44.8
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	5	44.5
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	13	44.4
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	18	44.2
(1,125)	1:X:72:TYR:C	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	7	42.8
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	3	42.7
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	11	42.6
(1,124)	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	1:X:73:ASN:N	13	41.6
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	18	40.4
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	1	39.4
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	13	39.1
(1,125)	1:X:72:TYR:C	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	13	38.9
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	18	37.3
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	11	37.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	11	36.1
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	15	35.5
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	12	35.5
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	17	35.4
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	3	34.5
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	12	34.5
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	3	33.5
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	6	33.4
(1,124)	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	1:X:73:ASN:N	15	33.2
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	17	31.8
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	14	31.3
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	7	30.5
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	17	30.2
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	8	30.2
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	6	29.8
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	5	29.4
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	20	29.3
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	7	28.6
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	15	28.4
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	11	28.2
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	14	28.0
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	13	27.8
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	6	27.6
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	14	26.5
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	3	26.2
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	3	26.0
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	2	25.6
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	8	25.0
(1,115)	1:X:66:ASP:C	1:X:67:PRO:N	1:X:67:PRO:CA	1:X:67:PRO:C	1	24.7
(1,217)	1:X:124:MET:C	1:X:125:ILE:N	1:X:125:ILE:CA	1:X:125:ILE:C	4	24.4
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	7	24.3
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	5	24.3
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	5	24.3
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	9	24.3
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	16	24.2
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	13	23.5
(1,47)	1:X:29:ILE:C	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	14	23.2
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	19	23.0
(1,217)	1:X:124:MET:C	1:X:125:ILE:N	1:X:125:ILE:CA	1:X:125:ILE:C	1	22.8
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	18	22.7
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	19	22.6
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	7	22.6
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	17	22.4
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	8	22.3
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	10	22.2
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	14	22.1
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	2	22.0
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	2	21.7
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	16	21.6
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	9	21.4
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	20	21.4

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	8	21.1
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	20	20.9
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	18	20.7
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	6	20.7
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	12	20.6
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	19	20.6
(1,71)	1:X:43:GLU:C	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	20	20.5
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	17	20.4
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	10	20.1
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	4	20.1
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	7	20.1
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	11	19.9
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	20	19.7
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	12	19.6
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	15	19.4
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	16	19.0
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	3	18.9
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	11	18.7
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	8	18.7
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	4	18.7
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	14	18.6
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	18	18.6
(1,47)	1:X:29:ILE:C	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1	18.3
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	9	18.3
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	17	18.2
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	8	18.2
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	3	17.9
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	5	17.9
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	16	17.9
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	7	17.7
(1,71)	1:X:43:GLU:C	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	16	17.5
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	19	17.3
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	9	17.3
(1,125)	1:X:72:TYR:C	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	15	17.2
(1,72)	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	1:X:45:GLY:N	16	16.5
(1,171)	1:X:97:GLU:C	1:X:98:GLU:N	1:X:98:GLU:CA	1:X:98:GLU:C	10	16.4
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	2	16.4
