



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 01:21 AM UTC

PDB ID : 4A5V / pdb_00004a5v
BMRB ID : 18039
Title : Solution structure ensemble of the two N-terminal apple domains (residues 58-231) of Toxoplasma gondii microneme protein 4
Authors : Marchant, J.; Cowper, B.; Liu, Y.; Lai, L.; Pinzan, C.; Marq, J.B.; Friedrich, N.; Sawmynaden, K.; Chai, W.; Childs, R.A.; Saouros, S.; Simpson, P.; Barreira, M.C.R.; Feizi, T.; Soldati-Favre, D.; Matthews, S.
Deposited on : 2011-10-28

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

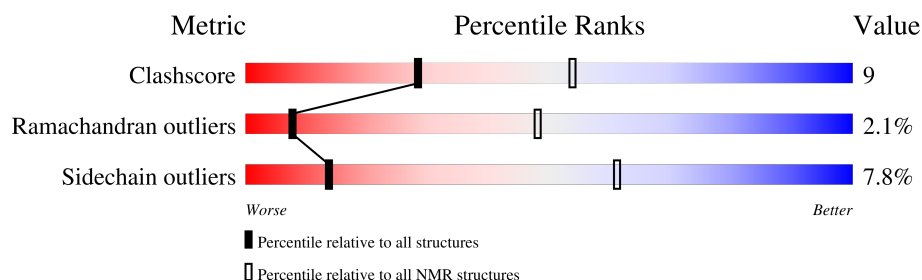
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	161	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:161 (157)	0.29	6

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 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	3, 6, 7, 9, 10
2	2, 4, 8
Single-model clusters	1; 5

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2302 atoms, of which 1105 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MICRONEMAL PROTEIN 4.

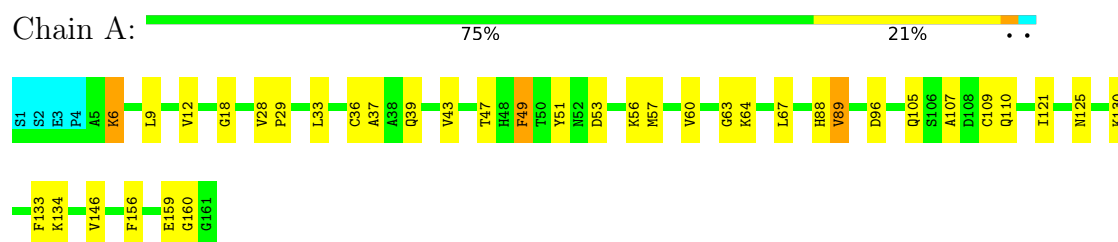
Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2302	725	1105	207	250	15	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: MICRONEMAL PROTEIN 4

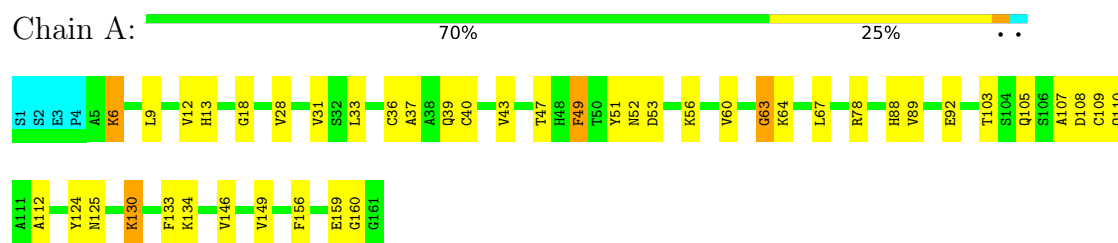


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

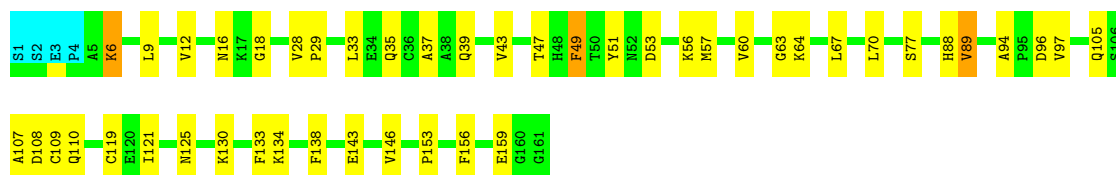
• Molecule 1: MICRONEMAL PROTEIN 4



4.2.2 Score per residue for model 2

• Molecule 1: MICRONEMAL PROTEIN 4





4.2.3 Score per residue for model 3

- Molecule 1: MICRONEMAL PROTEIN 4

Chain A: 92% 6% .



4.2.4 Score per residue for model 4

- Molecule 1: MICRONEMAL PROTEIN 4

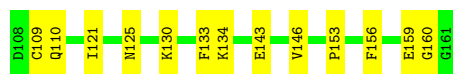
Chain A: 68% 26% . .



4.2.5 Score per residue for model 5

- Molecule 1: MICRONEMAL PROTEIN 4

Chain A: 70% 25% . .



4.2.6 Score per residue for model 6 (medoid)

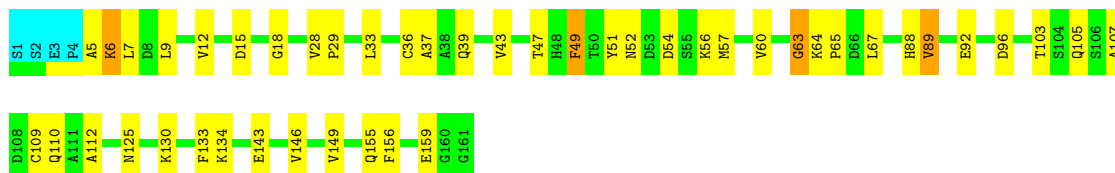
- Molecule 1: MICRONEMAL PROTEIN 4

Chain A: 91% 7% .



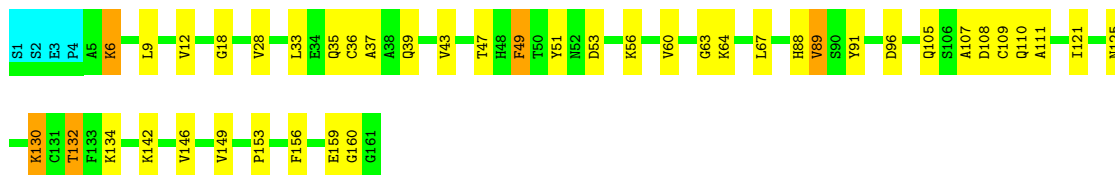
4.2.7 Score per residue for model 7

- Molecule 1: MICRONEMAL PROTEIN 4



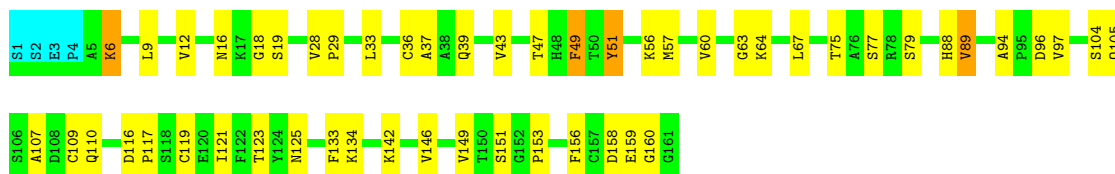
4.2.8 Score per residue for model 8

- Molecule 1: MICRONEMAL PROTEIN 4



4.2.9 Score per residue for model 9

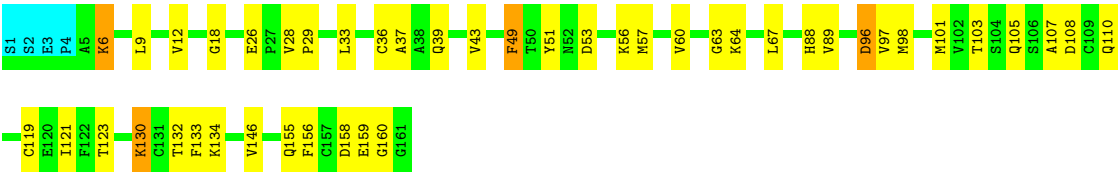
- Molecule 1: MICRONEMAL PROTEIN 4



4.2.10 Score per residue for model 10

- Molecule 1: MICRONEMAL PROTEIN 4





5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA*.

Of the 40 calculated structures, 10 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	1.2
NMRView	structure solution	
TALOS	structure solution	
ARIA	structure solution	
CNS	structure solution	

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	1772
Number of shifts mapped to atoms	1772
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1169	1080	1080	19±10
All	All	11690	10800	8640	193

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LYS:HZ2	1:A:53:ASP:HA	0.69	1.45	1	6
1:A:33:LEU:HD22	1:A:51:TYR:CD2	0.69	2.22	1	8
1:A:98:MET:HB2	1:A:133:PHE:CD1	0.69	2.23	10	1
1:A:37:ALA:HA	1:A:49:PHE:CE2	0.68	2.23	9	8
1:A:88:HIS:HA	1:A:146:VAL:O	0.63	1.93	7	8
1:A:36:CYS:SG	1:A:51:TYR:HD1	0.62	2.18	4	1
1:A:125:ASN:HD22	1:A:149:VAL:HG12	0.59	1.58	8	1
1:A:9:LEU:HD22	1:A:51:TYR:OH	0.58	1.98	7	7
1:A:89:VAL:HG21	1:A:142:LYS:HE2	0.57	1.76	8	1
1:A:130:LYS:NZ	1:A:132:THR:HG23	0.57	2.14	8	1
1:A:18:GLY:O	1:A:67:LEU:HA	0.57	2.00	1	8
1:A:133:PHE:C	1:A:134:LYS:HD2	0.56	2.25	9	6
1:A:130:LYS:HB3	1:A:130:LYS:NZ	0.56	2.14	1	1
1:A:6:LYS:HD3	1:A:56:LYS:HA	0.52	1.79	1	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:VAL:HG21	1:A:119:CYS:HA	0.52	1.81	10	3
1:A:156:PHE:HB2	1:A:159:GLU:HB2	0.51	1.82	8	8
1:A:79:SER:HB3	1:A:110:GLN:OE1	0.51	2.06	4	2
1:A:39:GLN:O	1:A:43:VAL:HG12	0.50	2.06	9	7
1:A:125:ASN:ND2	1:A:149:VAL:HG12	0.49	2.22	4	4
1:A:19:SER:OG	1:A:75:THR:HG21	0.49	2.07	9	1
1:A:110:GLN:CD	1:A:156:PHE:HA	0.49	2.33	1	6
1:A:6:LYS:HE2	1:A:33:LEU:HD23	0.49	1.85	1	1
1:A:49:PHE:CE2	1:A:78:ARG:HA	0.48	2.42	1	2
1:A:79:SER:HB2	1:A:110:GLN:NE2	0.48	2.23	5	1
1:A:29:PRO:HA	1:A:57:MET:HA	0.48	1.86	2	6
1:A:52:ASN:O	1:A:56:LYS:HA	0.47	2.09	1	1
1:A:47:THR:HG21	1:A:63:GLY:HA2	0.47	1.87	9	5
1:A:121:ILE:HG22	1:A:153:PRO:HA	0.47	1.87	8	5
1:A:91:TYR:OH	1:A:142:LYS:HE3	0.47	2.10	8	1
1:A:6:LYS:HD2	1:A:31:VAL:O	0.46	2.10	1	1
1:A:89:VAL:HA	1:A:143:GLU:O	0.46	2.10	5	4
1:A:89:VAL:HG21	1:A:142:LYS:HE3	0.46	1.87	9	1
1:A:36:CYS:O	1:A:39:GLN:HB3	0.46	2.11	4	5
1:A:67:LEU:CD1	1:A:103:THR:HB	0.46	2.41	7	3
1:A:112:ALA:HB3	1:A:133:PHE:CE2	0.45	2.46	1	1
1:A:16:ASN:HB2	1:A:70:LEU:O	0.45	2.11	2	1
1:A:33:LEU:HD22	1:A:51:TYR:CG	0.45	2.46	7	5
1:A:13:HIS:NE2	1:A:103:THR:HA	0.45	2.27	1	1
1:A:77:SER:HB2	1:A:107:ALA:O	0.45	2.12	4	2
1:A:47:THR:OG1	1:A:63:GLY:HA2	0.45	2.12	1	2
1:A:6:LYS:HD2	1:A:6:LYS:H	0.44	1.71	1	1
1:A:107:ALA:O	1:A:110:GLN:HB3	0.44	2.13	2	7
1:A:36:CYS:SG	1:A:51:TYR:CD1	0.44	3.07	4	4
1:A:13:HIS:CE1	1:A:67:LEU:HD13	0.44	2.48	5	1
1:A:40:CYS:SG	1:A:78:ARG:HB3	0.43	2.53	1	2
1:A:77:SER:HB3	1:A:107:ALA:HB1	0.43	1.89	5	2
1:A:49:PHE:CE1	1:A:51:TYR:OH	0.43	2.70	9	1
1:A:96:ASP:HA	1:A:134:LYS:HD3	0.43	1.89	10	1
1:A:5:ALA:O	1:A:7:LEU:HG	0.43	2.14	7	1
1:A:94:ALA:HB2	1:A:138:PHE:HA	0.43	1.89	2	1
1:A:49:PHE:CD1	1:A:49:PHE:N	0.42	2.87	4	1
1:A:92:GLU:HA	1:A:134:LYS:HE3	0.42	1.91	5	4
1:A:97:VAL:HG23	1:A:98:MET:HG3	0.42	1.92	10	1
1:A:125:ASN:N	1:A:130:LYS:O	0.42	2.51	5	3
1:A:6:LYS:HZ2	1:A:53:ASP:CA	0.42	2.24	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LEU:HG	1:A:10:SER:H	0.42	1.75	5	1
1:A:123:THR:HA	1:A:151:SER:HA	0.42	1.91	4	2
1:A:156:PHE:CB	1:A:159:GLU:HB2	0.42	2.45	4	3
1:A:116:ASP:CG	1:A:117:PRO:HD2	0.41	2.40	9	1
1:A:101:MET:O	1:A:130:LYS:HA	0.41	2.15	10	1
1:A:124:TYR:HA	1:A:130:LYS:O	0.41	2.16	1	1
1:A:111:ALA:HA	1:A:156:PHE:CE1	0.41	2.51	8	1
1:A:52:ASN:OD1	1:A:54:ASP:HB3	0.41	2.15	7	1
1:A:94:ALA:O	1:A:134:LYS:HG3	0.41	2.15	9	1
1:A:11:CYS:SG	1:A:76:ALA:HB1	0.41	2.56	4	1
1:A:146:VAL:O	1:A:149:VAL:HG22	0.40	2.15	7	1
1:A:123:THR:HB	1:A:132:THR:OG1	0.40	2.17	10	1
1:A:65:PRO:HD2	1:A:112:ALA:HB2	0.40	1.92	7	1
1:A:10:SER:HB2	1:A:80:CYS:CB	0.40	2.45	4	1
1:A:47:THR:CG2	1:A:63:GLY:HA2	0.40	2.47	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	156/161 (97%)	139±4 (89±3%)	12±1 (8±1%)	3±1 (2±1%)	8	48
All	All	1545/1610 (96%)	1390 (90%)	122 (8%)	33 (2%)	8	48

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	64	LYS	10
1	A	6	LYS	8
1	A	160	GLY	7
1	A	63	GLY	4
1	A	16	ASN	2
1	A	158	ASP	2

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	129/133 (97%)	118±3 (91±2%)	10±2 (8±1%)	14 61
All	All	1277/1330 (96%)	1178 (92%)	99 (8%)	14 61

All 22 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	28	VAL	10
1	A	60	VAL	10
1	A	89	VAL	10
1	A	105	GLN	10
1	A	12	VAL	9
1	A	49	PHE	9
1	A	109	CYS	9
1	A	96	ASP	9
1	A	108	ASP	4
1	A	130	LYS	3
1	A	121	ILE	2
1	A	51	TYR	2
1	A	15	ASP	2
1	A	155	GLN	2
1	A	64	LYS	1
1	A	75	THR	1
1	A	77	SER	1
1	A	35	GLN	1
1	A	132	THR	1
1	A	134	LYS	1
1	A	104	SER	1
1	A	26	GLU	1

6.3.3 RNA ⓘ

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 oligosaccharides 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 91% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `new_1.str.csh`

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	1772
Number of shifts mapped to atoms	1772
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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
$^{13}\text{C}_\alpha$	160	0.26 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	146	0.22 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}'$	154	0.25 ± 0.18	None needed (< 0.5 ppm)
^{15}N	150	0.18 ± 0.25	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 91%, i.e. 1742 atoms were assigned a chemical shift out of a possible 1908. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	775/785 (99%)	318/321 (99%)	309/314 (98%)	148/150 (99%)
Sidechain	873/982 (89%)	589/632 (93%)	273/314 (87%)	11/36 (31%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	94/141 (67%)	46/71 (65%)	48/65 (74%)	0/5 (0%)
Overall	1742/1908 (91%)	953/1024 (93%)	630/693 (91%)	159/191 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1772 atoms were assigned a chemical shift out of a possible 1948. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	787/803 (98%)	323/328 (98%)	314/322 (98%)	150/153 (98%)
Sidechain	891/1004 (89%)	601/646 (93%)	279/322 (87%)	11/36 (31%)
Aromatic	94/141 (67%)	46/71 (65%)	48/65 (74%)	0/5 (0%)
Overall	1772/1948 (91%)	970/1045 (93%)	641/709 (90%)	161/194 (83%)

7.1.4 Statistically unusual chemical shifts ⓘ

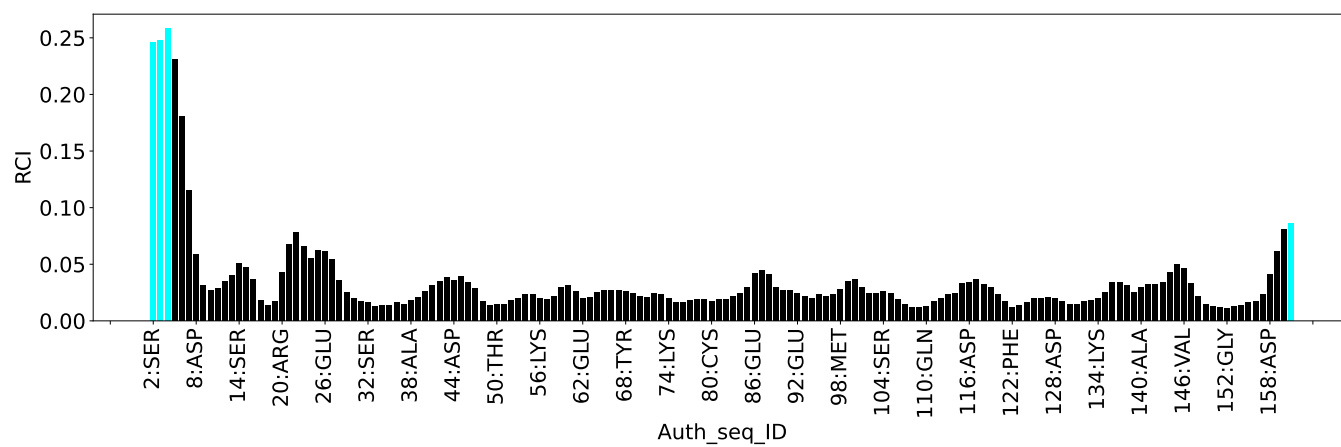
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	61	LYS	HB2	0.14	0.58 – 2.97	-6.9
1	A	78	ARG	HD2	1.79	1.97 – 4.26	-5.8
1	A	78	ARG	HB2	0.38	0.52 – 3.08	-5.5

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3572
Intra-residue ($ i-j =0$)	1134
Sequential ($ i-j =1$)	731
Medium range ($ i-j >1$ and $ i-j <5$)	472
Long range ($ i-j \geq 5$)	1207
Inter-chain	0
Hydrogen bond restraints	22
Disulfide bond restraints	6
Total dihedral-angle restraints	190
Number of unmapped restraints	0
Number of restraints per residue	23.4
Number of long range restraints per residue ¹	7.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	167.4	0.2
0.2-0.5 (Medium)	315.8	0.5
>0.5 (Large)	280.2	2.72

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)	16.0	8.04
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