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	20	16.1
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	20	16.1
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	3	15.9
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	19	15.7
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	8	15.4
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	13	15.3
(1,1)	1:X:4:LEU:C	1:X:5:GLU:N	1:X:5:GLU:CA	1:X:5:GLU:C	15	15.3
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	9	15.1
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	20	14.8
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	14	14.8
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	7	14.7
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	16	14.7
(1,180)	1:X:102:VAL:N	1:X:102:VAL:CA	1:X:102:VAL:C	1:X:103:LEU:N	9	14.6
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	17	14.6

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	14	14.5
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	9	14.4
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	5	14.4
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	14	13.9
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	5	13.9
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	3	13.7
(1,72)	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	1:X:45:GLY:N	20	13.6
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	6	13.5
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	5	13.5
(1,52)	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	1:X:35:THR:N	5	13.4
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	7	13.4
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	16	13.3
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	18	13.1
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	17	13.0
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	15	12.7
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	17	12.7
(1,53)	1:X:34:SER:C	1:X:35:THR:N	1:X:35:THR:CA	1:X:35:THR:C	5	12.6
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	19	12.5
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	3	12.5
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	13	12.5
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	2	12.4
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	18	12.4
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	15	12.0
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	17	12.0
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	19	11.9
(1,171)	1:X:97:GLU:C	1:X:98:GLU:N	1:X:98:GLU:CA	1:X:98:GLU:C	17	11.8
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	5	11.8
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	2	11.7
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	2	11.7
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	19	11.6
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	18	11.5
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	8	11.5
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	11	11.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	7	11.4
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	8	11.4
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	17	11.4
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	18	11.4
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	10	11.3
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	6	11.1
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	15	11.0
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	7	11.0
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	9	11.0
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	15	10.8
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	3	10.8
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	7	10.6
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	15	10.5
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	17	10.4
(1,146)	1:X:84:PRO:N	1:X:84:PRO:CA	1:X:84:PRO:C	1:X:85:LEU:N	11	10.4
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	4	10.3
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	20	10.3
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	16	10.3

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	13	10.1
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	11	9.9
(1,217)	1:X:124:MET:C	1:X:125:ILE:N	1:X:125:ILE:CA	1:X:125:ILE:C	2	9.9
(1,192)	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	1:X:111:ARG:N	3	9.9
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	8	9.9
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	12	9.8
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	18	9.8
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	10	9.7
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	7	9.7
(1,161)	1:X:92:ALA:C	1:X:93:ARG:N	1:X:93:ARG:CA	1:X:93:ARG:C	17	9.7
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	3	9.7
(1,52)	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	1:X:35:THR:N	13	9.6
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	8	9.6
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1	9.6
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	15	9.6
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	1	9.5
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	14	9.5
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	2	9.5
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	12	9.5
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	11	9.5
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	9	9.4
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	8	9.3
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	7	9.3
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	2	9.2
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1	9.2
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	1	9.2
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	12	9.2
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	6	9.2
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	20	9.1
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	10	9.1
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	7	9.1
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	8	9.0
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	14	8.9
(1,262)	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	1:X:148:PRO:N	8	8.9
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	12	8.8
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	6	8.8
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	16	8.7
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	16	8.5
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	10	8.5
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	14	8.4
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	5	8.4
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	7	8.4
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	8	8.4
(1,112)	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	1:X:66:ASP:N	10	8.4
(1,52)	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	1:X:35:THR:N	17	8.2
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	2	8.2
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	17	8.2
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	6	8.2
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	15	8.1
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	14	8.1
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	14	8.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:X:64:VAL:C	1:X:65:GLU:N	1:X:65:GLU:CA	1:X:65:GLU:C	4	8.0
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	1	7.9
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	7	7.9
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	10	7.9
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	7	7.9
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	2	7.9
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	17	7.8
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	8	7.8
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	20	7.8
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	5	7.7
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	1	7.7
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	2	7.7
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	4	7.7
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	1	7.7
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	12	7.7
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	11	7.7
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	14	7.6
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	3	7.6
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	9	7.6
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	13	7.6
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	14	7.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	3	7.5
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	3	7.4
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	17	7.4
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	15	7.4
(1,219)	1:X:125:ILE:C	1:X:126:THR:N	1:X:126:THR:CA	1:X:126:THR:C	20	7.4
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	9	7.4
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	13	7.4
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	20	7.3
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	17	7.3
(1,127)	1:X:73:ASN:C	1:X:74:LEU:N	1:X:74:LEU:CA	1:X:74:LEU:C	1	7.3
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	8	7.2
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	4	7.2
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	15	7.2
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	13	7.1
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	17	7.1
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	3	7.1
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	4	7.0
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	6	6.9
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	18	6.9
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	8	6.9
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	5	6.9
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	1	6.9
(1,53)	1:X:34:SER:C	1:X:35:THR:N	1:X:35:THR:CA	1:X:35:THR:C	17	6.8
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	10	6.8
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	2	6.8
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	15	6.7
(1,210)	1:X:119:ALA:N	1:X:119:ALA:CA	1:X:119:ALA:C	1:X:120:VAL:N	9	6.7
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	3	6.6
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	20	6.6
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	17	6.6

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	16	6.6
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	18	6.6
(1,137)	1:X:78:SER:C	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	11	6.6
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	16	6.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	5	6.5
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	6	6.5
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	13	6.4
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	6	6.4
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	4	6.4
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	15	6.3
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	15	6.3
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	16	6.3
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	11	6.3
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	18	6.3
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	2	6.3
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	14	6.2
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	3	6.2
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	1	6.2
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	18	6.1
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	20	6.1
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	16	6.1
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	11	6.1
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	5	6.1
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	19	6.1
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	16	6.0
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	10	6.0
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	17	6.0
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	16	6.0
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	2	5.9
(1,149)	1:X:86:PHE:C	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	14	5.9
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	20	5.9
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	10	5.9
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	20	5.9
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	17	5.9
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	1	5.8
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	10	5.8
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	1	5.8
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	20	5.8
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	12	5.8