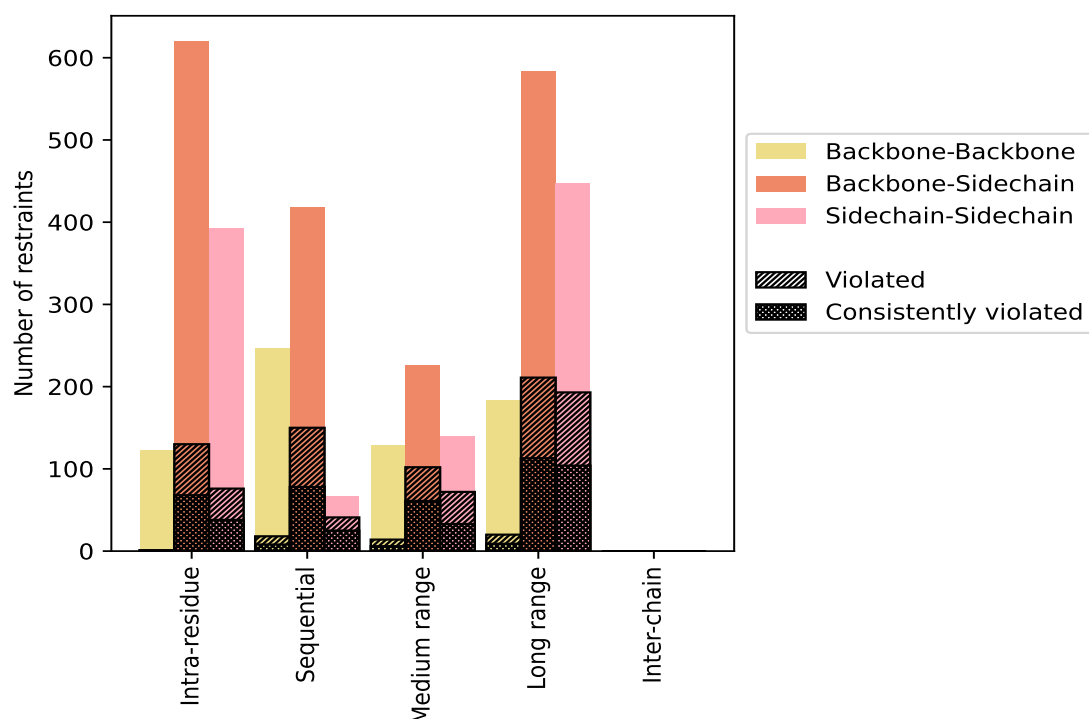
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	1134	31.7	207	18.3	5.8	107	9.4	3.0
Backbone-Backbone	122	3.4	1	0.8	0.0	1	0.8	0.0
Backbone-Sidechain	620	17.4	130	21.0	3.6	68	11.0	1.9
Sidechain-Sidechain	392	11.0	76	19.4	2.1	38	9.7	1.1
Sequential (i-j =1)	731	20.5	209	28.6	5.9	111	15.2	3.1
Backbone-Backbone	247	6.9	18	7.3	0.5	8	3.2	0.2
Backbone-Sidechain	418	11.7	150	35.9	4.2	78	18.7	2.2
Sidechain-Sidechain	66	1.8	41	62.1	1.1	25	37.9	0.7
Medium range (i-j >1 & i-j <5)	472	13.2	188	39.8	5.3	100	21.2	2.8
Backbone-Backbone	128	3.6	14	10.9	0.4	6	4.7	0.2
Backbone-Sidechain	204	5.7	102	50.0	2.9	61	29.9	1.7
Sidechain-Sidechain	140	3.9	72	51.4	2.0	33	23.6	0.9
Long range (i-j ≥5)	1207	33.8	424	35.1	11.9	226	18.7	6.3
Backbone-Backbone	183	5.1	20	10.9	0.6	9	4.9	0.3
Backbone-Sidechain	583	16.3	211	36.2	5.9	113	19.4	3.2
Sidechain-Sidechain	441	12.3	193	43.8	5.4	104	23.6	2.9
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	22	0.6	0	0.0	0.0	0	0.0	0.0
Disulfide bond	6	0.2	0	0.0	0.0	0	0.0	0.0
Total	3572	100.0	1028	28.8	28.8	544	15.2	15.2
Backbone-Backbone	680	19.0	53	7.8	1.5	24	3.5	0.7
Backbone-Sidechain	1847	51.7	593	32.1	16.6	320	17.3	9.0
Sidechain-Sidechain	1045	29.3	382	36.6	10.7	200	19.1	5.6

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

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



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

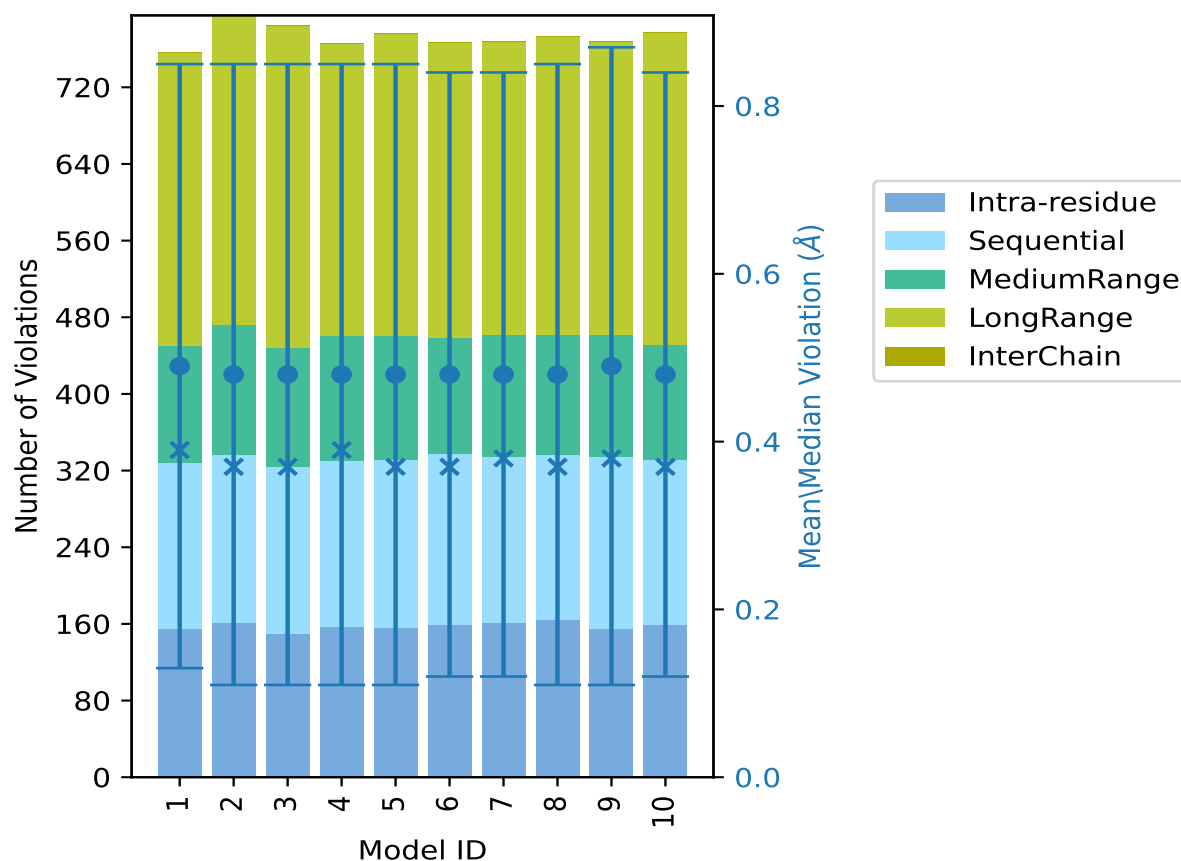
9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	155	173	122	306	0	756	0.49	2.45	0.36	0.39
2	161	176	135	323	0	795	0.48	2.37	0.37	0.37
3	150	174	124	336	0	784	0.48	2.23	0.37	0.37
4	157	173	131	305	0	766	0.48	2.35	0.37	0.39
5	156	175	130	315	0	776	0.48	2.25	0.37	0.37
6	159	178	122	308	0	767	0.48	2.35	0.36	0.37
7	161	173	128	306	0	768	0.48	2.52	0.36	0.38
8	164	172	126	311	0	773	0.48	2.37	0.37	0.37
9	155	179	128	306	0	768	0.49	2.39	0.38	0.38
10	159	172	120	326	0	777	0.48	2.72	0.36	0.37

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

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2516(IR:927, SQ:522, MR:284, LR:783, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
26	20	16	43	0	105	1	10.0
12	14	14	23	0	63	2	20.0
10	6	8	12	0	36	3	30.0

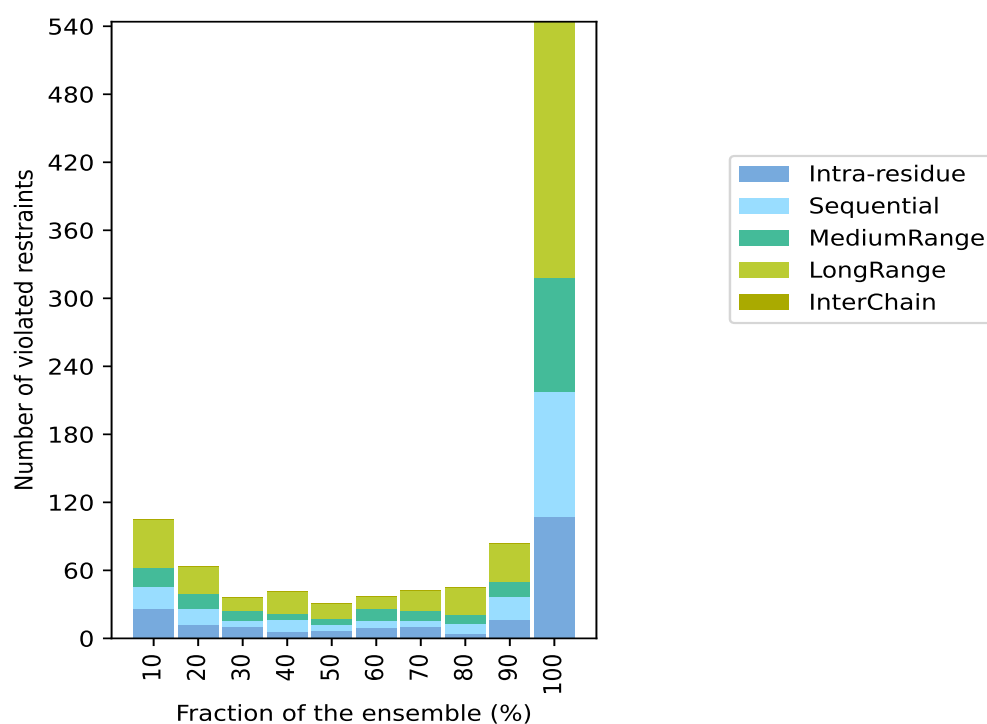
Continued on next page...

Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
6	10	6	19	0	41	4	40.0
7	5	5	14	0	31	5	50.0
9	7	10	11	0	37	6	60.0
10	6	8	18	0	42	7	70.0
4	9	8	24	0	45	8	80.0
16	21	13	34	0	84	9	90.0
107	111	100	226	0	544	10	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

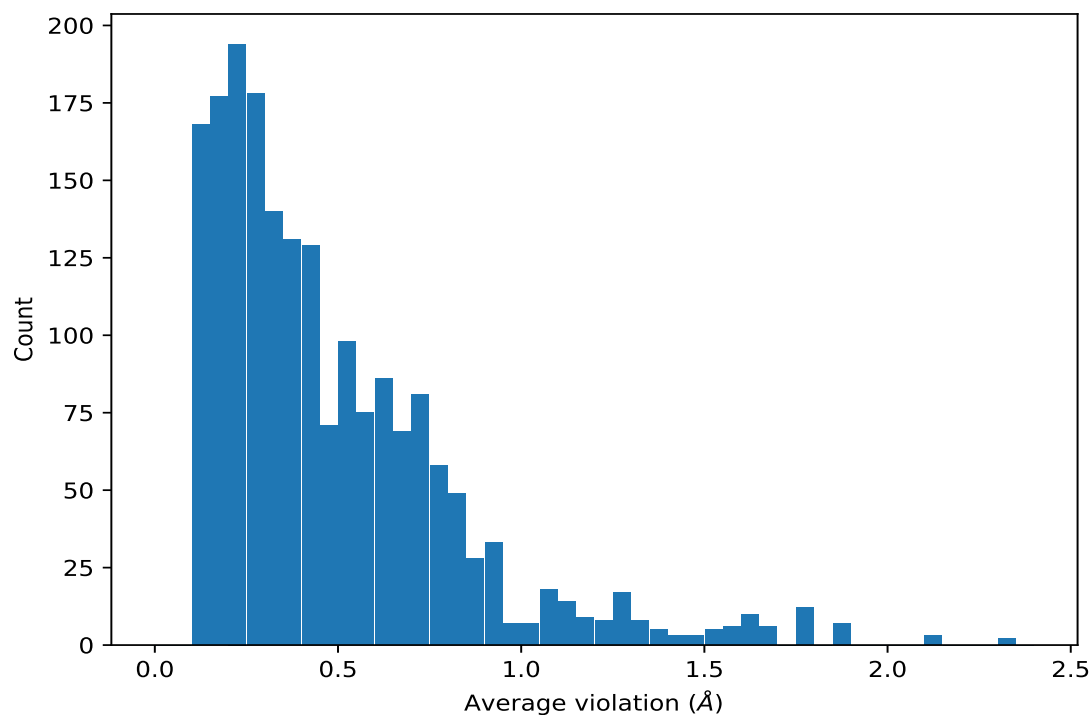


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	10	2.33	0.12	2.36
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG12	10	2.33	0.12	2.36
(1,2927)	1:31:A:VAL:HG22	1:57:A:MET:HG3	10	2.12	0.1	2.15
(1,2927)	1:31:A:VAL:HG21	1:57:A:MET:HG3	10	2.12	0.1	2.15
(1,2927)	1:31:A:VAL:HG23	1:57:A:MET:HG3	10	2.12	0.1	2.15
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	10	1.89	0.08	1.87
(1,2698)	1:73:A:GLY:HA3	1:74:A:LYS:HB3	10	1.89	0.08	1.87
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	10	1.89	0.27	1.88
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD2	10	1.88	0.27	1.98
(1,2788)	1:142:A:LYS:HE2	1:142:A:LYS:H	10	1.88	0.27	1.98
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD1	10	1.88	0.27	1.98
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	10	1.85	0.11	1.81
(1,2976)	1:112:A:ALA:HB3	1:98:A:MET:HG2	10	1.79	0.15	1.81
(1,2976)	1:26:A:GLU:HB2	1:23:A:THR:HG23	10	1.79	0.15	1.81
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG22	10	1.79	0.15	1.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG23	10	1.79	0.15	1.81
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG21	10	1.79	0.15	1.81
(1,2976)	1:26:A:GLU:HB2	1:23:A:THR:HG22	10	1.79	0.15	1.81
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	10	1.78	0.13	1.76
(1,2604)	1:149:A:VAL:HG21	1:92:A:GLU:HG3	10	1.75	0.14	1.78
(1,2604)	1:149:A:VAL:HG23	1:92:A:GLU:HG3	10	1.75	0.14	1.78
(1,2604)	1:149:A:VAL:HG22	1:92:A:GLU:HG3	10	1.75	0.14	1.78
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD13	10	1.67	0.11	1.69
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD11	10	1.67	0.11	1.69
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD12	10	1.67	0.11	1.69
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB2	10	1.67	0.12	1.68
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB3	10	1.67	0.12	1.68
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB1	10	1.67	0.12	1.68
(1,3142)	1:47:A:THR:HG21	1:62:A:GLU:HG2	10	1.64	0.03	1.64
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HG2	10	1.64	0.03	1.64
(1,3142)	1:47:A:THR:HG21	1:62:A:GLU:HB2	10	1.64	0.03	1.64
(1,3142)	1:47:A:THR:HG22	1:62:A:GLU:HB2	10	1.64	0.03	1.64
(1,3142)	1:47:A:THR:HG22	1:62:A:GLU:HG2	10	1.64	0.03	1.64
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HB2	10	1.64	0.03	1.64
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD13	10	1.6	0.11	1.6
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD12	10	1.6	0.11	1.6
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD11	10	1.6	0.11	1.6
(1,2894)	1:80:A:CYS:HB2	1:9:A:LEU:HB3	10	1.59	0.07	1.62
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	10	1.59	0.07	1.62
(1,2894)	1:36:A:CYS:HB3	1:35:A:GLN:HB2	10	1.59	0.07	1.62
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	10	1.57	0.03	1.58
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	10	1.55	0.05	1.56
(1,3274)	1:67:A:LEU:H	1:68:A:TYR:HB2	10	1.53	0.2	1.58
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	10	1.53	0.2	1.58
(1,1476)	1:33:A:LEU:HD11	1:14:A:SER:HB2	10	1.5	0.6	1.89
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	10	1.5	0.6	1.89
(1,1476)	1:33:A:LEU:HD13	1:14:A:SER:HB2	10	1.5	0.6	1.89
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB3	10	1.45	0.01	1.45
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB2	10	1.45	0.01	1.45
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB1	10	1.45	0.01	1.45
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	10	1.44	0.06	1.46
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	10	1.44	0.09	1.45
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	10	1.42	0.21	1.36
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	10	1.36	0.1	1.36
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	10	1.36	0.18	1.46
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	10	1.36	0.05	1.36
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	10	1.35	0.01	1.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	10	1.35	0.47	1.2
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	10	1.32	0.04	1.32
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG22	10	1.32	0.06	1.32
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG21	10	1.32	0.06	1.32
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG23	10	1.32	0.06	1.32
(1,2936)	1:59:A:HIS:HB2	1:61:A:LYS:HD2	10	1.32	0.06	1.32
(1,339)	1:149:A:VAL:HG22	1:88:A:HIS:HB2	10	1.31	0.05	1.32
(1,339)	1:149:A:VAL:HG21	1:88:A:HIS:HB2	10	1.31	0.05	1.32
(1,339)	1:149:A:VAL:HG23	1:88:A:HIS:HB2	10	1.31	0.05	1.32
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	10	1.28	0.13	1.27
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	10	1.27	0.6	1.56
(1,329)	1:100:A:ALA:HB2	1:130:A:LYS:HE2	10	1.27	0.6	1.56
(1,329)	1:100:A:ALA:HB1	1:130:A:LYS:HE2	10	1.27	0.6	1.56
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB2	10	1.27	0.19	1.23
(1,2634)	1:112:A:ALA:HB1	1:111:A:ALA:HB1	10	1.27	0.19	1.23
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB1	10	1.27	0.19	1.23
(1,2634)	1:112:A:ALA:HB3	1:111:A:ALA:HB2	10	1.27	0.19	1.23
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB3	10	1.27	0.19	1.23
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	10	1.26	0.06	1.25
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG21	10	1.26	0.06	1.25
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG23	10	1.26	0.06	1.25
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	10	1.26	0.14	1.32
(1,3494)	1:55:A:SER:H	1:57:A:MET:HB2	10	1.26	0.14	1.32
(1,3494)	1:55:A:SER:H	1:6:A:LYS:HD2	10	1.26	0.14	1.32
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	10	1.25	0.24	1.31
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	10	1.25	0.05	1.24
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG23	10	1.23	0.05	1.25
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG21	10	1.23	0.05	1.25
(1,171)	1:12:A:VAL:HG21	1:74:A:LYS:HB2	10	1.22	0.03	1.22
(1,171)	1:12:A:VAL:HG23	1:74:A:LYS:HB2	10	1.22	0.03	1.22
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	10	1.22	0.09	1.22
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	10	1.2	0.01	1.2
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG21	10	1.19	0.14	1.14
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG23	10	1.19	0.14	1.14
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG22	10	1.19	0.14	1.14
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	10	1.15	0.11	1.18
(1,2960)	1:78:A:ARG:HB2	1:77:A:SER:HA	10	1.15	0.11	1.18
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG23	10	1.15	0.05	1.15
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG21	10	1.15	0.05	1.15
(1,3320)	1:39:A:GLN:H	1:60:A:VAL:HG12	10	1.15	0.05	1.15
(1,2530)	1:13:A:HIS:HD2	1:67:A:LEU:HG	10	1.14	0.33	1.28
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	10	1.14	0.33	1.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	10	1.13	0.08	1.1
(1,3368)	1:129:A:GLN:H	1:149:A:VAL:HG11	10	1.12	0.18	1.16
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG23	10	1.12	0.18	1.16
(1,3368)	1:129:A:GLN:H	1:149:A:VAL:HG12	10	1.12	0.18	1.16
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG22	10	1.12	0.18	1.16
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG21	10	1.12	0.18	1.16
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	10	1.1	0.19	1.16
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	10	1.1	0.05	1.1
(1,2929)	1:135:A:GLY:H	1:97:A:VAL:HB	10	1.1	0.05	1.1
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB3	10	1.09	0.06	1.11
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB1	10	1.09	0.06	1.11
(1,3092)	1:49:A:PHE:H	1:76:A:ALA:HB1	10	1.09	0.06	1.11
(1,3092)	1:49:A:PHE:H	1:76:A:ALA:HB3	10	1.09	0.06	1.11
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB2	10	1.09	0.06	1.11
(1,1611)	1:7:A:LEU:HD11	1:4:A:PRO:HD3	10	1.06	0.22	1.08
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	10	1.06	0.22	1.08
(1,1611)	1:7:A:LEU:HD12	1:4:A:PRO:HD3	10	1.06	0.22	1.08
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB1	10	1.06	0.1	1.04
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB3	10	1.06	0.1	1.04
(1,2494)	1:49:A:PHE:HD2	1:37:A:ALA:HB1	10	1.06	0.1	1.04
(1,2494)	1:49:A:PHE:HD2	1:37:A:ALA:HB3	10	1.06	0.1	1.04
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB2	10	1.06	0.1	1.04
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	10	1.05	0.03	1.05
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	10	1.05	0.06	1.06
(1,2629)	1:111:A:ALA:HB1	1:110:A:GLN:H	10	1.05	0.06	1.06
(1,2629)	1:111:A:ALA:HB3	1:110:A:GLN:H	10	1.05	0.06	1.06
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	10	1.03	0.02	1.04
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD23	10	1.01	0.01	1.01
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD22	10	1.01	0.01	1.01
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD21	10	1.01	0.01	1.01
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	10	1.0	0.11	1.04
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	10	0.95	0.18	1.0
(1,2667)	1:94:A:ALA:HB2	1:121:A:ILE:HG12	10	0.95	0.09	0.96
(1,2667)	1:94:A:ALA:HB1	1:121:A:ILE:HG12	10	0.95	0.09	0.96
(1,2667)	1:94:A:ALA:HB3	1:121:A:ILE:HG12	10	0.95	0.09	0.96
(1,2636)	1:37:A:ALA:HB2	1:33:A:LEU:HA	10	0.95	0.05	0.96
(1,2636)	1:37:A:ALA:HB3	1:33:A:LEU:HA	10	0.95	0.05	0.96
(1,2636)	1:37:A:ALA:HB1	1:33:A:LEU:HA	10	0.95	0.05	0.96
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE3	10	0.94	0.05	0.94
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	10	0.94	0.05	0.94
(1,2892)	1:80:A:CYS:HB2	1:11:A:CYS:HB2	10	0.94	0.05	0.94
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	10	0.94	0.08	0.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3264)	1:96:A:ASP:H	1:134:A:LYS:HB3	10	0.94	0.08	0.97
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	10	0.93	0.04	0.93
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB2	10	0.93	0.04	0.93
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB1	10	0.93	0.04	0.93
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG23	10	0.93	0.1	0.93
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG22	10	0.93	0.1	0.93
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG21	10	0.93	0.1	0.93
(1,2851)	1:100:A:ALA:HB3	1:101:A:MET:HB2	10	0.93	0.1	0.93
(1,2851)	1:100:A:ALA:HB1	1:101:A:MET:HB2	10	0.93	0.1	0.93
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD13	10	0.92	0.04	0.92
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD11	10	0.92	0.04	0.92
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD12	10	0.92	0.04	0.92
(1,2822)	1:52:A:ASN:HB3	1:57:A:MET:HB2	10	0.92	0.04	0.91
(1,2822)	1:108:A:ASP:HB3	1:67:A:LEU:HG	10	0.92	0.04	0.91
(1,2583)	1:146:A:VAL:HG12	1:143:A:GLU:HB3	10	0.92	0.08	0.92
(1,2583)	1:146:A:VAL:HG11	1:143:A:GLU:HB3	10	0.92	0.08	0.92
(1,2583)	1:146:A:VAL:HG13	1:143:A:GLU:HB3	10	0.92	0.08	0.92
(1,2595)	1:75:A:THR:HG21	1:13:A:HIS:HB2	10	0.92	0.31	1.07
(1,2595)	1:75:A:THR:HG22	1:48:A:HIS:HB3	10	0.92	0.31	1.07
(1,2595)	1:75:A:THR:HG22	1:13:A:HIS:HB2	10	0.92	0.31	1.07
(1,2595)	1:75:A:THR:HG21	1:48:A:HIS:HB3	10	0.92	0.31	1.07
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	10	0.9	0.1	0.93
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	10	0.9	0.33	0.84
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB3	10	0.9	0.05	0.9
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB1	10	0.9	0.05	0.9
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB2	10	0.9	0.05	0.9
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG23	10	0.9	0.06	0.9
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG21	10	0.9	0.06	0.9
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG22	10	0.9	0.06	0.9
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	10	0.89	0.03	0.88
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD22	10	0.89	0.03	0.9
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD23	10	0.89	0.03	0.9
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD21	10	0.89	0.03	0.9
(1,1663)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	10	0.89	0.06	0.88
(1,1663)	1:149:A:VAL:HG12	1:148:A:GLY:HA2	10	0.89	0.06	0.88
(1,1663)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	10	0.89	0.06	0.88
(1,2852)	1:101:A:MET:HB2	1:65:A:PRO:HB2	10	0.89	0.12	0.9
(1,2852)	1:112:A:ALA:HB2	1:101:A:MET:HB2	10	0.89	0.12	0.9
(1,2852)	1:112:A:ALA:HB3	1:101:A:MET:HB2	10	0.89	0.12	0.9
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	10	0.88	0.11	0.85
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	10	0.87	0.01	0.87
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	10	0.87	0.03	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2836)	1:141:A:PHE:HB3	1:134:A:LYS:HG2	10	0.87	0.03	0.87
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB3	10	0.87	0.03	0.87
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	10	0.86	0.1	0.91
(1,2568)	1:43:A:VAL:HG22	1:60:A:VAL:HB	10	0.85	0.14	0.91
(1,2568)	1:149:A:VAL:HG13	1:125:A:ASN:HB2	10	0.85	0.14	0.91
(1,2568)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	10	0.85	0.14	0.91
(1,2568)	1:43:A:VAL:HG21	1:60:A:VAL:HB	10	0.85	0.14	0.91
(1,2568)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	10	0.85	0.14	0.91
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD13	10	0.85	0.06	0.84
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	10	0.85	0.06	0.84
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD12	10	0.85	0.06	0.84
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB3	10	0.84	0.15	0.87
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB2	10	0.84	0.15	0.87
(1,2713)	1:148:A:GLY:HA2	1:147:A:LEU:HB2	10	0.84	0.15	0.87
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB1	10	0.84	0.15	0.87
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	10	0.84	0.02	0.84
(1,2974)	1:98:A:MET:HG2	1:113:A:CYS:HA	10	0.84	0.09	0.82
(1,2974)	1:98:A:MET:HG2	1:119:A:CYS:HB3	10	0.84	0.09	0.82
(1,2974)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	10	0.84	0.09	0.82
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	10	0.84	0.47	0.61
(1,2908)	1:110:A:GLN:HG2	1:79:A:SER:HB2	10	0.84	0.47	0.61
(1,3093)	1:76:A:ALA:HB3	1:80:A:CYS:HA	10	0.84	0.15	0.84
(1,3093)	1:76:A:ALA:HB1	1:80:A:CYS:HA	10	0.84	0.15	0.84
(1,3093)	1:76:A:ALA:HB2	1:80:A:CYS:HA	10	0.84	0.15	0.84
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB3	10	0.84	0.03	0.83
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB2	10	0.84	0.03	0.83
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB1	10	0.84	0.03	0.83
(1,295)	1:28:A:VAL:HG23	1:39:A:GLN:HG3	10	0.83	0.05	0.82
(1,295)	1:28:A:VAL:HG21	1:39:A:GLN:HG3	10	0.83	0.05	0.82
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG3	10	0.83	0.08	0.86
(1,3327)	1:90:A:SER:H	1:89:A:VAL:HG11	10	0.83	0.08	0.86
(1,3327)	1:90:A:SER:H	1:89:A:VAL:HG13	10	0.83	0.08	0.86
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG2	10	0.83	0.08	0.86
(1,3098)	1:67:A:LEU:HD11	1:67:A:LEU:HA	10	0.83	0.03	0.83
(1,3098)	1:67:A:LEU:HD13	1:67:A:LEU:HA	10	0.83	0.03	0.83
(1,3098)	1:67:A:LEU:HD12	1:67:A:LEU:HA	10	0.83	0.03	0.83
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.82	0.02	0.81
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD23	10	0.81	0.24	0.78
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD21	10	0.81	0.24	0.78
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD22	10	0.81	0.24	0.78
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	10	0.81	0.1	0.82
(1,2569)	1:97:A:VAL:HG11	1:120:A:GLU:HB2	10	0.81	0.1	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2569)	1:97:A:VAL:HG13	1:120:A:GLU:HB2	10	0.81	0.1	0.82
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG21	10	0.8	0.14	0.78
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG23	10	0.8	0.14	0.78
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG22	10	0.8	0.14	0.78
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG22	10	0.8	0.1	0.8
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG21	10	0.8	0.1	0.8
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG23	10	0.8	0.1	0.8
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	10	0.8	0.03	0.79
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG21	10	0.8	0.2	0.86
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG23	10	0.8	0.2	0.86
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG22	10	0.8	0.2	0.86
(1,1642)	1:47:A:THR:HG23	1:111:A:ALA:HB1	10	0.79	0.06	0.81
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB3	10	0.79	0.06	0.81
(1,1642)	1:47:A:THR:HG23	1:111:A:ALA:HB3	10	0.79	0.06	0.81
(1,1642)	1:47:A:THR:HG21	1:111:A:ALA:HB1	10	0.79	0.06	0.81
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB1	10	0.79	0.06	0.81
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB2	10	0.79	0.06	0.81
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	10	0.79	0.1	0.74
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB3	10	0.79	0.04	0.78
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB2	10	0.79	0.04	0.78
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB1	10	0.79	0.04	0.78
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	10	0.79	0.12	0.81
(1,2982)	1:105:A:GLN:HG2	1:108:A:ASP:HA	10	0.79	0.12	0.81
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	10	0.79	0.64	0.56
(1,420)	1:111:A:ALA:HB1	1:65:A:PRO:HG2	10	0.79	0.64	0.56
(1,420)	1:111:A:ALA:HB3	1:65:A:PRO:HG2	10	0.79	0.64	0.56
(1,197)	1:99:A:THR:H	1:99:A:THR:HG23	10	0.78	0.03	0.8
(1,197)	1:99:A:THR:H	1:99:A:THR:HG22	10	0.78	0.03	0.8
(1,197)	1:99:A:THR:H	1:99:A:THR:HG21	10	0.78	0.03	0.8
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	10	0.78	0.27	0.88
(1,2944)	1:60:A:VAL:HB	1:23:A:THR:HG22	10	0.78	0.27	0.88
(1,2944)	1:60:A:VAL:HB	1:23:A:THR:HG21	10	0.78	0.27	0.88
(1,2662)	1:24:A:ILE:HG23	1:62:A:GLU:HG3	10	0.78	0.05	0.78
(1,2662)	1:24:A:ILE:HG22	1:62:A:GLU:HG3	10	0.78	0.05	0.78
(1,2662)	1:24:A:ILE:HG21	1:62:A:GLU:HG3	10	0.78	0.05	0.78
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	10	0.78	0.06	0.77
(1,3132)	1:23:A:THR:HG23	1:59:A:HIS:HD2	10	0.78	0.06	0.77
(1,3132)	1:23:A:THR:HG22	1:59:A:HIS:HD2	10	0.78	0.06	0.77
(1,2589)	1:60:A:VAL:HG21	1:24:A:ILE:HA	10	0.77	0.06	0.74
(1,2589)	1:60:A:VAL:HG22	1:24:A:ILE:HA	10	0.77	0.06	0.74
(1,2589)	1:60:A:VAL:HG23	1:24:A:ILE:HA	10	0.77	0.06	0.74
(1,2859)	1:71:A:THR:HG21	1:16:A:ASN:HB2	10	0.77	0.25	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2859)	1:71:A:THR:HG23	1:16:A:ASN:HB2	10	0.77	0.25	0.86
(1,2859)	1:71:A:THR:HG22	1:16:A:ASN:HB2	10	0.77	0.25	0.86
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG12	10	0.76	0.08	0.72
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG11	10	0.76	0.08	0.72
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG13	10	0.76	0.08	0.72
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	10	0.76	0.07	0.76
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG11	10	0.76	0.07	0.76
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG13	10	0.76	0.07	0.76
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	10	0.76	0.03	0.75
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	10	0.76	0.25	0.76
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	10	0.76	0.09	0.78
(1,2585)	1:97:A:VAL:HG12	1:134:A:LYS:HG3	10	0.76	0.09	0.78
(1,2585)	1:97:A:VAL:HG11	1:134:A:LYS:HG3	10	0.76	0.09	0.78
(1,2585)	1:97:A:VAL:HG12	1:134:A:LYS:HB2	10	0.76	0.09	0.78
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB3	10	0.75	0.03	0.76
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB2	10	0.75	0.03	0.76
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB1	10	0.75	0.03	0.76
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	10	0.75	0.04	0.76
(1,108)	1:31:A:VAL:HG23	1:58:A:CYS:HA	10	0.75	0.04	0.75
(1,108)	1:31:A:VAL:HG22	1:58:A:CYS:HA	10	0.75	0.04	0.75
(1,108)	1:31:A:VAL:HG21	1:58:A:CYS:HA	10	0.75	0.04	0.75
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB2	10	0.74	0.06	0.75
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB2	10	0.74	0.06	0.75
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB1	10	0.74	0.06	0.75
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB3	10	0.74	0.06	0.75
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB3	10	0.74	0.06	0.75
(1,2592)	1:75:A:THR:HG21	1:13:A:HIS:H	10	0.74	0.09	0.74
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG22	10	0.74	0.09	0.74
(1,2592)	1:75:A:THR:HG22	1:13:A:HIS:H	10	0.74	0.09	0.74
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG21	10	0.74	0.09	0.74
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG23	10	0.74	0.09	0.74
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB2	10	0.74	0.07	0.75
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB1	10	0.74	0.07	0.75
(1,3427)	1:113:A:CYS:H	1:110:A:GLN:HG2	10	0.74	0.07	0.75
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB3	10	0.74	0.07	0.75
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	10	0.74	0.06	0.76
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	10	0.73	0.08	0.72
(1,1277)	1:89:A:VAL:HG21	1:142:A:LYS:HD2	10	0.73	0.08	0.74
(1,1277)	1:89:A:VAL:HG22	1:142:A:LYS:HD2	10	0.73	0.08	0.74
(1,1277)	1:89:A:VAL:HG23	1:142:A:LYS:HD2	10	0.73	0.08	0.74