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	2	5.8
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	13	5.7
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	12	5.6
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	13	5.6
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	7	5.5
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	9	5.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	17	5.5
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	19	5.5
(1,146)	1:X:84:PRO:N	1:X:84:PRO:CA	1:X:84:PRO:C	1:X:85:LEU:N	4	5.5
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	8	5.4
(1,71)	1:X:43:GLU:C	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	5	5.4
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	10	5.4

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	4	5.4
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	7	5.4
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	15	5.4
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	20	5.3
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	8	5.3
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	9	5.3
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	11	5.3
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	14	5.3
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	11	5.3
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	6	5.3
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	12	5.2
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	14	5.2
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1	5.2
(1,125)	1:X:72:TYR:C	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	14	5.2
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	10	5.1
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	15	5.1
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	6	5.1
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	6	5.1
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	10	5.1
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	7	5.1
(1,131)	1:X:75:GLU:C	1:X:76:VAL:N	1:X:76:VAL:CA	1:X:76:VAL:C	16	5.1
(1,121)	1:X:70:VAL:C	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	16	5.1
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	13	5.0
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	12	5.0
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	15	5.0
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	20	4.9
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	19	4.9
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	9	4.9
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	15	4.9
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	9	4.9
(1,109)	1:X:63:ASP:C	1:X:64:VAL:N	1:X:64:VAL:CA	1:X:64:VAL:C	1	4.9
(1,55)	1:X:35:THR:C	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	14	4.8
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	5	4.8
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	9	4.8
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	4	4.8
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	14	4.7
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	18	4.7
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	5	4.7
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	6	4.7
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	5	4.7
(1,196)	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	1:X:113:TRP:N	11	4.7
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	18	4.7
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	13	4.7
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	4	4.7
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	4	4.7
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	7	4.6
(1,262)	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	1:X:148:PRO:N	4	4.6
(1,214)	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	1:X:122:GLY:N	7	4.6
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	5	4.6
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	18	4.6
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	4	4.6

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,147)	1:X:84:PRO:C	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	3	4.6
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	9	4.6
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	5	4.5
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	3	4.5
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	15	4.5
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	10	4.5
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	1	4.5
(1,14)	1:X:11:MET:N	1:X:11:MET:CA	1:X:11:MET:C	1:X:12:ILE:N	5	4.5
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	14	4.5
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	8	4.4
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	17	4.4
(1,244)	1:X:138:LEU:N	1:X:138:LEU:CA	1:X:138:LEU:C	1:X:139:SER:N	19	4.4
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	1	4.4
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	4	4.4
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	1	4.4
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	2	4.4
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	8	4.4
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	2	4.3
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	13	4.3
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	14	4.3
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	3	4.3
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	13	4.3
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	17	4.3
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	8	4.3
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	20	4.3
(1,160)	1:X:92:ALA:N	1:X:92:ALA:CA	1:X:92:ALA:C	1:X:93:ARG:N	19	4.3
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	3	4.3
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	6	4.2
(1,67)	1:X:41:ASP:C	1:X:42:SER:N	1:X:42:SER:CA	1:X:42:SER:C	3	4.2
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	14	4.2
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	8	4.2
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	19	4.2
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	17	4.2
(1,197)	1:X:112:LYS:C	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1	4.2
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	9	4.2
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	11	4.2
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	19	4.2
(1,119)	1:X:68:ILE:C	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	12	4.2
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	2	4.2