(1,1277)	1:89:A:VAL:HG22	1:142:A:LYS:HD3	10	0.73	0.08	0.74
(1,3073)	1:33:A:LEU:HD13	1:9:A:LEU:HB3	10	0.73	0.05	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD12	10	0.73	0.05	0.72
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD13	10	0.73	0.05	0.72
(1,3073)	1:33:A:LEU:HD11	1:9:A:LEU:HB3	10	0.73	0.05	0.72
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	10	0.72	0.11	0.77
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	10	0.72	0.31	0.88
(1,2549)	1:67:A:LEU:HD23	1:17:A:LYS:HE3	10	0.72	0.31	0.88
(1,2549)	1:67:A:LEU:HD21	1:17:A:LYS:HE3	10	0.72	0.31	0.88
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB2	10	0.72	0.07	0.72
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB1	10	0.72	0.07	0.72
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB3	10	0.72	0.07	0.72
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	10	0.72	0.07	0.72
(1,2850)	1:100:A:ALA:HB2	1:101:A:MET:HB3	10	0.72	0.07	0.72
(1,2850)	1:100:A:ALA:HB1	1:101:A:MET:HB3	10	0.72	0.07	0.72
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	10	0.72	0.05	0.74
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB3	10	0.72	0.05	0.74
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	10	0.72	0.06	0.72
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD11	10	0.72	0.02	0.72
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD13	10	0.72	0.02	0.72
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD12	10	0.72	0.02	0.72
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	10	0.72	0.02	0.72
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	10	0.72	0.02	0.72
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG11	10	0.72	0.02	0.72
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG22	10	0.72	0.08	0.71
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG23	10	0.72	0.08	0.71
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG21	10	0.72	0.08	0.71
(1,2560)	1:151:A:SER:H	1:89:A:VAL:HG22	10	0.72	0.08	0.71
(1,2560)	1:151:A:SER:H	1:89:A:VAL:HG23	10	0.72	0.08	0.71
(1,2560)	1:151:A:SER:H	1:89:A:VAL:HG21	10	0.72	0.08	0.71
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	10	0.71	0.03	0.72
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD23	10	0.71	0.12	0.74
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD22	10	0.71	0.12	0.74
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD21	10	0.71	0.12	0.74
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	10	0.71	0.54	0.39
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD23	10	0.71	0.54	0.39
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD21	10	0.71	0.54	0.39
(1,3331)	1:38:A:ALA:H	1:34:A:GLU:HB2	10	0.7	0.04	0.71
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	10	0.7	0.04	0.71
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	10	0.7	0.17	0.72
(1,3004)	1:56:A:LYS:H	1:6:A:LYS:HD2	10	0.7	0.17	0.72
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB2	10	0.7	0.09	0.72
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB1	10	0.7	0.09	0.72
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG21	10	0.7	0.09	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB3	10	0.7	0.09	0.72
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG22	10	0.7	0.09	0.72
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG23	10	0.7	0.09	0.72
(1,2594)	1:28:A:VAL:HG23	1:39:A:GLN:HA	10	0.7	0.08	0.7
(1,2594)	1:28:A:VAL:HG21	1:39:A:GLN:HA	10	0.7	0.08	0.7
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	10	0.7	0.08	0.65
(1,3176)	1:74:A:LYS:H	1:12:A:VAL:HG23	10	0.7	0.08	0.65
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	10	0.7	0.0	0.7
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	10	0.69	0.06	0.68
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	10	0.69	0.06	0.68
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG12	10	0.69	0.05	0.68
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG13	10	0.69	0.05	0.68
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG11	10	0.69	0.05	0.68
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	10	0.69	0.05	0.67
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	10	0.69	0.12	0.69
(1,2675)	1:24:A:ILE:HD13	1:61:A:LYS:HB3	10	0.69	0.05	0.7
(1,2675)	1:24:A:ILE:HD12	1:61:A:LYS:HB3	10	0.69	0.05	0.7
(1,2675)	1:24:A:ILE:HD11	1:61:A:LYS:HB3	10	0.69	0.05	0.7
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG21	10	0.69	0.02	0.68
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG23	10	0.69	0.02	0.68
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG22	10	0.69	0.02	0.68
(1,2642)	1:24:A:ILE:HG22	1:46:A:CYS:H	10	0.69	0.09	0.68
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG21	10	0.69	0.09	0.68
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG23	10	0.69	0.09	0.68
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG22	10	0.69	0.09	0.68
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	10	0.69	0.07	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	10	0.69	0.01	0.69
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD12	10	0.68	0.03	0.68
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD11	10	0.68	0.03	0.68
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD13	10	0.68	0.03	0.68
(1,3138)	1:12:A:VAL:HG13	1:51:A:TYR:HE2	10	0.68	0.03	0.68
(1,3138)	1:12:A:VAL:HG12	1:51:A:TYR:HE2	10	0.68	0.03	0.68
(1,3138)	1:12:A:VAL:HG11	1:51:A:TYR:HE2	10	0.68	0.03	0.68
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG13	10	0.68	0.09	0.68
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG12	10	0.68	0.09	0.68
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG11	10	0.68	0.09	0.68
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	10	0.68	0.4	0.55
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	10	0.68	0.07	0.66
(1,2824)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	10	0.68	0.08	0.65
(1,2824)	1:149:A:VAL:HG13	1:125:A:ASN:HB2	10	0.68	0.08	0.65
(1,2824)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	10	0.68	0.08	0.65
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG21	10	0.67	0.06	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,210)	1:149:A:VAL:HG11	1:123:A:THR:HG23	10	0.67	0.06	0.69
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG23	10	0.67	0.06	0.69
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG22	10	0.67	0.06	0.69
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG22	10	0.67	0.06	0.69
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG23	10	0.67	0.06	0.69
(1,2614)	1:42:A:ALA:HB3	1:39:A:GLN:HG3	10	0.67	0.05	0.66
(1,2614)	1:42:A:ALA:HB2	1:39:A:GLN:HG3	10	0.67	0.05	0.66
(1,2614)	1:42:A:ALA:HB1	1:39:A:GLN:HG3	10	0.67	0.05	0.66
(1,2488)	1:142:A:LYS:HB3	1:91:A:TYR:HD2	10	0.66	0.09	0.67
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	10	0.66	0.09	0.67
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	10	0.66	0.01	0.66
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG21	10	0.66	0.02	0.66
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG22	10	0.66	0.02	0.66
(1,2655)	1:97:A:VAL:HG23	1:134:A:LYS:HB2	10	0.66	0.12	0.64
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HG3	10	0.66	0.12	0.64
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HB2	10	0.66	0.12	0.64
(1,2655)	1:97:A:VAL:HG22	1:134:A:LYS:HB2	10	0.66	0.12	0.64
(1,2603)	1:149:A:VAL:HG23	1:147:A:LEU:HA	10	0.66	0.04	0.64
(1,2603)	1:149:A:VAL:HG22	1:147:A:LEU:HA	10	0.66	0.04	0.64
(1,2603)	1:149:A:VAL:HG21	1:147:A:LEU:HA	10	0.66	0.04	0.64
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	10	0.66	0.04	0.66
(1,2671)	1:24:A:ILE:HD12	1:60:A:VAL:HA	10	0.66	0.07	0.66
(1,2671)	1:24:A:ILE:HD11	1:60:A:VAL:HA	10	0.66	0.07	0.66
(1,2671)	1:24:A:ILE:HD13	1:60:A:VAL:HA	10	0.66	0.07	0.66
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD13	10	0.65	0.09	0.68
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD12	10	0.65	0.09	0.68
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD11	10	0.65	0.09	0.68
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	10	0.65	0.12	0.66
(1,1604)	1:33:A:LEU:HD23	1:51:A:TYR:HA	10	0.65	0.06	0.66
(1,1604)	1:33:A:LEU:HD21	1:51:A:TYR:HA	10	0.65	0.06	0.66
(1,1604)	1:33:A:LEU:HD22	1:51:A:TYR:HA	10	0.65	0.06	0.66
(1,2708)	1:116:A:ASP:HB3	1:115:A:ALA:HB1	10	0.64	0.12	0.64
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	10	0.64	0.12	0.64
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	10	0.64	0.01	0.64
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	10	0.64	0.05	0.63
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD3	10	0.64	0.05	0.63
(1,2653)	1:97:A:VAL:HG21	1:121:A:ILE:H	10	0.64	0.1	0.68
(1,2653)	1:97:A:VAL:HG22	1:121:A:ILE:H	10	0.64	0.1	0.68
(1,2653)	1:97:A:VAL:HG23	1:121:A:ILE:H	10	0.64	0.1	0.68
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB2	10	0.64	0.12	0.64
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB1	10	0.64	0.12	0.64
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB3	10	0.64	0.12	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3133)	1:123:A:THR:HG22	1:150:A:THR:HA	10	0.64	0.06	0.62
(1,3133)	1:123:A:THR:HG21	1:150:A:THR:HA	10	0.64	0.06	0.62
(1,3133)	1:123:A:THR:HG23	1:150:A:THR:HA	10	0.64	0.06	0.62
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG21	10	0.63	0.08	0.63
(1,2613)	1:53:A:ASP:HA	1:33:A:LEU:HD22	10	0.63	0.08	0.63
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG23	10	0.63	0.08	0.63
(1,2613)	1:53:A:ASP:HA	1:33:A:LEU:HD23	10	0.63	0.08	0.63
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	10	0.63	0.03	0.63
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD23	10	0.63	0.04	0.62
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD21	10	0.63	0.04	0.62
(1,3122)	1:7:A:LEU:HD23	1:5:A:ALA:H	10	0.63	0.04	0.62
(1,3122)	1:7:A:LEU:HD22	1:5:A:ALA:H	10	0.63	0.04	0.62
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD22	10	0.63	0.04	0.62
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE2	10	0.63	0.18	0.68
(1,2590)	1:102:A:VAL:HG13	1:17:A:LYS:HE2	10	0.63	0.18	0.68
(1,2590)	1:102:A:VAL:HG12	1:17:A:LYS:HE2	10	0.63	0.18	0.68
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE3	10	0.63	0.18	0.68
(1,2590)	1:102:A:VAL:HG13	1:17:A:LYS:HE3	10	0.63	0.18	0.68
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG21	10	0.62	0.12	0.64
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG22	10	0.62	0.12	0.64
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG23	10	0.62	0.12	0.64
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	10	0.62	0.1	0.63
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG23	10	0.62	0.04	0.62
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG22	10	0.62	0.04	0.62
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG21	10	0.62	0.04	0.62
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	10	0.62	0.15	0.62
(1,2958)	1:86:A:GLU:HB2	1:89:A:VAL:H	10	0.62	0.15	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	10	0.62	0.0	0.62
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD21	10	0.62	0.11	0.59
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD22	10	0.62	0.11	0.59
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD23	10	0.62	0.11	0.59
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	10	0.61	0.01	0.61
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD13	10	0.61	0.05	0.62
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD13	10	0.61	0.05	0.62
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD12	10	0.61	0.05	0.62
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD12	10	0.61	0.05	0.62
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG12	10	0.61	0.06	0.58
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG11	10	0.61	0.06	0.58
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG13	10	0.61	0.06	0.58
(1,3447)	1:50:A:THR:H	1:75:A:THR:HG23	10	0.61	0.06	0.58
(1,2539)	1:70:A:LEU:HD12	1:70:A:LEU:H	10	0.61	0.02	0.61
(1,2539)	1:70:A:LEU:HD11	1:70:A:LEU:H	10	0.61	0.02	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2539)	1:70:A:LEU:HD13	1:70:A:LEU:H	10	0.61	0.02	0.61
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD23	10	0.61	0.07	0.62
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD21	10	0.61	0.07	0.62
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD22	10	0.61	0.07	0.62
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD12	10	0.6	0.05	0.61
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD13	10	0.6	0.05	0.61
(1,404)	1:37:A:ALA:HB1	1:9:A:LEU:HD13	10	0.6	0.05	0.61
(1,404)	1:37:A:ALA:HB3	1:9:A:LEU:HD13	10	0.6	0.05	0.61
(1,404)	1:37:A:ALA:HB1	1:9:A:LEU:HD11	10	0.6	0.05	0.61
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG23	10	0.6	0.06	0.62
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG22	10	0.6	0.06	0.62
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG21	10	0.6	0.06	0.62
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	10	0.6	0.03	0.6
(1,487)	1:24:A:ILE:HG23	1:43:A:VAL:HB	10	0.6	0.03	0.6
(1,487)	1:24:A:ILE:HG22	1:43:A:VAL:HB	10	0.6	0.03	0.6
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	10	0.6	0.09	0.58
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	10	0.6	0.11	0.57
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HG	10	0.6	0.11	0.57
(1,2577)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	10	0.6	0.04	0.6
(1,2577)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	10	0.6	0.04	0.6
(1,416)	1:21:A:ALA:HB3	1:62:A:GLU:HB3	10	0.6	0.07	0.62
(1,416)	1:21:A:ALA:HB1	1:62:A:GLU:HB3	10	0.6	0.07	0.62
(1,416)	1:21:A:ALA:HB2	1:62:A:GLU:HB3	10	0.6	0.07	0.62
(1,284)	1:146:A:VAL:HG21	1:143:A:GLU:HA	10	0.6	0.04	0.6
(1,284)	1:146:A:VAL:HG23	1:143:A:GLU:HA	10	0.6	0.04	0.6
(1,284)	1:146:A:VAL:HG22	1:143:A:GLU:HA	10	0.6	0.04	0.6
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	10	0.6	0.11	0.56
(1,2511)	1:107:A:ALA:HB1	1:85:A:PHE:HZ	10	0.6	0.11	0.56
(1,2529)	1:115:A:ALA:HB1	1:116:A:ASP:HA	10	0.59	0.05	0.6
(1,2529)	1:115:A:ALA:HB2	1:116:A:ASP:HA	10	0.59	0.05	0.6
(1,2529)	1:115:A:ALA:HB3	1:116:A:ASP:HA	10	0.59	0.05	0.6
(1,2640)	1:114:A:ALA:HB2	1:113:A:CYS:HB3	10	0.59	0.06	0.6
(1,2640)	1:114:A:ALA:HB2	1:110:A:GLN:HA	10	0.59	0.06	0.6
(1,2640)	1:114:A:ALA:HB1	1:110:A:GLN:HA	10	0.59	0.06	0.6
(1,2640)	1:114:A:ALA:HB1	1:113:A:CYS:HB3	10	0.59	0.06	0.6
(1,2640)	1:114:A:ALA:HB3	1:110:A:GLN:HA	10	0.59	0.06	0.6
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG11	10	0.59	0.03	0.58
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG13	10	0.59	0.03	0.58
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG12	10	0.59	0.03	0.58
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG11	10	0.59	0.03	0.58
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG13	10	0.59	0.03	0.58
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG12	10	0.59	0.04	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG11	10	0.59	0.04	0.6
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG13	10	0.59	0.04	0.6
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG22	10	0.59	0.03	0.58
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG21	10	0.59	0.03	0.58
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG23	10	0.59	0.03	0.58
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	10	0.58	0.03	0.58
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG22	10	0.58	0.05	0.6
(1,1664)	1:89:A:VAL:HG12	1:123:A:THR:HG21	10	0.58	0.05	0.6
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG21	10	0.58	0.05	0.6
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG23	10	0.58	0.05	0.6
(1,1664)	1:89:A:VAL:HG13	1:123:A:THR:HG23	10	0.58	0.05	0.6
(1,1664)	1:89:A:VAL:HG13	1:123:A:THR:HG21	10	0.58	0.05	0.6
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	10	0.58	0.06	0.6
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB3	10	0.58	0.1	0.57
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB1	10	0.58	0.1	0.57
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB2	10	0.58	0.1	0.57
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	10	0.58	0.05	0.57
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD22	10	0.57	0.02	0.57
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD23	10	0.57	0.02	0.57
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD21	10	0.57	0.02	0.57
(1,269)	1:75:A:THR:HG21	1:77:A:SER:H	10	0.57	0.05	0.56
(1,269)	1:75:A:THR:HG23	1:77:A:SER:H	10	0.57	0.05	0.56
(1,269)	1:75:A:THR:HG22	1:77:A:SER:H	10	0.57	0.05	0.56
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG22	10	0.57	0.05	0.56
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG21	10	0.57	0.05	0.56
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG23	10	0.57	0.05	0.56
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	10	0.57	0.04	0.59
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	10	0.57	0.05	0.57
(1,2969)	1:92:A:GLU:HB2	1:93:A:GLY:HA2	10	0.57	0.05	0.57
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	10	0.56	0.07	0.56
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	10	0.56	0.15	0.63
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG22	10	0.56	0.06	0.54
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG23	10	0.56	0.06	0.54
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG21	10	0.56	0.06	0.54
(1,2932)	1:146:A:VAL:H	1:143:A:GLU:HB3	10	0.56	0.06	0.58
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	10	0.56	0.06	0.58
(1,335)	1:149:A:VAL:HG23	1:149:A:VAL:HA	10	0.56	0.01	0.56
(1,335)	1:149:A:VAL:HG22	1:149:A:VAL:HA	10	0.56	0.01	0.56
(1,335)	1:149:A:VAL:HG21	1:149:A:VAL:HA	10	0.56	0.01	0.56
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	10	0.55	0.03	0.55
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	10	0.55	0.12	0.58
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	10	0.55	0.05	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2690)	1:94:A:ALA:HA	1:134:A:LYS:HB3	10	0.55	0.05	0.54
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG22	10	0.55	0.03	0.56
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG21	10	0.55	0.03	0.56
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG23	10	0.55	0.03	0.56
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	10	0.55	0.05	0.55
(1,328)	1:100:A:ALA:HB2	1:101:A:MET:HA	10	0.55	0.05	0.55
(1,328)	1:100:A:ALA:HB1	1:101:A:MET:HA	10	0.55	0.05	0.55
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	10	0.55	0.16	0.52
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	10	0.55	0.01	0.55
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD22	10	0.55	0.14	0.6
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD21	10	0.55	0.14	0.6
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD23	10	0.55	0.14	0.6
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG13	10	0.54	0.04	0.56
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG12	10	0.54	0.04	0.56
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG11	10	0.54	0.04	0.56
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	10	0.54	0.06	0.54
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	10	0.54	0.09	0.55
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG3	10	0.54	0.09	0.55
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	10	0.54	0.05	0.56
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	10	0.53	0.03	0.54
(1,495)	1:94:A:ALA:HB2	1:134:A:LYS:HA	10	0.53	0.1	0.5
(1,495)	1:94:A:ALA:HB1	1:134:A:LYS:HA	10	0.53	0.1	0.5
(1,495)	1:94:A:ALA:HB3	1:134:A:LYS:HA	10	0.53	0.1	0.5
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	10	0.53	0.05	0.52
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	10	0.53	0.05	0.52
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG11	10	0.53	0.05	0.52
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	10	0.53	0.13	0.63
(1,486)	1:24:A:ILE:HG22	1:60:A:VAL:HB	10	0.53	0.02	0.53
(1,486)	1:24:A:ILE:HG21	1:60:A:VAL:HB	10	0.53	0.02	0.53
(1,486)	1:24:A:ILE:HG23	1:60:A:VAL:HB	10	0.53	0.02	0.53
(1,2624)	1:37:A:ALA:HB2	1:36:A:CYS:HB3	10	0.52	0.03	0.52
(1,2624)	1:37:A:ALA:HB3	1:36:A:CYS:HB3	10	0.52	0.03	0.52
(1,2624)	1:37:A:ALA:HB1	1:36:A:CYS:HB3	10	0.52	0.03	0.52
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	10	0.52	0.09	0.54
(1,288)	1:146:A:VAL:HG22	1:143:A:GLU:HG3	10	0.52	0.08	0.54
(1,288)	1:146:A:VAL:HG21	1:143:A:GLU:HG3	10	0.52	0.08	0.54
(1,288)	1:146:A:VAL:HG23	1:143:A:GLU:HG3	10	0.52	0.08	0.54
(1,2952)	1:101:A:MET:HG3	1:103:A:THR:HA	10	0.52	0.04	0.52
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	10	0.52	0.04	0.52
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD13	10	0.52	0.03	0.52
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD12	10	0.52	0.03	0.52
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD11	10	0.52	0.03	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	10	0.52	0.0	0.52
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG23	10	0.52	0.05	0.5
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG22	10	0.52	0.05	0.5
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG21	10	0.52	0.05	0.5
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	10	0.52	0.01	0.52
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB3	10	0.52	0.04	0.52
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB1	10	0.52	0.04	0.52
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB2	10	0.52	0.04	0.52
(1,2848)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	10	0.52	0.06	0.5
(1,2848)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	10	0.52	0.06	0.5
(1,2848)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	10	0.52	0.06	0.5
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	10	0.51	0.05	0.51
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG21	10	0.51	0.05	0.51
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG23	10	0.51	0.05	0.51
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG22	10	0.51	0.05	0.51
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	10	0.51	0.01	0.51
(1,2907)	1:110:A:GLN:HG2	1:77:A:SER:HB2	10	0.51	0.07	0.52
(1,2907)	1:84:A:CYS:HB3	1:154:A:LYS:HB3	10	0.51	0.07	0.52
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	10	0.51	0.21	0.44
(1,3520)	1:39:A:GLN:HE22	1:60:A:VAL:HG13	10	0.51	0.21	0.44
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	10	0.51	0.21	0.44
(1,3520)	1:39:A:GLN:HE22	1:60:A:VAL:HG11	10	0.51	0.21	0.44
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB1	10	0.51	0.03	0.5
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB2	10	0.51	0.03	0.5
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB3	10	0.51	0.03	0.5
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG22	10	0.51	0.04	0.52
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG23	10	0.51	0.04	0.52
(1,2825)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	10	0.5	0.05	0.51
(1,2825)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	10	0.5	0.05	0.51
(1,2825)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	10	0.5	0.05	0.51
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	10	0.5	0.04	0.51
(1,396)	1:107:A:ALA:HB2	1:77:A:SER:HB2	10	0.5	0.18	0.46
(1,396)	1:107:A:ALA:HB1	1:77:A:SER:HB2	10	0.5	0.18	0.46
(1,396)	1:107:A:ALA:HB3	1:77:A:SER:HB2	10	0.5	0.18	0.46
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	10	0.5	0.04	0.5
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG23	10	0.5	0.04	0.49
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG21	10	0.5	0.04	0.49
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG22	10	0.5	0.04	0.49
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD21	10	0.5	0.14	0.53
(1,3155)	1:70:A:LEU:HD21	1:17:A:LYS:H	10	0.5	0.14	0.53
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD23	10	0.5	0.14	0.53
(1,3155)	1:70:A:LEU:HD22	1:17:A:LYS:H	10	0.5	0.14	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD22	10	0.5	0.14	0.53
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG21	10	0.49	0.13	0.5
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG22	10	0.49	0.13	0.5
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG23	10	0.49	0.13	0.5
(1,3094)	1:76:A:ALA:HB3	1:77:A:SER:HB3	10	0.49	0.08	0.48
(1,3094)	1:76:A:ALA:HB1	1:77:A:SER:HB3	10	0.49	0.08	0.48
(1,3094)	1:76:A:ALA:HB2	1:77:A:SER:HB3	10	0.49	0.08	0.48
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	10	0.49	0.15	0.49
(1,2665)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	10	0.49	0.07	0.48
(1,2665)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	10	0.49	0.07	0.48
(1,2665)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	10	0.49	0.07	0.48
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	10	0.48	0.04	0.48
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	10	0.48	0.02	0.48
(1,1018)	1:121:A:ILE:HG21	1:120:A:GLU:HG3	10	0.48	0.05	0.48
(1,1018)	1:120:A:GLU:HG3	1:121:A:ILE:HG22	10	0.48	0.05	0.48
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB2	10	0.48	0.1	0.5
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB3	10	0.48	0.1	0.5
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB1	10	0.48	0.1	0.5
(1,1542)	1:76:A:ALA:HB1	1:75:A:THR:HA	10	0.48	0.04	0.47
(1,1542)	1:76:A:ALA:HB2	1:75:A:THR:HA	10	0.48	0.04	0.47
(1,1542)	1:76:A:ALA:HB3	1:75:A:THR:HA	10	0.48	0.04	0.47
(1,331)	1:149:A:VAL:HG23	1:146:A:VAL:H	10	0.47	0.04	0.46
(1,331)	1:149:A:VAL:HG22	1:146:A:VAL:H	10	0.47	0.04	0.46
(1,331)	1:149:A:VAL:HG21	1:146:A:VAL:H	10	0.47	0.04	0.46
(1,2615)	1:42:A:ALA:HB3	1:43:A:VAL:HB	10	0.47	0.03	0.48
(1,2615)	1:42:A:ALA:HB2	1:43:A:VAL:HB	10	0.47	0.03	0.48
(1,2615)	1:42:A:ALA:HB1	1:43:A:VAL:HB	10	0.47	0.03	0.48
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	10	0.47	0.08	0.46
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	10	0.47	0.14	0.48
(1,3496)	1:135:A:GLY:H	1:97:A:VAL:HB	10	0.47	0.14	0.48
(1,3496)	1:135:A:GLY:H	1:95:A:PRO:HB3	10	0.47	0.14	0.48
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	10	0.47	0.01	0.46
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD23	10	0.47	0.01	0.46
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD21	10	0.47	0.01	0.46
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG22	10	0.46	0.12	0.43
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG21	10	0.46	0.12	0.43
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG23	10	0.46	0.12	0.43
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	10	0.46	0.04	0.46
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	10	0.46	0.02	0.46
(1,3493)	1:129:A:GLN:HE21	1:128:A:ASP:HB3	10	0.46	0.13	0.46
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	10	0.46	0.13	0.46
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD23	10	0.46	0.04	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD21	10	0.46	0.04	0.45
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD22	10	0.46	0.04	0.45
(1,167)	1:150:A:THR:HG23	1:85:A:PHE:HB2	10	0.46	0.09	0.46
(1,167)	1:150:A:THR:HG21	1:85:A:PHE:HB2	10	0.46	0.09	0.46
(1,167)	1:150:A:THR:HG22	1:85:A:PHE:HB2	10	0.46	0.09	0.46
(1,2817)	1:56:A:LYS:H	1:54:A:ASP:HB3	10	0.46	0.03	0.45
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	10	0.46	0.03	0.45
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	10	0.45	0.08	0.45
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD22	10	0.45	0.06	0.44
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD23	10	0.45	0.06	0.44
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD21	10	0.45	0.06	0.44
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	10	0.45	0.04	0.44
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD11	10	0.45	0.07	0.46
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD13	10	0.45	0.07	0.46
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD12	10	0.45	0.07	0.46
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG22	10	0.45	0.09	0.48
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG23	10	0.45	0.09	0.48
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG21	10	0.45	0.09	0.48
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	10	0.44	0.07	0.44
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG22	10	0.44	0.02	0.45
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG23	10	0.44	0.02	0.45
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG21	10	0.44	0.02	0.45
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG22	10	0.44	0.09	0.46
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG21	10	0.44	0.09	0.46
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD13	10	0.44	0.04	0.44
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD11	10	0.44	0.04	0.44
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD12	10	0.44	0.04	0.44
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	10	0.44	0.12	0.44
(1,2866)	1:159:A:GLU:HG3	1:156:A:PHE:HD2	10	0.44	0.12	0.44
(1,2866)	1:159:A:GLU:HG3	1:156:A:PHE:HD1	10	0.44	0.12	0.44
(1,2831)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	10	0.44	0.04	0.44
(1,2831)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	10	0.44	0.04	0.44
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG23	10	0.44	0.05	0.42
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG21	10	0.44	0.05	0.42
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG22	10	0.44	0.05	0.42
(1,165)	1:150:A:THR:HG21	1:123:A:THR:HA	10	0.43	0.04	0.42
(1,165)	1:150:A:THR:HG22	1:123:A:THR:HA	10	0.43	0.04	0.42
(1,165)	1:150:A:THR:HG23	1:123:A:THR:HA	10	0.43	0.04	0.42
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	10	0.43	0.04	0.42
(1,2548)	1:31:A:VAL:HG13	1:30:A:ASP:HA	10	0.43	0.04	0.42
(1,2548)	1:31:A:VAL:HG11	1:30:A:ASP:HA	10	0.43	0.04	0.42
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	10	0.43	0.06	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD13	10	0.43	0.07	0.44
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD11	10	0.43	0.07	0.44
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD12	10	0.43	0.07	0.44
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD13	10	0.43	0.07	0.44
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD11	10	0.43	0.07	0.44
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	10	0.43	0.01	0.43
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB1	10	0.43	0.03	0.43
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB2	10	0.43	0.03	0.43
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB3	10	0.43	0.03	0.43
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG12	10	0.43	0.04	0.42
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG13	10	0.43	0.04	0.42
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG11	10	0.43	0.04	0.42
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE3	10	0.43	0.13	0.47
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE2	10	0.43	0.13	0.47
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	10	0.43	0.07	0.46
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD23	10	0.43	0.07	0.46
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD22	10	0.43	0.07	0.46
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG3	10	0.43	0.02	0.42
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	10	0.43	0.02	0.42
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	10	0.42	0.04	0.43
(1,2867)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	10	0.42	0.02	0.42
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	10	0.42	0.02	0.42
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	10	0.42	0.19	0.4
(1,3339)	1:156:A:PHE:H	1:155:A:GLN:HG3	10	0.42	0.19	0.4
(1,2719)	1:25:A:GLY:HA2	1:26:A:GLU:HB3	10	0.42	0.09	0.4
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	10	0.42	0.09	0.4
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB3	10	0.42	0.09	0.4
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG21	10	0.42	0.03	0.42
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG22	10	0.42	0.03	0.42
(1,282)	1:146:A:VAL:HG21	1:88:A:HIS:HA	10	0.42	0.06	0.42
(1,282)	1:146:A:VAL:HG23	1:88:A:HIS:HA	10	0.42	0.06	0.42
(1,282)	1:146:A:VAL:HG22	1:88:A:HIS:HA	10	0.42	0.06	0.42
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	10	0.42	0.13	0.48
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	10	0.42	0.04	0.42
(1,2643)	1:31:A:VAL:HG22	1:57:A:MET:HA	10	0.42	0.09	0.43
(1,2643)	1:31:A:VAL:HG21	1:57:A:MET:HA	10	0.42	0.09	0.43
(1,2643)	1:31:A:VAL:HG23	1:57:A:MET:HA	10	0.42	0.09	0.43
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	10	0.41	0.12	0.37
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD2	10	0.41	0.12	0.37
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG11	10	0.41	0.16	0.48
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG13	10	0.41	0.16	0.48
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG12	10	0.41	0.16	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG23	10	0.41	0.04	0.4
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG21	10	0.41	0.04	0.4
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB1	10	0.41	0.01	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB3	10	0.41	0.01	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB2	10	0.41	0.01	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG21	10	0.41	0.02	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG23	10	0.41	0.02	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG22	10	0.41	0.02	0.41
(1,411)	1:21:A:ALA:HB1	1:48:A:HIS:HD2	10	0.41	0.06	0.42
(1,411)	1:21:A:ALA:HB2	1:48:A:HIS:HD2	10	0.41	0.06	0.42
(1,411)	1:21:A:ALA:HB3	1:48:A:HIS:HD2	10	0.41	0.06	0.42
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD13	10	0.4	0.09	0.41
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	10	0.4	0.09	0.41
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD12	10	0.4	0.09	0.41
(1,386)	1:112:A:ALA:HB1	1:114:A:ALA:H	10	0.4	0.04	0.4
(1,386)	1:112:A:ALA:HB3	1:114:A:ALA:H	10	0.4	0.04	0.4
(1,386)	1:112:A:ALA:HB2	1:114:A:ALA:H	10	0.4	0.04	0.4
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	10	0.4	0.08	0.39
(1,2992)	1:16:A:ASN:H	1:13:A:HIS:HB3	10	0.4	0.08	0.39
(1,2558)	1:149:A:VAL:HG11	1:126:A:GLU:H	10	0.4	0.08	0.43
(1,2558)	1:149:A:VAL:HG13	1:126:A:GLU:H	10	0.4	0.08	0.43
(1,2558)	1:149:A:VAL:HG12	1:126:A:GLU:H	10	0.4	0.08	0.43
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG22	10	0.4	0.03	0.4
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG21	10	0.4	0.03	0.4
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG23	10	0.4	0.03	0.4
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	10	0.4	0.09	0.38
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HB3	10	0.4	0.12	0.45
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	10	0.4	0.12	0.45
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG2	10	0.4	0.12	0.45
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	10	0.4	0.05	0.41
(1,2967)	1:159:A:GLU:HB3	1:156:A:PHE:HD2	10	0.4	0.05	0.41
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG23	10	0.4	0.04	0.39
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG22	10	0.4	0.04	0.39
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG21	10	0.4	0.04	0.39
(1,488)	1:24:A:ILE:HG23	1:62:A:GLU:HG2	10	0.39	0.03	0.39
(1,488)	1:24:A:ILE:HG22	1:62:A:GLU:HG2	10	0.39	0.03	0.39
(1,488)	1:24:A:ILE:HG21	1:62:A:GLU:HG2	10	0.39	0.03	0.39
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	10	0.39	0.02	0.4
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD11	10	0.39	0.07	0.4
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD13	10	0.39	0.07	0.4
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD12	10	0.39	0.07	0.4
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	10	0.39	0.01	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD11	10	0.39	0.07	0.38
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD13	10	0.39	0.07	0.38
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD12	10	0.39	0.07	0.38
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	10	0.39	0.05	0.38
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	10	0.39	0.08	0.39
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG11	10	0.39	0.04	0.39
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG13	10	0.39	0.04	0.39
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG12	10	0.39	0.04	0.39
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	10	0.39	0.06	0.4
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB1	10	0.39	0.11	0.4
(1,2503)	1:85:A:PHE:HE1	1:110:A:GLN:HG2	10	0.39	0.11	0.4
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB3	10	0.39	0.11	0.4
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB2	10	0.39	0.11	0.4
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	10	0.39	0.09	0.36
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD13	10	0.38	0.06	0.38
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD11	10	0.38	0.06	0.38
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD12	10	0.38	0.06	0.38
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	10	0.38	0.05	0.38
(1,2714)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	10	0.38	0.06	0.37
(1,2714)	1:149:A:VAL:HG12	1:148:A:GLY:HA2	10	0.38	0.06	0.37
(1,2714)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	10	0.38	0.06	0.37
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	10	0.38	0.07	0.38
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD22	10	0.38	0.07	0.38
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD23	10	0.38	0.07	0.38
(1,3166)	1:131:A:CYS:HA	1:130:A:LYS:HG2	10	0.38	0.08	0.36
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG21	10	0.38	0.08	0.36
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG22	10	0.38	0.08	0.36
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG23	10	0.38	0.08	0.36
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG3	10	0.38	0.02	0.38
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	10	0.38	0.02	0.38
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	10	0.37	0.05	0.38
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD22	10	0.37	0.05	0.38
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD23	10	0.37	0.05	0.38
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	10	0.37	0.13	0.36
(1,1673)	1:147:A:LEU:HD22	1:147:A:LEU:HD12	10	0.37	0.01	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD11	10	0.37	0.01	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD12	10	0.37	0.01	0.38
(1,1673)	1:147:A:LEU:HD22	1:147:A:LEU:HD13	10	0.37	0.01	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD13	10	0.37	0.01	0.38
(1,1673)	1:147:A:LEU:HD21	1:147:A:LEU:HD13	10	0.37	0.01	0.38
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD12	10	0.37	0.02	0.36
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD11	10	0.37	0.02	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD13	10	0.37	0.02	0.36
(1,2639)	1:114:A:ALA:HB3	1:156:A:PHE:HE2	10	0.37	0.14	0.32
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB3	10	0.37	0.14	0.32
(1,2639)	1:114:A:ALA:HB2	1:156:A:PHE:HE2	10	0.37	0.14	0.32
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB2	10	0.37	0.14	0.32
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	10	0.37	0.11	0.43
(1,499)	1:94:A:ALA:HB3	1:138:A:PHE:HB2	10	0.37	0.04	0.36
(1,499)	1:94:A:ALA:HB2	1:138:A:PHE:HB2	10	0.37	0.04	0.36
(1,499)	1:94:A:ALA:HB1	1:138:A:PHE:HB2	10	0.37	0.04	0.36
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	10	0.37	0.07	0.38
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB1	10	0.37	0.07	0.38
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB3	10	0.37	0.07	0.38
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB3	10	0.36	0.04	0.36
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB2	10	0.36	0.04	0.36
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB1	10	0.36	0.04	0.36
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	10	0.36	0.09	0.37
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD13	10	0.36	0.07	0.38
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	10	0.36	0.07	0.38
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD11	10	0.36	0.07	0.38
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	10	0.36	0.07	0.34
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG2	10	0.36	0.11	0.35
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	10	0.36	0.11	0.35
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	10	0.36	0.06	0.36
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	10	0.36	0.09	0.36
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB3	10	0.36	0.08	0.36
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB2	10	0.36	0.08	0.36
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB1	10	0.36	0.08	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG12	10	0.36	0.03	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG11	10	0.36	0.03	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG13	10	0.36	0.03	0.36
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	10	0.36	0.08	0.38
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	10	0.35	0.05	0.37
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	10	0.35	0.05	0.37
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG13	10	0.35	0.05	0.37
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	10	0.35	0.07	0.36
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	10	0.35	0.14	0.34
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	10	0.35	0.01	0.35
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	10	0.35	0.04	0.34
(1,2805)	1:10:A:SER:H	1:9:A:LEU:HB2	10	0.35	0.04	0.34
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	10	0.35	0.0	0.35
(1,304)	1:75:A:THR:H	1:75:A:THR:HG21	10	0.35	0.08	0.32
(1,304)	1:75:A:THR:H	1:75:A:THR:HG23	10	0.35	0.08	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,304)	1:75:A:THR:H	1:75:A:THR:HG22	10	0.35	0.08	0.32
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	10	0.35	0.08	0.37
(1,456)	1:38:A:ALA:HB3	1:35:A:GLN:HG3	10	0.34	0.08	0.34
(1,456)	1:38:A:ALA:HB2	1:35:A:GLN:HG3	10	0.34	0.08	0.34
(1,456)	1:38:A:ALA:HB1	1:35:A:GLN:HG3	10	0.34	0.08	0.34
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	10	0.34	0.04	0.34
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	10	0.34	0.03	0.33
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB1	10	0.34	0.03	0.33
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB3	10	0.34	0.03	0.33
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	10	0.34	0.02	0.35
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	10	0.34	0.05	0.32
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	10	0.34	0.06	0.34
(1,1000)	1:112:A:ALA:HB1	1:109:A:CYS:HB2	10	0.34	0.06	0.36