(1,109)	1:X:63:ASP:C	1:X:64:VAL:N	1:X:64:VAL:CA	1:X:64:VAL:C	10	4.2
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	12	4.1
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	7	4.1
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	12	4.1
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	9	4.1
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	6	4.1
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	14	4.1
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	12	4.1
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	3	4.1
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	15	4.1
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	18	4.1
(1,142)	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	1:X:83:ARG:N	17	4.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	8	4.1
(1,92)	1:X:55:SER:N	1:X:55:SER:CA	1:X:55:SER:C	1:X:56:HIS:N	7	4.0
(1,66)	1:X:41:ASP:N	1:X:41:ASP:CA	1:X:41:ASP:C	1:X:42:SER:N	7	4.0
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	3	4.0
(1,214)	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	1:X:122:GLY:N	16	4.0
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	11	4.0
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	5	4.0
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	11	4.0
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	3	4.0
(1,122)	1:X:71:ALA:N	1:X:71:ALA:CA	1:X:71:ALA:C	1:X:72:TYR:N	16	4.0
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	19	3.9
(1,251)	1:X:141:ILE:C	1:X:142:GLN:N	1:X:142:GLN:CA	1:X:142:GLN:C	5	3.9
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	19	3.9
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	10	3.9
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	14	3.9
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	3	3.9
(1,1)	1:X:4:LEU:C	1:X:5:GLU:N	1:X:5:GLU:CA	1:X:5:GLU:C	19	3.9
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	8	3.8
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	2	3.8
(1,236)	1:X:134:GLU:N	1:X:134:GLU:CA	1:X:134:GLU:C	1:X:135:VAL:N	1	3.8
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	1	3.8
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	10	3.8
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	16	3.8
(1,109)	1:X:63:ASP:C	1:X:64:VAL:N	1:X:64:VAL:CA	1:X:64:VAL:C	17	3.8
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	18	3.7
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	1	3.7
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	6	3.7
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	11	3.7
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	12	3.7
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	14	3.7
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	5	3.7
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	20	3.7
(1,125)	1:X:72:TYR:C	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	5	3.7
(1,78)	1:X:48:VAL:N	1:X:48:VAL:CA	1:X:48:VAL:C	1:X:49:ASP:N	17	3.6
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	5	3.6
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	2	3.6
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	7	3.6
(1,164)	1:X:94:PHE:N	1:X:94:PHE:CA	1:X:94:PHE:C	1:X:95:VAL:N	12	3.6
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1	3.6
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	13	3.6
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	10	3.5
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	16	3.5
(1,47)	1:X:29:ILE:C	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	18	3.5
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	1	3.5
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	10	3.5
(1,219)	1:X:125:ILE:C	1:X:126:THR:N	1:X:126:THR:CA	1:X:126:THR:C	10	3.5
(1,199)	1:X:113:TRP:C	1:X:114:GLN:N	1:X:114:GLN:CA	1:X:114:GLN:C	1	3.5
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	12	3.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	13	3.5
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	9	3.5
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	19	3.5

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	4	3.5
(1,139)	1:X:80:GLY:C	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	6	3.5
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	13	3.5
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	1	3.5
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	1	3.4
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	17	3.4
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	16	3.4
(1,236)	1:X:134:GLU:N	1:X:134:GLU:CA	1:X:134:GLU:C	1:X:135:VAL:N	7	3.4
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	13	3.4
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	20	3.4
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	18	3.4
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	8	3.4
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	18	3.4
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	3	3.3
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	5	3.3
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	17	3.3
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	6	3.3
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	4	3.3
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	10	3.3
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	1	3.3
(1,147)	1:X:84:PRO:C	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	12	3.3
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	6	3.3
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	16	3.3
(1,131)	1:X:75:GLU:C	1:X:76:VAL:N	1:X:76:VAL:CA	1:X:76:VAL:C	13	3.3
(1,109)	1:X:63:ASP:C	1:X:64:VAL:N	1:X:64:VAL:CA	1:X:64:VAL:C	20	3.3
(1,92)	1:X:55:SER:N	1:X:55:SER:CA	1:X:55:SER:C	1:X:56:HIS:N	3	3.2
(1,82)	1:X:50:ASP:N	1:X:50:ASP:CA	1:X:50:ASP:C	1:X:51:CYS:N	6	3.2
(1,72)	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	1:X:45:GLY:N	11	3.2
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	11	3.2
(1,34)	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	1:X:22:GLU:N	11	3.2
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	19	3.2
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	13	3.2
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	3	3.2
(1,214)	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	1:X:122:GLY:N	18	3.2
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	7	3.2
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	2	3.2
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	8	3.2
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	12	3.2