(1,1000)	1:112:A:ALA:HB3	1:109:A:CYS:HB2	10	0.34	0.06	0.36
(1,1000)	1:112:A:ALA:HB2	1:109:A:CYS:HB2	10	0.34	0.06	0.36
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	10	0.34	0.09	0.36
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	10	0.34	0.04	0.34
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	10	0.34	0.07	0.36
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG21	10	0.33	0.16	0.34
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG23	10	0.33	0.16	0.34
(1,188)	1:67:A:LEU:HD22	1:75:A:THR:HG22	10	0.33	0.16	0.34
(1,188)	1:67:A:LEU:HD22	1:75:A:THR:HG23	10	0.33	0.16	0.34
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG22	10	0.33	0.16	0.34
(1,188)	1:67:A:LEU:HD21	1:75:A:THR:HG23	10	0.33	0.16	0.34
(1,2566)	1:103:A:THR:HG22	1:102:A:VAL:HA	10	0.33	0.1	0.3
(1,2566)	1:103:A:THR:HG21	1:102:A:VAL:HA	10	0.33	0.1	0.3
(1,2566)	1:103:A:THR:HG23	1:102:A:VAL:HA	10	0.33	0.1	0.3
(1,2834)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	10	0.33	0.05	0.34
(1,2834)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	10	0.33	0.05	0.34
(1,2834)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	10	0.33	0.05	0.34
(1,228)	1:89:A:VAL:HG22	1:142:A:LYS:HA	10	0.33	0.09	0.32
(1,228)	1:89:A:VAL:HG23	1:142:A:LYS:HA	10	0.33	0.09	0.32
(1,228)	1:89:A:VAL:HG21	1:142:A:LYS:HA	10	0.33	0.09	0.32
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD11	10	0.33	0.05	0.32
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD12	10	0.33	0.05	0.32
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD13	10	0.33	0.05	0.32
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	10	0.33	0.05	0.34
(1,176)	1:31:A:VAL:HG12	1:58:A:CYS:HB2	10	0.33	0.05	0.34
(1,176)	1:31:A:VAL:HG13	1:58:A:CYS:HB2	10	0.33	0.05	0.34
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	10	0.33	0.13	0.26
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	10	0.33	0.15	0.32
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD23	10	0.32	0.05	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD12	10	0.32	0.05	0.34
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.32	0.05	0.34
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD11	10	0.32	0.05	0.34
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	10	0.32	0.01	0.32
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB1	10	0.32	0.03	0.31
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB3	10	0.32	0.03	0.31
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB2	10	0.32	0.03	0.31
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	10	0.32	0.01	0.32
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG21	10	0.32	0.04	0.32
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG23	10	0.32	0.04	0.32
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG22	10	0.32	0.04	0.32
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD13	10	0.32	0.02	0.32
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD12	10	0.32	0.02	0.32
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD11	10	0.32	0.02	0.32
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	10	0.32	0.05	0.32
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	10	0.32	0.1	0.3
(1,290)	1:102:A:VAL:HG23	1:131:A:CYS:H	10	0.32	0.1	0.3
(1,290)	1:102:A:VAL:HG21	1:131:A:CYS:H	10	0.32	0.1	0.3
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	10	0.32	0.08	0.32
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	10	0.32	0.04	0.31
(1,2757)	1:97:A:VAL:H	1:133:A:PHE:HB3	10	0.32	0.04	0.31
(1,415)	1:21:A:ALA:HB2	1:66:A:ASP:HB2	10	0.31	0.04	0.32
(1,415)	1:21:A:ALA:HB3	1:66:A:ASP:HB2	10	0.31	0.04	0.32
(1,415)	1:21:A:ALA:HB1	1:66:A:ASP:HB2	10	0.31	0.04	0.32
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	10	0.31	0.04	0.32
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	10	0.31	0.03	0.31
(1,1075)	1:31:A:VAL:HG21	1:36:A:CYS:HB3	10	0.31	0.03	0.32
(1,1075)	1:31:A:VAL:HG23	1:36:A:CYS:HB3	10	0.31	0.03	0.32
(1,1075)	1:31:A:VAL:HG22	1:36:A:CYS:HB3	10	0.31	0.03	0.32
(1,3137)	1:12:A:VAL:HG12	1:11:A:CYS:H	10	0.31	0.03	0.3
(1,3137)	1:12:A:VAL:HG11	1:11:A:CYS:H	10	0.31	0.03	0.3
(1,3137)	1:12:A:VAL:HG13	1:11:A:CYS:H	10	0.31	0.03	0.3
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	10	0.31	0.04	0.32
(1,408)	1:140:A:ALA:HB3	1:140:A:ALA:HA	10	0.31	0.01	0.31
(1,408)	1:140:A:ALA:HB1	1:140:A:ALA:HA	10	0.31	0.01	0.31
(1,408)	1:140:A:ALA:HB2	1:140:A:ALA:HA	10	0.31	0.01	0.31
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	10	0.31	0.08	0.28
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	10	0.3	0.09	0.34
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	10	0.3	0.04	0.3
(1,3097)	1:67:A:LEU:HD12	1:102:A:VAL:H	10	0.3	0.11	0.28
(1,3097)	1:67:A:LEU:HD11	1:102:A:VAL:H	10	0.3	0.11	0.28
(1,3097)	1:67:A:LEU:HD13	1:102:A:VAL:H	10	0.3	0.11	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG21	10	0.3	0.06	0.29
(1,342)	1:149:A:VAL:HG23	1:123:A:THR:HG23	10	0.3	0.06	0.29
(1,342)	1:149:A:VAL:HG22	1:123:A:THR:HG23	10	0.3	0.06	0.29
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG22	10	0.3	0.06	0.29
(1,342)	1:149:A:VAL:HG23	1:123:A:THR:HG22	10	0.3	0.06	0.29
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG23	10	0.3	0.06	0.29
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	10	0.3	0.07	0.3
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG11	10	0.3	0.07	0.3
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG13	10	0.3	0.07	0.3
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	10	0.3	0.05	0.31
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	10	0.3	0.07	0.31
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	10	0.3	0.04	0.31
(1,1541)	1:76:A:ALA:HB1	1:51:A:TYR:HE2	10	0.3	0.08	0.27
(1,1541)	1:76:A:ALA:HB2	1:51:A:TYR:HE2	10	0.3	0.08	0.27
(1,1541)	1:76:A:ALA:HB3	1:51:A:TYR:HE2	10	0.3	0.08	0.27
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	10	0.3	0.02	0.3
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB3	10	0.3	0.02	0.3
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	10	0.3	0.08	0.28
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	10	0.3	0.01	0.3
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	10	0.29	0.06	0.3
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	10	0.29	0.08	0.32
(1,2656)	1:156:A:PHE:H	1:155:A:GLN:HA	10	0.29	0.08	0.32
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD12	10	0.29	0.01	0.29
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD11	10	0.29	0.01	0.29
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	10	0.29	0.01	0.29
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	10	0.29	0.08	0.32
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG21	10	0.29	0.03	0.3
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG22	10	0.29	0.03	0.3
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG23	10	0.29	0.03	0.3
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB1	10	0.29	0.0	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB3	10	0.29	0.0	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB2	10	0.29	0.0	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	10	0.29	0.0	0.29
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	10	0.29	0.04	0.29
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	10	0.29	0.08	0.26
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	10	0.29	0.05	0.28
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	10	0.28	0.02	0.29
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB1	10	0.28	0.03	0.29
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB2	10	0.28	0.03	0.29
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB3	10	0.28	0.03	0.29
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG11	10	0.28	0.02	0.29
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG13	10	0.28	0.02	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG12	10	0.28	0.02	0.29
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	10	0.28	0.01	0.29
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	10	0.28	0.09	0.26
(1,2916)	1:134:A:LYS:HB3	1:138:A:PHE:H	10	0.28	0.09	0.26
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG12	10	0.28	0.02	0.28
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG11	10	0.28	0.02	0.28
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG13	10	0.28	0.02	0.28
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	10	0.28	0.08	0.28
(1,3187)	1:76:A:ALA:H	1:13:A:HIS:HB2	10	0.28	0.08	0.28
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	10	0.28	0.09	0.3
(1,741)	1:41:A:LYS:HE3	1:38:A:ALA:HA	10	0.28	0.09	0.3
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	10	0.28	0.03	0.28
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	10	0.28	0.02	0.29
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	10	0.28	0.03	0.28
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	10	0.28	0.01	0.28
(1,1156)	1:102:A:VAL:HG11	1:102:A:VAL:HB	10	0.28	0.01	0.28
(1,1156)	1:102:A:VAL:HG13	1:102:A:VAL:HB	10	0.28	0.01	0.28
(1,1156)	1:102:A:VAL:HG12	1:102:A:VAL:HB	10	0.28	0.01	0.28
(1,1156)	1:102:A:VAL:HG23	1:102:A:VAL:HB	10	0.28	0.01	0.28
(1,2673)	1:24:A:ILE:HD13	1:62:A:GLU:HG3	10	0.28	0.02	0.28
(1,2673)	1:24:A:ILE:HD12	1:62:A:GLU:HG3	10	0.28	0.02	0.28
(1,2673)	1:24:A:ILE:HD11	1:62:A:GLU:HG3	10	0.28	0.02	0.28
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	10	0.27	0.23	0.21
(1,3164)	1:75:A:THR:HG22	1:19:A:SER:HA	10	0.27	0.06	0.3
(1,3164)	1:75:A:THR:HG21	1:19:A:SER:HA	10	0.27	0.06	0.3
(1,3164)	1:75:A:THR:HG23	1:19:A:SER:HA	10	0.27	0.06	0.3
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	10	0.27	0.05	0.28
(1,2760)	1:18:A:GLY:HA2	1:19:A:SER:HA	10	0.27	0.05	0.28
(1,235)	1:103:A:THR:HG21	1:124:A:TYR:HD2	10	0.27	0.09	0.26
(1,235)	1:103:A:THR:HG23	1:124:A:TYR:HD2	10	0.27	0.09	0.26
(1,235)	1:103:A:THR:HG22	1:124:A:TYR:HD2	10	0.27	0.09	0.26
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	10	0.27	0.08	0.29
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	10	0.27	0.02	0.26
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG23	10	0.27	0.01	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG22	10	0.27	0.01	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG21	10	0.27	0.01	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG13	10	0.27	0.03	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG12	10	0.27	0.03	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG11	10	0.27	0.03	0.27
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	10	0.26	0.05	0.26
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	10	0.26	0.04	0.27
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG21	10	0.26	0.02	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG23	10	0.26	0.02	0.27
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG22	10	0.26	0.02	0.27
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG21	10	0.26	0.05	0.27
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG22	10	0.26	0.05	0.27
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG23	10	0.26	0.05	0.27
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	10	0.26	0.01	0.26
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	10	0.26	0.02	0.26
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG22	10	0.26	0.05	0.27
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG21	10	0.26	0.05	0.27
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG23	10	0.26	0.05	0.27
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	10	0.26	0.02	0.26
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	10	0.26	0.02	0.26
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG11	10	0.26	0.02	0.26
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	10	0.26	0.02	0.26
(1,240)	1:28:A:VAL:HG11	1:29:A:PRO:HD2	10	0.26	0.02	0.26
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB3	10	0.26	0.02	0.26
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB2	10	0.26	0.02	0.26
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB1	10	0.26	0.02	0.26
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB1	10	0.26	0.04	0.27
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB2	10	0.26	0.04	0.27
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB3	10	0.26	0.04	0.27
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB3	10	0.26	0.01	0.26
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB2	10	0.26	0.01	0.26
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB1	10	0.26	0.01	0.26
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	10	0.26	0.07	0.24
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	10	0.26	0.02	0.26
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB1	10	0.25	0.06	0.25
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB3	10	0.25	0.06	0.25
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB2	10	0.25	0.06	0.25
(1,2567)	1:43:A:VAL:HG12	1:43:A:VAL:HB	10	0.25	0.01	0.25
(1,2567)	1:43:A:VAL:HG11	1:43:A:VAL:HB	10	0.25	0.01	0.25
(1,2567)	1:43:A:VAL:HG13	1:43:A:VAL:HB	10	0.25	0.01	0.25
(1,2567)	1:12:A:VAL:HG21	1:12:A:VAL:HB	10	0.25	0.01	0.25
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD12	10	0.25	0.01	0.26
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD11	10	0.25	0.01	0.26
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD13	10	0.25	0.01	0.26
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	10	0.25	0.0	0.25
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG13	10	0.25	0.03	0.24
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG12	10	0.25	0.03	0.24
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG11	10	0.25	0.03	0.24
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	10	0.25	0.01	0.25
(1,356)	1:115:A:ALA:HB1	1:116:A:ASP:HA	10	0.25	0.05	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,356)	1:115:A:ALA:HB2	1:116:A:ASP:HA	10	0.25	0.05	0.26
(1,356)	1:115:A:ALA:HB3	1:116:A:ASP:HA	10	0.25	0.05	0.26
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	10	0.25	0.01	0.24
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG12	10	0.25	0.01	0.24
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	10	0.25	0.04	0.24
(1,2692)	1:153:A:PRO:HD3	1:152:A:GLY:HA3	10	0.25	0.06	0.26
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	10	0.25	0.06	0.26
(1,3000)	1:64:A:LYS:HD2	1:116:A:ASP:HA	10	0.25	0.05	0.25
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	10	0.25	0.05	0.25
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	10	0.24	0.02	0.25
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG2	10	0.24	0.02	0.25
(1,709)	1:144:A:ARG:HD3	1:144:A:ARG:HG3	10	0.24	0.02	0.25
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	10	0.24	0.04	0.25
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	10	0.24	0.0	0.24
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB3	10	0.24	0.03	0.24
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB2	10	0.24	0.03	0.24
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB1	10	0.24	0.03	0.24
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	10	0.24	0.08	0.22
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	10	0.24	0.03	0.24
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	10	0.24	0.02	0.24
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	10	0.23	0.02	0.24
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	10	0.23	0.15	0.16
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	10	0.23	0.03	0.23
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	10	0.23	0.02	0.22
(1,3338)	1:156:A:PHE:H	1:156:A:PHE:HA	10	0.23	0.02	0.23
(1,3338)	1:156:A:PHE:H	1:155:A:GLN:HA	10	0.23	0.02	0.23
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	10	0.22	0.01	0.22
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	10	0.22	0.07	0.24
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	10	0.22	0.03	0.22
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD23	10	0.22	0.01	0.22
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD21	10	0.22	0.01	0.22
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD22	10	0.22	0.01	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG13	10	0.22	0.01	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG12	10	0.22	0.01	0.22
(1,2942)	1:12:A:VAL:HG22	1:12:A:VAL:HB	10	0.22	0.01	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG11	10	0.22	0.01	0.22
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	10	0.22	0.04	0.22
(1,2672)	1:24:A:ILE:HD12	1:46:A:CYS:HB3	10	0.22	0.05	0.22
(1,2672)	1:24:A:ILE:HD11	1:46:A:CYS:HB3	10	0.22	0.05	0.22
(1,2672)	1:24:A:ILE:HD13	1:46:A:CYS:HB3	10	0.22	0.05	0.22
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	10	0.22	0.06	0.22
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	10	0.21	0.08	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3158)	1:9:A:LEU:HD23	1:9:A:LEU:HG	10	0.21	0.01	0.22
(1,3158)	1:9:A:LEU:HD22	1:9:A:LEU:HG	10	0.21	0.01	0.22
(1,3158)	1:9:A:LEU:HD21	1:9:A:LEU:HG	10	0.21	0.01	0.22
(1,2506)	1:31:A:VAL:HG12	1:29:A:PRO:HA	10	0.21	0.07	0.2
(1,2506)	1:31:A:VAL:HG13	1:29:A:PRO:HA	10	0.21	0.07	0.2
(1,2506)	1:31:A:VAL:HG11	1:29:A:PRO:HA	10	0.21	0.07	0.2
(1,2506)	1:150:A:THR:HA	1:89:A:VAL:HG12	10	0.21	0.07	0.2
(1,2506)	1:150:A:THR:HA	1:89:A:VAL:HG13	10	0.21	0.07	0.2
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG12	10	0.21	0.04	0.2
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG11	10	0.21	0.04	0.2
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG13	10	0.21	0.04	0.2
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	10	0.2	0.02	0.2
(1,3041)	1:118:A:SER:HB3	1:117:A:PRO:HG2	10	0.2	0.02	0.2
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	10	0.2	0.04	0.2
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB1	10	0.2	0.02	0.2
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB2	10	0.2	0.02	0.2
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB3	10	0.2	0.02	0.2
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG21	10	0.2	0.05	0.2
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG23	10	0.2	0.05	0.2
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG22	10	0.2	0.05	0.2
(1,2485)	1:91:A:TYR:HD1	1:91:A:TYR:HE1	10	0.2	0.0	0.2
(1,2485)	1:91:A:TYR:HD2	1:91:A:TYR:HE2	10	0.2	0.0	0.2
(1,2485)	1:68:A:TYR:HD2	1:68:A:TYR:HE2	10	0.2	0.0	0.2
(1,2485)	1:68:A:TYR:HD1	1:68:A:TYR:HE1	10	0.2	0.0	0.2
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	10	0.2	0.05	0.2
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	10	0.19	0.03	0.17
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	10	0.19	0.0	0.19
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	10	0.19	0.01	0.19
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	10	0.19	0.07	0.16
(1,357)	1:115:A:ALA:HB3	1:115:A:ALA:HA	10	0.18	0.01	0.18
(1,357)	1:115:A:ALA:HB1	1:115:A:ALA:HA	10	0.18	0.01	0.18
(1,357)	1:115:A:ALA:HB2	1:115:A:ALA:HA	10	0.18	0.01	0.18
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	10	0.18	0.02	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD23	10	0.18	0.01	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD21	10	0.18	0.01	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD22	10	0.18	0.01	0.18
(1,211)	1:146:A:VAL:HG11	1:149:A:VAL:H	10	0.18	0.02	0.18
(1,211)	1:146:A:VAL:HG13	1:149:A:VAL:H	10	0.18	0.02	0.18
(1,211)	1:146:A:VAL:HG12	1:149:A:VAL:H	10	0.18	0.02	0.18
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	10	0.17	0.03	0.18
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB2	10	0.17	0.03	0.18
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	10	0.17	0.01	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,174)	1:31:A:VAL:HG11	1:31:A:VAL:HA	10	0.17	0.01	0.17
(1,174)	1:31:A:VAL:HG12	1:31:A:VAL:HA	10	0.17	0.01	0.17
(1,2625)	1:112:A:ALA:HB1	1:109:A:CYS:HB3	10	0.17	0.03	0.18
(1,2625)	1:112:A:ALA:HB3	1:109:A:CYS:HB3	10	0.17	0.03	0.18
(1,2625)	1:112:A:ALA:HB2	1:109:A:CYS:HB3	10	0.17	0.03	0.18
(1,489)	1:24:A:ILE:HG21	1:24:A:ILE:HB	10	0.17	0.01	0.17
(1,489)	1:24:A:ILE:HG22	1:24:A:ILE:HB	10	0.17	0.01	0.17
(1,489)	1:24:A:ILE:HG23	1:24:A:ILE:HB	10	0.17	0.01	0.17
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD13	10	0.17	0.03	0.16
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD11	10	0.17	0.03	0.16
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD12	10	0.17	0.03	0.16
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	10	0.17	0.02	0.16
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	10	0.17	0.02	0.17
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	10	0.16	0.03	0.18
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG21	10	0.16	0.02	0.16
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG22	10	0.16	0.02	0.16
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG23	10	0.16	0.02	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	10	0.16	0.0	0.16
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	10	0.16	0.01	0.16
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD11	10	0.16	0.01	0.16
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD12	10	0.16	0.01	0.16
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD13	10	0.16	0.01	0.16
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	10	0.15	0.01	0.15
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	10	0.15	0.04	0.14
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	10	0.15	0.02	0.15
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB2	10	0.15	0.03	0.16
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB3	10	0.15	0.03	0.16
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB1	10	0.15	0.03	0.16
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	10	0.15	0.01	0.15
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	10	0.15	0.02	0.15
(1,1674)	1:28:A:VAL:HG13	1:28:A:VAL:HA	10	0.15	0.02	0.15
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB3	10	0.14	0.01	0.15
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB2	10	0.14	0.01	0.15
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB1	10	0.14	0.01	0.15
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	10	0.14	0.03	0.14
(1,2787)	1:56:A:LYS:HE2	1:56:A:LYS:HD3	10	0.14	0.03	0.14
(1,2787)	1:6:A:LYS:HE3	1:6:A:LYS:HD2	10	0.14	0.03	0.14
(1,243)	1:149:A:VAL:HG12	1:149:A:VAL:HG21	10	0.14	0.02	0.15
(1,243)	1:149:A:VAL:HG11	1:149:A:VAL:HG23	10	0.14	0.02	0.15
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG22	10	0.14	0.02	0.15
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG21	10	0.14	0.02	0.15
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG23	10	0.14	0.02	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,243)	1:149:A:VAL:HG12	1:149:A:VAL:HG23	10	0.14	0.02	0.15
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	10	0.14	0.0	0.14
(1,532)	1:24:A:ILE:HD11	1:24:A:ILE:HG12	10	0.14	0.01	0.14
(1,532)	1:24:A:ILE:HD13	1:24:A:ILE:HG12	10	0.14	0.01	0.14
(1,532)	1:24:A:ILE:HD12	1:24:A:ILE:HG12	10	0.14	0.01	0.14
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG21	10	0.14	0.03	0.13
(1,276)	1:97:A:VAL:HG11	1:97:A:VAL:HG22	10	0.14	0.03	0.13
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG22	10	0.14	0.03	0.13
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG23	10	0.14	0.03	0.13
(1,276)	1:97:A:VAL:HG13	1:97:A:VAL:HG21	10	0.14	0.03	0.13
(1,200)	1:71:A:THR:HG23	1:71:A:THR:HB	10	0.14	0.01	0.14
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	10	0.14	0.01	0.14
(1,200)	1:71:A:THR:HG22	1:71:A:THR:HB	10	0.14	0.01	0.14
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	10	0.13	0.01	0.13
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	10	0.13	0.02	0.13
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	10	0.13	0.01	0.13
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	10	0.12	0.0	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD11	10	0.12	0.01	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD13	10	0.12	0.01	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD23	10	0.12	0.01	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD21	10	0.12	0.01	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD12	10	0.12	0.01	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	10	0.12	0.0	0.12
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	9	1.62	0.05	1.62
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	9	1.57	0.28	1.65
(1,468)	1:97:A:VAL:HG22	1:98:A:MET:HG3	9	0.78	0.06	0.75
(1,468)	1:97:A:VAL:HG23	1:98:A:MET:HG3	9	0.78	0.06	0.75
(1,468)	1:97:A:VAL:HG21	1:98:A:MET:HG3	9	0.78	0.06	0.75
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	9	0.74	0.03	0.73
(1,2556)	1:71:A:THR:HG22	1:54:A:ASP:HB2	9	0.73	0.28	0.77
(1,2556)	1:71:A:THR:HG21	1:54:A:ASP:HB2	9	0.73	0.28	0.77
(1,2556)	1:71:A:THR:HG23	1:54:A:ASP:HB2	9	0.73	0.28	0.77
(1,218)	1:89:A:VAL:HG23	1:151:A:SER:HB2	9	0.73	0.19	0.81
(1,218)	1:89:A:VAL:HG21	1:151:A:SER:HB2	9	0.73	0.19	0.81
(1,218)	1:89:A:VAL:HG22	1:151:A:SER:HB2	9	0.73	0.19	0.81
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG22	9	0.67	0.06	0.67
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG21	9	0.67	0.06	0.67
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG23	9	0.67	0.06	0.67
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	9	0.61	0.06	0.63
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	9	0.61	0.07	0.6
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG23	9	0.57	0.15	0.54
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG22	9	0.57	0.15	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	9	0.54	0.17	0.54
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB3	9	0.51	0.11	0.53
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB2	9	0.51	0.11	0.53
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB1	9	0.51	0.11	0.53
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB3	9	0.5	0.11	0.46
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB2	9	0.5	0.11	0.46
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB1	9	0.5	0.11	0.46
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	9	0.5	0.22	0.57
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD3	9	0.47	0.08	0.45
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD2	9	0.47	0.08	0.45
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	9	0.44	0.02	0.44
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	9	0.44	0.01	0.44
(1,2716)	1:159:A:GLU:H	1:160:A:GLY:HA2	9	0.44	0.12	0.5
(1,2716)	1:160:A:GLY:HA2	1:156:A:PHE:HD2	9	0.44	0.12	0.5
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	9	0.43	0.16	0.45
(1,3055)	1:18:A:GLY:H	1:17:A:LYS:HD3	9	0.42	0.08	0.44
(1,3055)	1:144:A:ARG:HG3	1:144:A:ARG:H	9	0.42	0.08	0.44
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	9	0.41	0.17	0.49
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	9	0.38	0.03	0.4
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD22	9	0.38	0.09	0.41
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD21	9	0.38	0.09	0.41
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD23	9	0.38	0.09	0.41
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG21	9	0.36	0.05	0.37
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG22	9	0.36	0.05	0.37
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG23	9	0.36	0.05	0.37
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	9	0.35	0.26	0.27
(1,146)	1:9:A:LEU:HD22	1:37:A:ALA:HB2	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD21	1:37:A:ALA:HB2	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB3	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB1	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD21	1:37:A:ALA:HB1	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD22	1:37:A:ALA:HB3	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB2	9	0.35	0.12	0.37
(1,146)	1:9:A:LEU:HD22	1:37:A:ALA:HB1	9	0.35	0.12	0.37
(1,2561)	1:89:A:VAL:HG23	1:91:A:TYR:HD1	9	0.33	0.1	0.36
(1,2561)	1:89:A:VAL:HG21	1:91:A:TYR:HD1	9	0.33	0.1	0.36
(1,2561)	1:89:A:VAL:HG22	1:91:A:TYR:HD1	9	0.33	0.1	0.36
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	9	0.32	0.01	0.33
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG11	9	0.32	0.09	0.33
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG12	9	0.32	0.09	0.33
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG13	9	0.32	0.09	0.33
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	9	0.31	0.07	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD22	9	0.31	0.07	0.32
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD23	9	0.31	0.07	0.32
(1,3127)	1:132:A:THR:HG23	1:92:A:GLU:HG2	9	0.3	0.1	0.31
(1,3127)	1:132:A:THR:HG21	1:92:A:GLU:HG2	9	0.3	0.1	0.31
(1,3127)	1:132:A:THR:HG22	1:92:A:GLU:HG2	9	0.3	0.1	0.31
(1,692)	1:97:A:VAL:HG22	1:133:A:PHE:HB2	9	0.27	0.09	0.25
(1,692)	1:97:A:VAL:HG21	1:133:A:PHE:HB2	9	0.27	0.09	0.25
(1,692)	1:97:A:VAL:HG23	1:133:A:PHE:HB2	9	0.27	0.09	0.25
(1,1605)	1:33:A:LEU:HD21	1:74:A:LYS:HB3	9	0.26	0.07	0.27
(1,1605)	1:33:A:LEU:HD22	1:74:A:LYS:HB3	9	0.26	0.07	0.27
(1,1605)	1:33:A:LEU:HD23	1:74:A:LYS:HB3	9	0.26	0.07	0.27
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	9	0.26	0.08	0.28
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	9	0.26	0.29	0.16
(1,3449)	1:130:A:LYS:H	1:129:A:GLN:HB2	9	0.26	0.29	0.16
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG21	9	0.25	0.03	0.24
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG23	9	0.25	0.03	0.24
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG22	9	0.25	0.03	0.24
(1,2546)	1:150:A:THR:HG22	1:106:A:SER:HB2	9	0.25	0.1	0.27
(1,2546)	1:150:A:THR:HG23	1:106:A:SER:HB2	9	0.25	0.1	0.27
(1,2546)	1:150:A:THR:HG21	1:106:A:SER:HB2	9	0.25	0.1	0.27
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	9	0.25	0.1	0.25
(1,285)	1:146:A:VAL:HG22	1:90:A:SER:HA	9	0.24	0.05	0.25
(1,285)	1:146:A:VAL:HG21	1:90:A:SER:HA	9	0.24	0.05	0.25
(1,285)	1:146:A:VAL:HG23	1:90:A:SER:HA	9	0.24	0.05	0.25
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	9	0.24	0.02	0.24
(1,1606)	1:33:A:LEU:HD21	1:12:A:VAL:HB	9	0.23	0.06	0.25
(1,1606)	1:33:A:LEU:HD22	1:12:A:VAL:HB	9	0.23	0.06	0.25
(1,1606)	1:33:A:LEU:HD23	1:12:A:VAL:HB	9	0.23	0.06	0.25
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	9	0.23	0.04	0.22
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG13	9	0.23	0.04	0.22
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG11	9	0.23	0.04	0.22
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	9	0.23	0.08	0.25
(1,2764)	1:74:A:LYS:H	1:53:A:ASP:HB3	9	0.23	0.08	0.25
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	9	0.22	0.11	0.18
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HD3	9	0.22	0.07	0.19
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HG3	9	0.22	0.07	0.19
(1,2794)	1:64:A:LYS:HE3	1:64:A:LYS:HG3	9	0.22	0.07	0.19
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	9	0.22	0.07	0.19
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG22	9	0.22	0.03	0.23
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG23	9	0.22	0.03	0.23
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG21	9	0.22	0.03	0.23
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	9	0.22	0.05	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,169)	1:12:A:VAL:HG21	1:75:A:THR:H	9	0.21	0.02	0.22
(1,169)	1:12:A:VAL:HG23	1:75:A:THR:H	9	0.21	0.02	0.22
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	9	0.21	0.05	0.21
(1,3125)	1:123:A:THR:HG21	1:91:A:TYR:HD1	9	0.21	0.07	0.24
(1,3125)	1:123:A:THR:HG23	1:91:A:TYR:HD1	9	0.21	0.07	0.24
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	9	0.21	0.05	0.2
(1,358)	1:115:A:ALA:HB1	1:116:A:ASP:HB2	9	0.21	0.04	0.21
(1,358)	1:115:A:ALA:HB2	1:116:A:ASP:HB2	9	0.21	0.04	0.21
(1,358)	1:115:A:ALA:HB3	1:116:A:ASP:HB2	9	0.21	0.04	0.21
(1,1627)	1:132:A:THR:HG22	1:100:A:ALA:HB2	9	0.2	0.02	0.2
(1,1627)	1:132:A:THR:HG22	1:100:A:ALA:HB1	9	0.2	0.02	0.2
(1,1627)	1:132:A:THR:HG23	1:100:A:ALA:HB2	9	0.2	0.02	0.2
(1,1627)	1:132:A:THR:HG21	1:100:A:ALA:HB2	9	0.2	0.02	0.2
(1,1627)	1:132:A:THR:HG23	1:100:A:ALA:HB1	9	0.2	0.02	0.2
(1,1627)	1:132:A:THR:HG21	1:100:A:ALA:HB3	9	0.2	0.02	0.2
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG23	9	0.2	0.05	0.23
(1,3512)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	9	0.2	0.05	0.23
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG22	9	0.2	0.05	0.23
(1,3512)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	9	0.2	0.05	0.23
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	9	0.19	0.03	0.19
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG22	9	0.19	0.06	0.2
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG21	9	0.19	0.06	0.2
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG23	9	0.19	0.06	0.2
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	9	0.18	0.06	0.2
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	9	0.18	0.01	0.19
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	9	0.18	0.06	0.16
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	9	0.17	0.01	0.17
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	9	0.17	0.03	0.17
(1,401)	1:37:A:ALA:HB2	1:51:A:TYR:HE1	9	0.17	0.01	0.17
(1,401)	1:37:A:ALA:HB3	1:51:A:TYR:HE1	9	0.17	0.01	0.17
(1,401)	1:37:A:ALA:HB1	1:51:A:TYR:HE1	9	0.17	0.01	0.17
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	9	0.17	0.07	0.15
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB3	9	0.16	0.03	0.15
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB2	9	0.16	0.03	0.15
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB1	9	0.16	0.03	0.15
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	9	0.16	0.03	0.17
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	9	0.16	0.02	0.16
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	9	0.16	0.02	0.16
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	9	0.16	0.04	0.17
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	9	0.16	0.05	0.14
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB3	9	0.16	0.05	0.14
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	9	0.16	0.02	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	9	0.16	0.03	0.16
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD23	9	0.16	0.04	0.15
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD21	9	0.16	0.04	0.15
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD22	9	0.16	0.04	0.15
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG21	9	0.15	0.02	0.15
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG23	9	0.15	0.02	0.15
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG22	9	0.15	0.02	0.15
(1,2912)	1:153:A:PRO:HB2	1:121:A:ILE:HA	9	0.15	0.05	0.13
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	9	0.15	0.05	0.13
(1,41)	1:50:A:THR:HG22	1:75:A:THR:HA	9	0.15	0.02	0.15
(1,41)	1:50:A:THR:HG21	1:75:A:THR:HA	9	0.15	0.02	0.15
(1,41)	1:50:A:THR:HG23	1:75:A:THR:HA	9	0.15	0.02	0.15
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	9	0.15	0.02	0.14
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	9	0.14	0.01	0.14
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	9	0.13	0.02	0.13
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	9	0.13	0.01	0.13
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB2	9	0.13	0.01	0.12
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB1	9	0.13	0.01	0.12
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB3	9	0.13	0.01	0.12
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	9	0.12	0.0	0.12
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	9	0.12	0.02	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	9	0.12	0.01	0.12
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	8	0.7	0.06	0.68
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	8	0.6	0.07	0.62
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	8	0.59	0.41	0.42
(1,2785)	1:130:A:LYS:HE3	1:125:A:ASN:HD21	8	0.59	0.41	0.42
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	8	0.48	0.45	0.29
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	8	0.46	0.13	0.5
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB1	8	0.46	0.29	0.4
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB3	8	0.46	0.29	0.4
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB2	8	0.46	0.29	0.4
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	8	0.44	0.03	0.45
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	8	0.39	0.24	0.31
(1,1640)	1:47:A:THR:HG22	1:156:A:PHE:HE2	8	0.37	0.12	0.4
(1,1640)	1:47:A:THR:HG21	1:156:A:PHE:HE2	8	0.37	0.12	0.4
(1,1640)	1:47:A:THR:HG23	1:156:A:PHE:HE2	8	0.37	0.12	0.4
(1,3345)	1:150:A:THR:H	1:126:A:GLU:HB2	8	0.34	0.18	0.3
(1,3345)	1:150:A:THR:H	1:87:A:GLN:HG2	8	0.34	0.18	0.3
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	8	0.32	0.07	0.29
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	8	0.29	0.24	0.2
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	8	0.28	0.07	0.28
(1,2847)	1:91:A:TYR:HB2	1:151:A:SER:HB2	8	0.28	0.07	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG23	8	0.27	0.13	0.22
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG21	8	0.27	0.13	0.22
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG22	8	0.27	0.13	0.22
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	8	0.26	0.13	0.25
(1,1666)	1:9:A:LEU:HD23	1:33:A:LEU:HA	8	0.26	0.01	0.26
(1,1666)	1:9:A:LEU:HD22	1:33:A:LEU:HA	8	0.26	0.01	0.26
(1,1666)	1:9:A:LEU:HD21	1:33:A:LEU:HA	8	0.26	0.01	0.26
(1,2582)	1:97:A:VAL:HG11	1:135:A:GLY:HA2	8	0.26	0.11	0.24
(1,2582)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	8	0.26	0.11	0.24
(1,2582)	1:97:A:VAL:HG13	1:135:A:GLY:HA2	8	0.26	0.11	0.24
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	8	0.25	0.1	0.22
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG2	8	0.25	0.1	0.22
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG3	8	0.25	0.1	0.22
(1,242)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	8	0.24	0.02	0.24
(1,242)	1:43:A:VAL:HG22	1:46:A:CYS:HB2	8	0.24	0.02	0.24
(1,242)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	8	0.24	0.02	0.24
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	8	0.24	0.03	0.23
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	8	0.24	0.06	0.24
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG22	8	0.23	0.08	0.22
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG23	8	0.23	0.08	0.22
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG21	8	0.23	0.08	0.22
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	8	0.23	0.07	0.22
(1,3161)	1:132:A:THR:HG22	1:100:A:ALA:HB2	8	0.23	0.04	0.24
(1,3161)	1:100:A:ALA:HB2	1:130:A:LYS:HG2	8	0.23	0.04	0.24
(1,3161)	1:100:A:ALA:HB3	1:130:A:LYS:HG2	8	0.23	0.04	0.24
(1,3161)	1:132:A:THR:HG23	1:100:A:ALA:HB2	8	0.23	0.04	0.24
(1,3161)	1:132:A:THR:HG21	1:100:A:ALA:HB2	8	0.23	0.04	0.24
(1,3161)	1:132:A:THR:HG23	1:100:A:ALA:HB1	8	0.23	0.04	0.24
(1,3161)	1:100:A:ALA:HB1	1:130:A:LYS:HG2	8	0.23	0.04	0.24
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	8	0.22	0.05	0.22
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	8	0.21	0.04	0.22
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG23	8	0.21	0.07	0.22
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG22	8	0.21	0.07	0.22
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG21	8	0.21	0.07	0.22
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	8	0.2	0.04	0.2
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	8	0.2	0.04	0.19
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	8	0.2	0.02	0.2
(1,2901)	1:129:A:GLN:HG3	1:126:A:GLU:HA	8	0.2	0.02	0.2
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	8	0.2	0.06	0.19
(1,2633)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	8	0.18	0.03	0.17
(1,2633)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	8	0.18	0.03	0.17
(1,2633)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	8	0.18	0.03	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	8	0.17	0.04	0.16
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	8	0.16	0.04	0.15
(1,2735)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	8	0.15	0.02	0.16
(1,2735)	1:43:A:VAL:HG22	1:46:A:CYS:HB2	8	0.15	0.02	0.16
(1,2735)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	8	0.15	0.02	0.16
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	8	0.15	0.03	0.14
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	8	0.15	0.03	0.15
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG22	8	0.14	0.05	0.12
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG23	8	0.14	0.05	0.12
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG21	8	0.14	0.05	0.12
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	8	0.14	0.03	0.14
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	8	0.14	0.02	0.14
(1,3466)	1:52:A:ASN:H	1:57:A:MET:H	8	0.14	0.02	0.14
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	8	0.14	0.02	0.15
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	8	0.13	0.02	0.14
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	8	0.13	0.03	0.13
(1,2607)	1:149:A:VAL:HG11	1:149:A:VAL:HG23	8	0.13	0.02	0.13
(1,2607)	1:149:A:VAL:HG13	1:149:A:VAL:HG21	8	0.13	0.02	0.13
(1,2607)	1:149:A:VAL:HG13	1:149:A:VAL:HG23	8	0.13	0.02	0.13
(1,2607)	1:149:A:VAL:HG12	1:149:A:VAL:HG23	8	0.13	0.02	0.13
(1,2607)	1:149:A:VAL:HG22	1:146:A:VAL:HG11	8	0.13	0.02	0.13
(1,2607)	1:149:A:VAL:HG23	1:146:A:VAL:HG12	8	0.13	0.02	0.13
(1,2607)	1:149:A:VAL:HG12	1:149:A:VAL:HG21	8	0.13	0.02	0.13
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	7	1.77	0.5	1.95
(1,2723)	1:63:A:GLY:HA3	1:64:A:LYS:HD2	7	1.77	0.5	1.95
(1,2747)	1:82:A:ARG:HD3	1:85:A:PHE:HB3	7	1.23	0.56	1.11
(1,2747)	1:49:A:PHE:HB3	1:59:A:HIS:HB3	7	1.23	0.56	1.11
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	7	0.88	0.48	1.1
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB2	7	0.84	0.66	0.4
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB3	7	0.84	0.66	0.4
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	7	0.58	0.0	0.58
(1,3202)	1:100:A:ALA:H	1:96:A:ASP:HB3	7	0.37	0.15	0.35
(1,3202)	1:100:A:ALA:H	1:133:A:PHE:HB2	7	0.37	0.15	0.35
(1,380)	1:112:A:ALA:HB2	1:65:A:PRO:HG3	7	0.36	0.11	0.42
(1,380)	1:112:A:ALA:HB1	1:65:A:PRO:HG3	7	0.36	0.11	0.42
(1,380)	1:112:A:ALA:HB3	1:65:A:PRO:HG3	7	0.36	0.11	0.42
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	7	0.35	0.11	0.37
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	7	0.31	0.02	0.31
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	7	0.31	0.03	0.31
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	7	0.31	0.09	0.36
(1,216)	1:89:A:VAL:HG22	1:143:A:GLU:HA	7	0.29	0.01	0.29