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	9	3.1
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	8	3.1
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	9	3.1
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	14	3.1
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	13	3.1
(1,54)	1:X:35:THR:N	1:X:35:THR:CA	1:X:35:THR:C	1:X:36:LEU:N	14	3.1
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	3	3.1
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	5	3.1
(1,221)	1:X:126:THR:C	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	13	3.1
(1,214)	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	1:X:122:GLY:N	6	3.1
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	18	3.1
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	13	3.1
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	11	3.1

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	16	3.1
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	16	3.1
(1,159)	1:X:91:TYR:C	1:X:92:ALA:N	1:X:92:ALA:CA	1:X:92:ALA:C	20	3.1
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	7	3.1
(1,92)	1:X:55:SER:N	1:X:55:SER:CA	1:X:55:SER:C	1:X:56:HIS:N	8	3.0
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	5	3.0
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	7	3.0
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	7	3.0
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	7	3.0
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	15	3.0
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	18	3.0
(1,246)	1:X:139:SER:N	1:X:139:SER:CA	1:X:139:SER:C	1:X:140:ASN:N	19	3.0
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	8	3.0
(1,203)	1:X:115:GLY:C	1:X:116:VAL:N	1:X:116:VAL:CA	1:X:116:VAL:C	2	3.0
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	2	3.0
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	7	3.0
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	4	3.0
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	12	3.0
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	6	3.0
(1,138)	1:X:79:PRO:N	1:X:79:PRO:CA	1:X:79:PRO:C	1:X:80:GLY:N	20	3.0
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	16	3.0
(1,86)	1:X:52:ALA:N	1:X:52:ALA:CA	1:X:52:ALA:C	1:X:53:ASP:N	1	2.9
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	11	2.9
(1,56)	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	1:X:37:ARG:N	1	2.9
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	10	2.9
(1,221)	1:X:126:THR:C	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	6	2.9
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	2	2.9
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	3	2.9
(1,14)	1:X:11:MET:N	1:X:11:MET:CA	1:X:11:MET:C	1:X:12:ILE:N	15	2.9
(1,14)	1:X:11:MET:N	1:X:11:MET:CA	1:X:11:MET:C	1:X:12:ILE:N	20	2.9
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	6	2.9
(1,133)	1:X:76:VAL:C	1:X:77:SER:N	1:X:77:SER:CA	1:X:77:SER:C	14	2.9
(1,78)	1:X:48:VAL:N	1:X:48:VAL:CA	1:X:48:VAL:C	1:X:49:ASP:N	3	2.8
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	14	2.8
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	16	2.8
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	8	2.8
(1,193)	1:X:110:ARG:C	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	19	2.8
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	11	2.8
(1,161)	1:X:92:ALA:C	1:X:93:ARG:N	1:X:93:ARG:CA	1:X:93:ARG:C	15	2.8
(1,146)	1:X:84:PRO:N	1:X:84:PRO:CA	1:X:84:PRO:C	1:X:85:LEU:N	18	2.8
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	15	2.8
(1,133)	1:X:76:VAL:C	1:X:77:SER:N	1:X:77:SER:CA	1:X:77:SER:C	13	2.8
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	3	2.8
(1,114)	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	1:X:67:PRO:N	10	2.8
(1,81)	1:X:49:ASP:C	1:X:50:ASP:N	1:X:50:ASP:CA	1:X:50:ASP:C	9	2.7
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	20	2.7
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	14	2.7
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	17	2.7
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	20	2.7
(1,231)	1:X:131:GLY:C	1:X:132:LYS:N	1:X:132:LYS:CA	1:X:132:LYS:C	10	2.7
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	15	2.7

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,192)	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	1:X:111:ARG:N	12	2.7
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	3	2.7
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	3	2.6
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	13	2.6
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	1	2.6
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	6	2.6
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	2	2.6
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	7	2.6
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	19	2.6
(1,196)	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	1:X:113:TRP:N	6	2.6
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	11	2.6
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	19	2.6
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	19	2.5
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	2	2.5
(1,231)	1:X:131:GLY:C	1:X:132:LYS:N	1:X:132:LYS:CA	1:X:132:LYS:C	16	2.5
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	16	2.5
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	12	2.5
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	19	2.5
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	4	2.4
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	20	2.4
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	2	2.4
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	15	2.4
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	13	2.4
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	11	2.4
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	13	2.4
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	10	2.4
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	17	2.4
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	17	2.4
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	4	2.4
(1,168)	1:X:96:GLY:N	1:X:96:GLY:CA	1:X:96:GLY:C	1:X:97:GLU:N	11	2.4
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	4	2.4
(1,109)	1:X:63:ASP:C	1:X:64:VAL:N	1:X:64:VAL:CA	1:X:64:VAL:C	14	2.4
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1	2.3
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	19	2.3
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	5	2.3
(1,47)	1:X:29:ILE:C	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	16	2.3
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	6	2.3
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	13	2.3
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	18	2.3
(1,208)	1:X:118:LYS:N	1:X:118:LYS:CA	1:X:118:LYS:C	1:X:119:ALA:N	15	2.3
(1,186)	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	1:X:108:GLN:N	5	2.3
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	5	2.3
(1,168)	1:X:96:GLY:N	1:X:96:GLY:CA	1:X:96:GLY:C	1:X:97:GLU:N	4	2.3
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	12	2.3
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	15	2.3
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	5	2.2
(1,45)	1:X:28:PHE:C	1:X:29:ILE:N	1:X:29:ILE:CA	1:X:29:ILE:C	16	2.2
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	4	2.2
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	9	2.2
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	13	2.2
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	11	2.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	10	2.2
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	14	2.2
(1,152)	1:X:88:ALA:N	1:X:88:ALA:CA	1:X:88:ALA:C	1:X:89:GLU:N	6	2.2
(1,124)	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	1:X:73:ASN:N	2	2.2
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	2	2.1
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	6	2.1
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	14	2.1
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	10	2.1
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	4	2.1
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	7	2.1
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	4	2.1
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	16	2.1
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	8	2.1
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	20	2.1
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	19	2.1
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	10	2.1
(1,181)	1:X:102:VAL:C	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	9	2.1
(1,161)	1:X:92:ALA:C	1:X:93:ARG:N	1:X:93:ARG:CA	1:X:93:ARG:C	9	2.1
(1,14)	1:X:11:MET:N	1:X:11:MET:CA	1:X:11:MET:C	1:X:12:ILE:N	10	2.1
(1,120)	1:X:69:THR:N	1:X:69:THR:CA	1:X:69:THR:C	1:X:70:VAL:N	20	2.1
(1,71)	1:X:43:GLU:C	1:X:44:ASP:N	1:X:44:ASP:CA	1:X:44:ASP:C	6	2.0
(1,67)	1:X:41:ASP:C	1:X:42:SER:N	1:X:42:SER:CA	1:X:42:SER:C	4	2.0
(1,48)	1:X:30:ARG:N	1:X:30:ARG:CA	1:X:30:ARG:C	1:X:31:GLY:N	9	2.0
(1,45)	1:X:28:PHE:C	1:X:29:ILE:N	1:X:29:ILE:CA	1:X:29:ILE:C	19	2.0
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	1	2.0
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	11	2.0
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	15	2.0
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	7	2.0
(1,203)	1:X:115:GLY:C	1:X:116:VAL:N	1:X:116:VAL:CA	1:X:116:VAL:C	14	2.0
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	3	2.0
(1,140)	1:X:81:LEU:N	1:X:81:LEU:CA	1:X:81:LEU:C	1:X:82:ASP:N	10	2.0
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	9	1.9
(1,29)	1:X:18:ALA:C	1:X:19:LEU:N	1:X:19:LEU:CA	1:X:19:LEU:C	8	1.9
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	1	1.9
(1,199)	1:X:113:TRP:C	1:X:114:GLN:N	1:X:114:GLN:CA	1:X:114:GLN:C	3	1.9
(1,198)	1:X:113:TRP:N	1:X:113:TRP:CA	1:X:113:TRP:C	1:X:114:GLN:N	5	1.9
(1,194)	1:X:111:ARG:N	1:X:111:ARG:CA	1:X:111:ARG:C	1:X:112:LYS:N	16	1.9
(1,178)	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	1:X:102:VAL:N	16	1.9
(1,154)	1:X:89:GLU:N	1:X:89:GLU:CA	1:X:89:GLU:C	1:X:90:HIS:N	18	1.9
(1,148)	1:X:85:LEU:N	1:X:85:LEU:CA	1:X:85:LEU:C	1:X:86:PHE:N	9	1.9
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	14	1.9
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	4	1.8
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	15	1.8
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	9	1.8
(1,56)	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	1:X:37:ARG:N	19	1.8
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	5	1.8
(1,236)	1:X:134:GLU:N	1:X:134:GLU:CA	1:X:134:GLU:C	1:X:135:VAL:N	20	1.8
(1,214)	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	1:X:122:GLY:N	17	1.8
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	13	1.8
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	15	1.8
(1,181)	1:X:102:VAL:C	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	13	1.8

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,161)	1:X:92:ALA:C	1:X:93:ARG:N	1:X:93:ARG:CA	1:X:93:ARG:C	19	1.8
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	1	1.8
(1,130)	1:X:75:GLU:N	1:X:75:GLU:CA	1:X:75:GLU:C	1:X:76:VAL:N	14	1.8
(1,78)	1:X:48:VAL:N	1:X:48:VAL:CA	1:X:48:VAL:C	1:X:49:ASP:N	8	1.7
(1,75)	1:X:46:ILE:C	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	18	1.7
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	19	1.7
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	8	1.7
(1,41)	1:X:26:ILE:C	1:X:27:GLU:N	1:X:27:GLU:CA	1:X:27:GLU:C	11	1.7
(1,226)	1:X:129:VAL:N	1:X:129:VAL:CA	1:X:129:VAL:C	1:X:130:GLU:N	17	1.7
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	16	1.7
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	6	1.7
(1,187)	1:X:107:VAL:C	1:X:108:GLN:N	1:X:108:GLN:CA	1:X:108:GLN:C	4	1.7
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	2	1.7
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	1	1.7
(1,168)	1:X:96:GLY:N	1:X:96:GLY:CA	1:X:96:GLY:C	1:X:97:GLU:N	12	1.7
(1,130)	1:X:75:GLU:N	1:X:75:GLU:CA	1:X:75:GLU:C	1:X:76:VAL:N	19	1.7
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	12	1.7
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	12	1.7
(1,92)	1:X:55:SER:N	1:X:55:SER:CA	1:X:55:SER:C	1:X:56:HIS:N	19	1.6
(1,76)	1:X:47:ASN:N	1:X:47:ASN:CA	1:X:47:ASN:C	1:X:48:VAL:N	17	1.6
(1,67)	1:X:41:ASP:C	1:X:42:SER:N	1:X:42:SER:CA	1:X:42:SER:C	11	1.6
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	17	1.6
(1,53)	1:X:34:SER:C	1:X:35:THR:N	1:X:35:THR:CA	1:X:35:THR:C	13	1.6
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	8	1.6
(1,37)	1:X:24:VAL:C	1:X:25:GLY:N	1:X:25:GLY:CA	1:X:25:GLY:C	10	1.6
(1,31)	1:X:19:LEU:C	1:X:20:GLY:N	1:X:20:GLY:CA	1:X:20:GLY:C	8	1.6
(1,238)	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	1:X:136:PHE:N	12	1.6
(1,203)	1:X:115:GLY:C	1:X:116:VAL:N	1:X:116:VAL:CA	1:X:116:VAL:C	12	1.6
(1,203)	1:X:115:GLY:C	1:X:116:VAL:N	1:X:116:VAL:CA	1:X:116:VAL:C	19	1.6
(1,2)	1:X:5:GLU:N	1:X:5:GLU:CA	1:X:5:GLU:C	1:X:6:GLN:N	4	1.6
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1	1.6
(1,181)	1:X:102:VAL:C	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	11	1.6
(1,143)	1:X:82:ASP:C	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	6	1.6
(1,135)	1:X:77:SER:C	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	15	1.6
(1,73)	1:X:45:GLY:C	1:X:46:ILE:N	1:X:46:ILE:CA	1:X:46:ILE:C	8	1.5
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	2	1.5
(1,69)	1:X:42:SER:C	1:X:43:GLU:N	1:X:43:GLU:CA	1:X:43:GLU:C	15	1.5
(1,64)	1:X:40:ILE:N	1:X:40:ILE:CA	1:X:40:ILE:C	1:X:41:ASP:N	3	1.5
(1,45)	1:X:28:PHE:C	1:X:29:ILE:N	1:X:29:ILE:CA	1:X:29:ILE:C	12	1.5
(1,36)	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1:X:24:VAL:N	10	1.5
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	1	1.5
(1,33)	1:X:20:GLY:C	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	12	1.5
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	18	1.5
(1,244)	1:X:138:LEU:N	1:X:138:LEU:CA	1:X:138:LEU:C	1:X:139:SER:N	13	1.5
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	9	1.5
(1,216)	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	1:X:125:ILE:N	7	1.5
(1,207)	1:X:117:ILE:C	1:X:118:LYS:N	1:X:118:LYS:CA	1:X:118:LYS:C	1	1.5
(1,191)	1:X:109:ASN:C	1:X:110:ARG:N	1:X:110:ARG:CA	1:X:110:ARG:C	6	1.5
(1,169)	1:X:96:GLY:C	1:X:97:GLU:N	1:X:97:GLU:CA	1:X:97:GLU:C	11	1.5
(1,144)	1:X:83:ARG:N	1:X:83:ARG:CA	1:X:83:ARG:C	1:X:84:PRO:N	19	1.5
(1,141)	1:X:81:LEU:C	1:X:82:ASP:N	1:X:82:ASP:CA	1:X:82:ASP:C	10	1.5

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,136)	1:X:78:SER:N	1:X:78:SER:CA	1:X:78:SER:C	1:X:79:PRO:N	2	1.5
(1,117)	1:X:67:PRO:C	1:X:68:ILE:N	1:X:68:ILE:CA	1:X:68:ILE:C	19	1.5
(1,80)	1:X:49:ASP:N	1:X:49:ASP:CA	1:X:49:ASP:C	1:X:50:ASP:N	4	1.4
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	12	1.4
(1,261)	1:X:146:LEU:C	1:X:147:VAL:N	1:X:147:VAL:CA	1:X:147:VAL:C	12	1.4
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	19	1.4
(1,246)	1:X:139:SER:N	1:X:139:SER:CA	1:X:139:SER:C	1:X:140:ASN:N	3	1.4
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	17	1.4
(1,207)	1:X:117:ILE:C	1:X:118:LYS:N	1:X:118:LYS:CA	1:X:118:LYS:C	17	1.4
(1,203)	1:X:115:GLY:C	1:X:116:VAL:N	1:X:116:VAL:CA	1:X:116:VAL:C	18	1.4
(1,195)	1:X:111:ARG:C	1:X:112:LYS:N	1:X:112:LYS:CA	1:X:112:LYS:C	5	1.4
(1,190)	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	1:X:110:ARG:N	12	1.4
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	10	1.4
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	15	1.4
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	19	1.4
(1,168)	1:X:96:GLY:N	1:X:96:GLY:CA	1:X:96:GLY:C	1:X:97:GLU:N	15	1.4
(1,150)	1:X:87:THR:N	1:X:87:THR:CA	1:X:87:THR:C	1:X:88:ALA:N	9	1.4
(1,145)	1:X:83:ARG:C	1:X:84:PRO:N	1:X:84:PRO:CA	1:X:84:PRO:C	18	1.4
(1,134)	1:X:77:SER:N	1:X:77:SER:CA	1:X:77:SER:C	1:X:78:SER:N	1	1.4
(1,124)	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	1:X:73:ASN:N	10	1.4
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	13	1.4
(1,86)	1:X:52:ALA:N	1:X:52:ALA:CA	1:X:52:ALA:C	1:X:53:ASP:N	12	1.3
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	1	1.3
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	5	1.3
(1,42)	1:X:27:GLU:N	1:X:27:GLU:CA	1:X:27:GLU:C	1:X:28:PHE:N	2	1.3
(1,34)	1:X:21:PHE:N	1:X:21:PHE:CA	1:X:21:PHE:C	1:X:22:GLU:N	2	1.3
(1,244)	1:X:138:LEU:N	1:X:138:LEU:CA	1:X:138:LEU:C	1:X:139:SER:N	9	1.3
(1,237)	1:X:134:GLU:C	1:X:135:VAL:N	1:X:135:VAL:CA	1:X:135:VAL:C	5	1.3
(1,224)	1:X:128:THR:N	1:X:128:THR:CA	1:X:128:THR:C	1:X:129:VAL:N	7	1.3
(1,221)	1:X:126:THR:C	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	7	1.3
(1,212)	1:X:120:VAL:N	1:X:120:VAL:CA	1:X:120:VAL:C	1:X:121:ASP:N	4	1.3
(1,184)	1:X:104:ARG:N	1:X:104:ARG:CA	1:X:104:ARG:C	1:X:105:MET:N	20	1.3
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	3	1.3
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	15	1.3
(1,181)	1:X:102:VAL:C	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	12	1.3
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	16	1.3
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	17	1.3
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	19	1.3
(1,86)	1:X:52:ALA:N	1:X:52:ALA:CA	1:X:52:ALA:C	1:X:53:ASP:N	3	1.2
(1,66)	1:X:41:ASP:N	1:X:41:ASP:CA	1:X:41:ASP:C	1:X:42:SER:N	20	1.2
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	2	1.2
(1,38)	1:X:25:GLY:N	1:X:25:GLY:CA	1:X:25:GLY:C	1:X:26:ILE:N	10	1.2
(1,28)	1:X:18:ALA:N	1:X:18:ALA:CA	1:X:18:ALA:C	1:X:19:LEU:N	20	1.2
(1,250)	1:X:141:ILE:N	1:X:141:ILE:CA	1:X:141:ILE:C	1:X:142:GLN:N	8	1.2
(1,247)	1:X:139:SER:C	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	15	1.2
(1,230)	1:X:131:GLY:N	1:X:131:GLY:CA	1:X:131:GLY:C	1:X:132:LYS:N	12	1.2
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	18	1.2
(1,215)	1:X:123:GLU:C	1:X:124:MET:N	1:X:124:MET:CA	1:X:124:MET:C	15	1.2
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	19	1.2
(1,189)	1:X:108:GLN:C	1:X:109:ASN:N	1:X:109:ASN:CA	1:X:109:ASN:C	13	1.2
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	12	1.2

*Continued on next page...*

*Continued from previous page...*

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	6	1.2
(1,177)	1:X:100:THR:C	1:X:101:LEU:N	1:X:101:LEU:CA	1:X:101:LEU:C	15	1.2
(1,166)	1:X:95:VAL:N	1:X:95:VAL:CA	1:X:95:VAL:C	1:X:96:GLY:N	19	1.2
(1,113)	1:X:65:GLU:C	1:X:66:ASP:N	1:X:66:ASP:CA	1:X:66:ASP:C	8	1.2
(1,92)	1:X:55:SER:N	1:X:55:SER:CA	1:X:55:SER:C	1:X:56:HIS:N	1	1.1
(1,59)	1:X:37:ARG:C	1:X:38:ILE:N	1:X:38:ILE:CA	1:X:38:ILE:C	6	1.1
(1,56)	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	1:X:37:ARG:N	2	1.1
(1,55)	1:X:35:THR:C	1:X:36:LEU:N	1:X:36:LEU:CA	1:X:36:LEU:C	17	1.1
(1,51)	1:X:33:THR:C	1:X:34:SER:N	1:X:34:SER:CA	1:X:34:SER:C	9	1.1
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	4	1.1
(1,35)	1:X:22:GLU:C	1:X:23:LEU:N	1:X:23:LEU:CA	1:X:23:LEU:C	19	1.1
(1,248)	1:X:140:ASN:N	1:X:140:ASN:CA	1:X:140:ASN:C	1:X:141:ILE:N	18	1.1
(1,241)	1:X:136:PHE:C	1:X:137:ALA:N	1:X:137:ALA:CA	1:X:137:ALA:C	7	1.1
(1,222)	1:X:127:VAL:N	1:X:127:VAL:CA	1:X:127:VAL:C	1:X:128:THR:N	20	1.1
(1,213)	1:X:120:VAL:C	1:X:121:ASP:N	1:X:121:ASP:CA	1:X:121:ASP:C	15	1.1
(1,211)	1:X:119:ALA:C	1:X:120:VAL:N	1:X:120:VAL:CA	1:X:120:VAL:C	9	1.1
(1,185)	1:X:106:ALA:C	1:X:107:VAL:N	1:X:107:VAL:CA	1:X:107:VAL:C	20	1.1
(1,182)	1:X:103:LEU:N	1:X:103:LEU:CA	1:X:103:LEU:C	1:X:104:ARG:N	16	1.1
(1,153)	1:X:88:ALA:C	1:X:89:GLU:N	1:X:89:GLU:CA	1:X:89:GLU:C	14	1.1
(1,14)	1:X:11:MET:N	1:X:11:MET:CA	1:X:11:MET:C	1:X:12:ILE:N	17	1.1
(1,126)	1:X:73:ASN:N	1:X:73:ASN:CA	1:X:73:ASN:C	1:X:74:LEU:N	8	1.1
(1,123)	1:X:71:ALA:C	1:X:72:TYR:N	1:X:72:TYR:CA	1:X:72:TYR:C	16	1.1