(1,216)	1:89:A:VAL:HG21	1:143:A:GLU:HA	7	0.29	0.01	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,216)	1:89:A:VAL:HG23	1:143:A:GLU:HA	7	0.29	0.01	0.29
(1,501)	1:94:A:ALA:HB2	1:121:A:ILE:HD12	7	0.27	0.11	0.28
(1,501)	1:94:A:ALA:HB1	1:121:A:ILE:HD12	7	0.27	0.11	0.28
(1,501)	1:94:A:ALA:HB3	1:121:A:ILE:HD12	7	0.27	0.11	0.28
(1,501)	1:94:A:ALA:HB1	1:121:A:ILE:HD11	7	0.27	0.11	0.28
(1,501)	1:94:A:ALA:HB3	1:121:A:ILE:HD11	7	0.27	0.11	0.28
(1,2627)	1:111:A:ALA:HB3	1:156:A:PHE:HD1	7	0.27	0.1	0.23
(1,2627)	1:111:A:ALA:HB2	1:156:A:PHE:HD1	7	0.27	0.1	0.23
(1,2627)	1:111:A:ALA:HB1	1:156:A:PHE:HD1	7	0.27	0.1	0.23
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	7	0.26	0.03	0.26
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	7	0.24	0.07	0.26
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	7	0.23	0.06	0.22
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	7	0.23	0.01	0.23
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	7	0.22	0.07	0.21
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	7	0.21	0.04	0.21
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	7	0.18	0.02	0.18
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD12	7	0.18	0.02	0.18
(1,3080)	1:10:A:SER:H	1:10:A:SER:HB3	7	0.18	0.03	0.19
(1,3080)	1:11:A:CYS:H	1:10:A:SER:HB3	7	0.18	0.03	0.19
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	7	0.17	0.03	0.18
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	7	0.17	0.06	0.15
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG23	7	0.16	0.04	0.17
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG22	7	0.16	0.04	0.17
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG21	7	0.16	0.04	0.17
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD23	7	0.16	0.04	0.17
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD21	7	0.16	0.04	0.17
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD22	7	0.16	0.04	0.17
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	7	0.16	0.04	0.17
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	7	0.16	0.05	0.14
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	7	0.15	0.04	0.14
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	7	0.15	0.04	0.14
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG11	7	0.15	0.04	0.14
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	7	0.15	0.03	0.16
(1,2739)	1:122:A:PHE:HB3	1:109:A:CYS:HB2	7	0.15	0.03	0.16
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	7	0.15	0.04	0.16
(1,2797)	1:130:A:LYS:HE2	1:130:A:LYS:HD3	7	0.15	0.01	0.15
(1,2797)	1:130:A:LYS:HE3	1:130:A:LYS:HD2	7	0.15	0.01	0.15
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	7	0.14	0.02	0.14
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	7	0.14	0.01	0.14
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	7	0.13	0.01	0.13
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	7	0.13	0.01	0.12
(1,164)	1:150:A:THR:HG23	1:150:A:THR:HA	7	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,164)	1:150:A:THR:HG21	1:150:A:THR:HA	7	0.12	0.01	0.12
(1,164)	1:150:A:THR:HG22	1:150:A:THR:HA	7	0.12	0.01	0.12
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	7	0.12	0.02	0.12
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	7	0.12	0.0	0.12
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	7	0.12	0.02	0.11
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	7	0.12	0.01	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	7	0.11	0.0	0.11
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	6	1.01	0.17	1.07
(1,3461)	1:110:A:GLN:HE22	1:157:A:CYS:HB3	6	0.84	0.1	0.83
(1,3461)	1:155:A:GLN:HE22	1:154:A:LYS:HA	6	0.84	0.1	0.83
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG23	6	0.8	0.32	0.72
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG21	6	0.8	0.32	0.72
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG22	6	0.8	0.32	0.72
(1,3115)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	6	0.79	0.12	0.84
(1,3115)	1:56:A:LYS:HE3	1:56:A:LYS:HG2	6	0.79	0.12	0.84
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG22	6	0.54	0.22	0.62
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG21	6	0.54	0.22	0.62
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG23	6	0.54	0.22	0.62
(1,2641)	1:114:A:ALA:HB1	1:110:A:GLN:HG2	6	0.49	0.07	0.49
(1,2641)	1:114:A:ALA:HB3	1:110:A:GLN:HG2	6	0.49	0.07	0.49
(1,2641)	1:114:A:ALA:HB2	1:110:A:GLN:HG2	6	0.49	0.07	0.49
(1,1253)	1:67:A:LEU:HD23	1:65:A:PRO:HB2	6	0.44	0.23	0.38
(1,1253)	1:67:A:LEU:HD21	1:65:A:PRO:HB2	6	0.44	0.23	0.38
(1,2793)	1:40:A:CYS:HB2	1:46:A:CYS:HB3	6	0.42	0.11	0.45
(1,2793)	1:40:A:CYS:HB2	1:78:A:ARG:HA	6	0.42	0.11	0.45
(1,2793)	1:64:A:LYS:HE2	1:117:A:PRO:HD3	6	0.42	0.11	0.45
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	6	0.4	0.28	0.32
(1,2801)	1:41:A:LYS:H	1:40:A:CYS:HB2	6	0.35	0.11	0.38
(1,2801)	1:64:A:LYS:HE2	1:116:A:ASP:H	6	0.35	0.11	0.38
(1,2801)	1:64:A:LYS:HE3	1:116:A:ASP:H	6	0.35	0.11	0.38
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB3	6	0.31	0.23	0.22
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB2	6	0.31	0.23	0.22
(1,2664)	1:94:A:ALA:HB1	1:95:A:PRO:HD2	6	0.27	0.12	0.24
(1,2664)	1:94:A:ALA:HB2	1:95:A:PRO:HD2	6	0.27	0.12	0.24
(1,2664)	1:94:A:ALA:HB3	1:95:A:PRO:HD2	6	0.27	0.12	0.24
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	6	0.25	0.09	0.28
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	6	0.24	0.03	0.24
(1,1577)	1:64:A:LYS:HE2	1:64:A:LYS:HG2	6	0.23	0.03	0.24
(1,1577)	1:64:A:LYS:HE3	1:64:A:LYS:HG2	6	0.23	0.03	0.24
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	6	0.23	0.01	0.23
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG22	6	0.23	0.14	0.18
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG23	6	0.23	0.14	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3523)	1:31:A:VAL:H	1:30:A:ASP:HB3	6	0.22	0.05	0.24
(1,3523)	1:31:A:VAL:H	1:56:A:LYS:HE3	6	0.22	0.05	0.24
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	6	0.22	0.2	0.14
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	6	0.22	0.09	0.19
(1,231)	1:104:A:SER:H	1:103:A:THR:HG23	6	0.21	0.05	0.22
(1,231)	1:104:A:SER:H	1:103:A:THR:HG21	6	0.21	0.05	0.22
(1,231)	1:104:A:SER:H	1:103:A:THR:HG22	6	0.21	0.05	0.22
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	6	0.2	0.1	0.16
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD21	6	0.2	0.07	0.22
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD23	6	0.2	0.07	0.22
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD22	6	0.2	0.07	0.22
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	6	0.2	0.04	0.2
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB3	6	0.19	0.06	0.16
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB1	6	0.19	0.06	0.16
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB2	6	0.19	0.06	0.16
(1,388)	1:112:A:ALA:HB2	1:65:A:PRO:HD3	6	0.18	0.05	0.19
(1,388)	1:112:A:ALA:HB3	1:65:A:PRO:HD3	6	0.18	0.05	0.19
(1,388)	1:112:A:ALA:HB1	1:65:A:PRO:HD3	6	0.18	0.05	0.19
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG22	6	0.18	0.02	0.18
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG21	6	0.18	0.02	0.18
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG23	6	0.18	0.02	0.18
(1,2765)	1:133:A:PHE:HB2	1:97:A:VAL:H	6	0.17	0.02	0.18
(1,2765)	1:54:A:ASP:H	1:53:A:ASP:HB3	6	0.17	0.02	0.18
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	6	0.17	0.06	0.18
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	6	0.16	0.04	0.15
(1,2725)	1:160:A:GLY:HA3	1:159:A:GLU:HB2	6	0.16	0.02	0.16
(1,2725)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	6	0.16	0.02	0.16
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	6	0.16	0.03	0.16
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD22	6	0.14	0.04	0.14
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD23	6	0.14	0.04	0.14
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD21	6	0.14	0.04	0.14
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	6	0.12	0.01	0.12
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	6	0.12	0.01	0.12
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD12	6	0.12	0.02	0.11
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD11	6	0.12	0.02	0.11
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD13	6	0.12	0.02	0.11
(1,370)	1:5:A:ALA:HB1	1:5:A:ALA:HA	6	0.11	0.0	0.11
(1,370)	1:5:A:ALA:HB3	1:5:A:ALA:HA	6	0.11	0.0	0.11
(1,1584)	1:74:A:LYS:HG2	1:14:A:SER:HB2	5	0.53	0.21	0.44
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB3	5	0.52	0.44	0.26
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB2	5	0.52	0.44	0.26
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB1	5	0.52	0.44	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2786)	1:41:A:LYS:HE2	1:41:A:LYS:HG2	5	0.36	0.22	0.38
(1,2786)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	5	0.36	0.22	0.38
(1,184)	1:67:A:LEU:HD21	1:19:A:SER:HB3	5	0.36	0.02	0.36
(1,761)	1:64:A:LYS:HE2	1:115:A:ALA:HB1	5	0.3	0.06	0.32
(1,761)	1:64:A:LYS:HE2	1:115:A:ALA:HB2	5	0.3	0.06	0.32
(1,761)	1:64:A:LYS:HE3	1:115:A:ALA:HB1	5	0.3	0.06	0.32
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB3	5	0.26	0.08	0.28
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB1	5	0.26	0.08	0.28
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB2	5	0.26	0.08	0.28
(1,2531)	1:13:A:HIS:HD2	1:17:A:LYS:HB2	5	0.25	0.04	0.27
(1,2531)	1:75:A:THR:HG23	1:13:A:HIS:HD2	5	0.25	0.04	0.27
(1,2531)	1:75:A:THR:HG22	1:13:A:HIS:HD2	5	0.25	0.04	0.27
(1,964)	1:67:A:LEU:HD23	1:17:A:LYS:HB2	5	0.24	0.05	0.23
(1,964)	1:67:A:LEU:HD22	1:17:A:LYS:HB2	5	0.24	0.05	0.23
(1,964)	1:67:A:LEU:HD21	1:17:A:LYS:HB2	5	0.24	0.05	0.23
(1,742)	1:37:A:ALA:HB3	1:41:A:LYS:HE2	5	0.23	0.04	0.25
(1,742)	1:37:A:ALA:HB2	1:41:A:LYS:HE2	5	0.23	0.04	0.25
(1,742)	1:37:A:ALA:HB3	1:41:A:LYS:HE3	5	0.23	0.04	0.25
(1,2754)	1:136:A:ARG:HD3	1:120:A:GLU:HG3	5	0.23	0.09	0.21
(1,2402)	1:19:A:SER:H	1:19:A:SER:HB3	5	0.22	0.01	0.22
(1,494)	1:94:A:ALA:HB1	1:141:A:PHE:HD2	5	0.22	0.11	0.23
(1,494)	1:94:A:ALA:HB3	1:141:A:PHE:HD2	5	0.22	0.11	0.23
(1,494)	1:94:A:ALA:HB2	1:141:A:PHE:HD2	5	0.22	0.11	0.23
(1,2211)	1:17:A:LYS:H	1:73:A:GLY:HA2	5	0.22	0.08	0.2
(1,2510)	1:47:A:THR:HG22	1:156:A:PHE:HE2	5	0.21	0.08	0.18
(1,2510)	1:114:A:ALA:HB1	1:156:A:PHE:HE2	5	0.21	0.08	0.18
(1,2510)	1:47:A:THR:HG21	1:156:A:PHE:HE2	5	0.21	0.08	0.18
(1,2510)	1:114:A:ALA:HB2	1:156:A:PHE:HE2	5	0.21	0.08	0.18
(1,2510)	1:114:A:ALA:HB3	1:156:A:PHE:HE2	5	0.21	0.08	0.18
(1,3280)	1:103:A:THR:H	1:129:A:GLN:HB2	5	0.2	0.07	0.2
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG21	5	0.2	0.07	0.18
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG22	5	0.2	0.07	0.18
(1,3471)	1:57:A:MET:H	1:56:A:LYS:HG2	5	0.19	0.08	0.16
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG22	5	0.19	0.03	0.18
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG23	5	0.19	0.03	0.18
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG21	5	0.19	0.03	0.18
(1,2977)	1:26:A:GLU:HB3	1:26:A:GLU:H	5	0.19	0.07	0.16
(1,191)	1:127:A:HIS:HA	1:126:A:GLU:HB2	5	0.18	0.07	0.15
(1,3250)	1:91:A:TYR:H	1:92:A:GLU:HB2	5	0.18	0.07	0.13
(1,3250)	1:91:A:TYR:H	1:149:A:VAL:HB	5	0.18	0.07	0.13
(1,3023)	1:79:A:SER:HB3	1:156:A:PHE:HB2	5	0.16	0.04	0.14
(1,412)	1:21:A:ALA:HB1	1:61:A:LYS:HA	5	0.15	0.04	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,412)	1:21:A:ALA:HB2	1:61:A:LYS:HA	5	0.15	0.04	0.14
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG21	5	0.14	0.04	0.12
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG22	5	0.14	0.04	0.12
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG23	5	0.14	0.04	0.12
(1,733)	1:132:A:THR:H	1:131:A:CYS:HB2	5	0.14	0.03	0.13
(1,1555)	1:67:A:LEU:HD23	1:67:A:LEU:HD12	5	0.14	0.03	0.12
(1,1555)	1:67:A:LEU:HD23	1:67:A:LEU:HD11	5	0.14	0.03	0.12
(1,1555)	1:67:A:LEU:HD22	1:67:A:LEU:HD11	5	0.14	0.03	0.12
(1,428)	1:31:A:VAL:HG23	1:58:A:CYS:HB3	5	0.13	0.02	0.14
(1,428)	1:31:A:VAL:HG22	1:58:A:CYS:HB3	5	0.13	0.02	0.14
(1,428)	1:31:A:VAL:HG21	1:58:A:CYS:HB3	5	0.13	0.02	0.14
(1,2978)	1:26:A:GLU:HB3	1:27:A:PRO:HD3	5	0.12	0.01	0.11
(1,2978)	1:26:A:GLU:HB2	1:27:A:PRO:HD3	5	0.12	0.01	0.11
(1,177)	1:31:A:VAL:HG11	1:31:A:VAL:HB	5	0.11	0.01	0.11
(1,177)	1:31:A:VAL:HG12	1:31:A:VAL:HB	5	0.11	0.01	0.11
(1,177)	1:31:A:VAL:HG13	1:31:A:VAL:HB	5	0.11	0.01	0.11
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB2	5	0.11	0.01	0.11
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB3	5	0.11	0.01	0.11
(1,1678)	1:70:A:LEU:HG	1:70:A:LEU:HA	5	0.1	0.0	0.1
(1,3412)	1:115:A:ALA:H	1:112:A:ALA:HB2	4	1.11	0.04	1.1
(1,3412)	1:115:A:ALA:H	1:112:A:ALA:HB3	4	1.11	0.04	1.1
(1,3412)	1:16:A:ASN:HD22	1:71:A:THR:HG21	4	1.11	0.04	1.1
(1,1181)	1:64:A:LYS:HE2	1:64:A:LYS:HB2	4	0.88	0.04	0.88
(1,1181)	1:64:A:LYS:HE3	1:64:A:LYS:HB2	4	0.88	0.04	0.88
(1,2962)	1:65:A:PRO:HB3	1:67:A:LEU:HG	4	0.77	0.13	0.77
(1,3008)	1:130:A:LYS:HD3	1:130:A:LYS:HA	4	0.67	0.09	0.66
(1,3091)	1:94:A:ALA:HA	1:95:A:PRO:HA	4	0.5	0.08	0.54
(1,3091)	1:83:A:SER:HB2	1:157:A:CYS:HB2	4	0.5	0.08	0.54
(1,3209)	1:70:A:LEU:H	1:16:A:ASN:HB2	4	0.5	0.15	0.56
(1,3209)	1:70:A:LEU:H	1:69:A:ASP:HB3	4	0.5	0.15	0.56
(1,3113)	1:56:A:LYS:HG3	1:56:A:LYS:HE3	4	0.47	0.0	0.47
(1,3113)	1:56:A:LYS:HG3	1:56:A:LYS:HE2	4	0.47	0.0	0.47
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	4	0.43	0.3	0.42
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	4	0.43	0.3	0.42
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG21	4	0.43	0.3	0.42
(1,2269)	1:141:A:PHE:H	1:142:A:LYS:HB3	4	0.42	0.21	0.38
(1,21)	1:156:A:PHE:HD2	1:114:A:ALA:HB2	4	0.4	0.14	0.46
(1,21)	1:156:A:PHE:HD2	1:114:A:ALA:HB3	4	0.4	0.14	0.46
(1,173)	1:35:A:GLN:HE21	1:31:A:VAL:HG13	4	0.4	0.19	0.42
(1,173)	1:35:A:GLN:HE21	1:31:A:VAL:HG11	4	0.4	0.19	0.42
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG21	4	0.34	0.13	0.3
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG22	4	0.34	0.13	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG23	4	0.34	0.13	0.3
(1,899)	1:16:A:ASN:H	1:15:A:ASP:HB3	4	0.24	0.04	0.24
(1,1625)	1:132:A:THR:H	1:132:A:THR:HG21	4	0.24	0.08	0.25
(1,1625)	1:132:A:THR:H	1:132:A:THR:HG22	4	0.24	0.08	0.25
(1,305)	1:75:A:THR:HG23	1:19:A:SER:HB2	4	0.22	0.01	0.22
(1,305)	1:75:A:THR:HG22	1:19:A:SER:HB2	4	0.22	0.01	0.22
(1,1573)	1:65:A:PRO:HD2	1:64:A:LYS:HG3	4	0.2	0.06	0.23
(1,3240)	1:107:A:ALA:H	1:106:A:SER:HB2	4	0.2	0.06	0.22
(1,3240)	1:107:A:ALA:H	1:11:A:CYS:HB2	4	0.2	0.06	0.22
(1,982)	1:143:A:GLU:HG2	1:90:A:SER:HB3	4	0.2	0.03	0.2
(1,3027)	1:110:A:GLN:HB3	1:109:A:CYS:H	4	0.2	0.02	0.2
(1,3027)	1:110:A:GLN:HB3	1:156:A:PHE:HD1	4	0.2	0.02	0.2
(1,3152)	1:71:A:THR:HB	1:70:A:LEU:HD12	4	0.18	0.02	0.18
(1,3152)	1:71:A:THR:HB	1:70:A:LEU:HD11	4	0.18	0.02	0.18
(1,2502)	1:85:A:PHE:HE2	1:107:A:ALA:HA	4	0.17	0.06	0.15
(1,2502)	1:152:A:GLY:HA3	1:85:A:PHE:HE1	4	0.17	0.06	0.15
(1,3145)	1:52:A:ASN:HB2	1:50:A:THR:HG23	4	0.16	0.04	0.16
(1,3145)	1:52:A:ASN:HB2	1:50:A:THR:HG21	4	0.16	0.04	0.16
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG23	4	0.15	0.02	0.15
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG21	4	0.15	0.02	0.15
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG22	4	0.15	0.02	0.15
(1,2877)	1:61:A:LYS:HB3	1:23:A:THR:HA	4	0.15	0.03	0.13
(1,2877)	1:61:A:LYS:HB3	1:21:A:ALA:HA	4	0.15	0.03	0.13
(1,3296)	1:151:A:SER:H	1:86:A:GLU:HB3	4	0.14	0.03	0.15
(1,1963)	1:119:A:CYS:H	1:97:A:VAL:HG21	4	0.14	0.04	0.12
(1,1963)	1:119:A:CYS:H	1:97:A:VAL:HG23	4	0.14	0.04	0.12
(1,3021)	1:105:A:GLN:HB3	1:108:A:ASP:H	4	0.14	0.01	0.14
(1,2823)	1:125:A:ASN:HB3	1:129:A:GLN:H	4	0.14	0.01	0.14
(1,2823)	1:125:A:ASN:HD21	1:125:A:ASN:HB3	4	0.14	0.01	0.14
(1,3491)	1:18:A:GLY:H	1:68:A:TYR:HB3	4	0.13	0.02	0.12
(1,830)	1:57:A:MET:H	1:52:A:ASN:HB2	4	0.12	0.02	0.12
(1,1879)	1:94:A:ALA:H	1:141:A:PHE:HD2	4	0.12	0.02	0.12
(1,3251)	1:33:A:LEU:H	1:32:A:SER:HB2	4	0.12	0.01	0.12
(1,888)	1:101:A:MET:HB3	1:102:A:VAL:H	4	0.12	0.02	0.12
(1,1841)	1:107:A:ALA:H	1:11:A:CYS:HA	4	0.12	0.02	0.12
(1,2914)	1:142:A:LYS:HE3	1:142:A:LYS:HB2	4	0.12	0.01	0.12
(1,2914)	1:142:A:LYS:HE3	1:89:A:VAL:HB	4	0.12	0.01	0.12
(1,2740)	1:136:A:ARG:H	1:135:A:GLY:HA2	4	0.12	0.01	0.12
(1,2740)	1:145:A:GLY:H	1:145:A:GLY:HA3	4	0.12	0.01	0.12
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB2	4	0.12	0.01	0.12
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB1	4	0.12	0.01	0.12
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB3	4	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2004)	1:111:A:ALA:H	1:112:A:ALA:HB2	4	0.12	0.01	0.12
(1,2004)	1:111:A:ALA:H	1:112:A:ALA:HB3	4	0.12	0.01	0.12
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG22	4	0.11	0.01	0.11
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG21	4	0.11	0.01	0.11
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG23	4	0.11	0.01	0.11
(1,471)	1:112:A:ALA:H	1:109:A:CYS:HA	4	0.11	0.01	0.1
(1,2646)	1:38:A:ALA:HA	1:37:A:ALA:HA	4	0.1	0.0	0.1
(1,3022)	1:79:A:SER:HB3	1:156:A:PHE:HD1	3	0.43	0.05	0.45
(1,3022)	1:79:A:SER:HB3	1:159:A:GLU:H	3	0.43	0.05	0.45
(1,728)	1:17:A:LYS:HE2	1:17:A:LYS:HD2	3	0.38	0.0	0.38
(1,3486)	1:155:A:GLN:HE22	1:155:A:GLN:HG3	3	0.34	0.01	0.34
(1,3486)	1:155:A:GLN:HE22	1:155:A:GLN:HG2	3	0.34	0.01	0.34
(1,2745)	1:82:A:ARG:HD2	1:85:A:PHE:HD2	3	0.33	0.04	0.31
(1,2745)	1:82:A:ARG:HD2	1:85:A:PHE:HE2	3	0.33	0.04	0.31
(1,2710)	1:161:A:GLY:HA2	1:155:A:GLN:HG3	3	0.29	0.09	0.24
(1,2710)	1:161:A:GLY:HA2	1:155:A:GLN:HG2	3	0.29	0.09	0.24
(1,2326)	1:110:A:GLN:HE22	1:85:A:PHE:HE1	3	0.28	0.11	0.27
(1,3136)	1:52:A:ASN:H	1:50:A:THR:HG21	3	0.25	0.09	0.31
(1,3136)	1:52:A:ASN:H	1:50:A:THR:HG23	3	0.25	0.09	0.31
(1,3208)	1:70:A:LEU:H	1:16:A:ASN:HB3	3	0.25	0.14	0.16
(1,180)	1:66:A:ASP:H	1:67:A:LEU:HD21	3	0.24	0.08	0.28
(1,180)	1:66:A:ASP:H	1:67:A:LEU:HD23	3	0.24	0.08	0.28
(1,180)	1:66:A:ASP:H	1:67:A:LEU:HD22	3	0.24	0.08	0.28
(1,680)	1:20:A:ARG:H	1:20:A:ARG:HD3	3	0.23	0.08	0.23
(1,3509)	1:35:A:GLN:HE22	1:35:A:GLN:HA	3	0.21	0.08	0.24
(1,3509)	1:35:A:GLN:HE22	1:32:A:SER:HB2	3	0.21	0.08	0.24
(1,2844)	1:156:A:PHE:HB3	1:159:A:GLU:HB3	3	0.2	0.08	0.2
(1,1421)	1:108:A:ASP:HA	1:65:A:PRO:HG2	3	0.19	0.07	0.15
(1,2146)	1:154:A:LYS:H	1:121:A:ILE:HG22	3	0.19	0.02	0.2
(1,2146)	1:154:A:LYS:H	1:121:A:ILE:HG23	3	0.19	0.02	0.2
(1,2572)	1:35:A:GLN:HA	1:35:A:GLN:HG3	3	0.18	0.07	0.16
(1,3335)	1:136:A:ARG:H	1:136:A:ARG:HD3	3	0.17	0.02	0.17
(1,1062)	1:35:A:GLN:HG2	1:31:A:VAL:HA	3	0.17	0.03	0.18
(1,2803)	1:66:A:ASP:HB2	1:20:A:ARG:HB2	3	0.17	0.04	0.19
(1,3273)	1:47:A:THR:H	1:78:A:ARG:HG2	3	0.16	0.06	0.14
(1,651)	1:97:A:VAL:HG21	1:135:A:GLY:HA2	3	0.15	0.03	0.14
(1,651)	1:97:A:VAL:HG22	1:135:A:GLY:HA2	3	0.15	0.03	0.14
(1,3350)	1:127:A:HIS:H	1:128:A:ASP:HB2	3	0.15	0.04	0.13
(1,2766)	1:133:A:PHE:HB2	1:96:A:ASP:HA	3	0.14	0.03	0.12
(1,2766)	1:133:A:PHE:HB2	1:134:A:LYS:HA	3	0.14	0.03	0.12
(1,2879)	1:150:A:THR:HB	1:85:A:PHE:HD2	3	0.14	0.04	0.14
(1,277)	1:143:A:GLU:H	1:146:A:VAL:HG23	3	0.14	0.04	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,277)	1:143:A:GLU:H	1:146:A:VAL:HG22	3	0.14	0.04	0.12
(1,277)	1:143:A:GLU:H	1:146:A:VAL:HG21	3	0.14	0.04	0.12
(1,3422)	1:54:A:ASP:H	1:72:A:GLY:HA2	3	0.14	0.03	0.13
(1,2527)	1:17:A:LYS:HD2	1:17:A:LYS:HA	3	0.14	0.02	0.13
(1,3205)	1:131:A:CYS:H	1:103:A:THR:H	3	0.13	0.02	0.14
(1,251)	1:39:A:GLN:HA	1:42:A:ALA:HB3	3	0.13	0.01	0.13
(1,251)	1:39:A:GLN:HA	1:42:A:ALA:HB2	3	0.13	0.01	0.13
(1,2091)	1:56:A:LYS:H	1:56:A:LYS:HB3	3	0.13	0.02	0.13
(1,2403)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.12	0.0	0.12
(1,326)	1:100:A:ALA:H	1:100:A:ALA:HB2	3	0.12	0.01	0.12
(1,326)	1:100:A:ALA:H	1:100:A:ALA:HB1	3	0.12	0.01	0.12
(1,3238)	1:107:A:ALA:H	1:77:A:SER:HB3	3	0.12	0.02	0.11
(1,3410)	1:115:A:ALA:H	1:114:A:ALA:HA	3	0.11	0.0	0.11
(1,214)	1:146:A:VAL:HG11	1:146:A:VAL:HB	3	0.11	0.0	0.11
(1,214)	1:146:A:VAL:HG12	1:146:A:VAL:HB	3	0.11	0.0	0.11
(1,1482)	1:153:A:PRO:HG2	1:154:A:LYS:HB2	3	0.11	0.0	0.11
(1,2085)	1:102:A:VAL:H	1:101:A:MET:H	3	0.1	0.0	0.1
(1,1190)	1:59:A:HIS:HB2	1:61:A:LYS:HE3	2	1.16	0.01	1.16
(1,770)	1:81:A:ASP:HB2	1:79:A:SER:HB2	2	1.05	0.49	1.05
(1,1863)	1:21:A:ALA:H	1:61:A:LYS:HE2	2	1.02	0.04	1.02
(1,3185)	1:76:A:ALA:H	1:78:A:ARG:H	2	0.87	0.02	0.87
(1,704)	1:21:A:ALA:HB1	1:61:A:LYS:HE2	2	0.71	0.07	0.71
(1,704)	1:21:A:ALA:HB2	1:61:A:LYS:HE2	2	0.71	0.07	0.71
(1,2858)	1:16:A:ASN:HB3	1:71:A:THR:HG23	2	0.61	0.03	0.61
(1,2858)	1:16:A:ASN:HB3	1:71:A:THR:HG22	2	0.61	0.03	0.61
(1,2749)	1:82:A:ARG:HD3	1:82:A:ARG:HB2	2	0.58	0.01	0.58
(1,44)	1:151:A:SER:HB3	1:123:A:THR:HA	2	0.56	0.01	0.56
(1,3459)	1:118:A:SER:H	1:118:A:SER:HB2	2	0.54	0.4	0.54
(1,3456)	1:125:A:ASN:HD21	1:92:A:GLU:HG2	2	0.54	0.42	0.54
(1,3456)	1:125:A:ASN:HD21	1:128:A:ASP:HB2	2	0.54	0.42	0.54
(1,3538)	1:152:A:GLY:H	1:151:A:SER:HB2	2	0.54	0.03	0.54
(1,3380)	1:16:A:ASN:HD21	1:71:A:THR:HG23	2	0.53	0.23	0.53
(1,3380)	1:16:A:ASN:HD21	1:71:A:THR:HG21	2	0.53	0.23	0.53
(1,1185)	1:59:A:HIS:HB3	1:61:A:LYS:HE3	2	0.44	0.01	0.44
(1,2637)	1:140:A:ALA:HB1	1:137:A:GLY:HA2	2	0.42	0.05	0.42
(1,2379)	1:35:A:GLN:HE22	1:31:A:VAL:HG13	2	0.4	0.01	0.4
(1,2379)	1:35:A:GLN:HE22	1:31:A:VAL:HG12	2	0.4	0.01	0.4
(1,3220)	1:13:A:HIS:H	1:12:A:VAL:H	2	0.36	0.01	0.36
(1,1133)	1:39:A:GLN:HE21	1:39:A:GLN:HG2	2	0.35	0.0	0.35
(1,3502)	1:87:A:GLN:HE21	1:88:A:HIS:HA	2	0.35	0.09	0.35
(1,3502)	1:87:A:GLN:HE21	1:150:A:THR:HA	2	0.35	0.09	0.35
(1,238)	1:103:A:THR:HG23	1:101:A:MET:HG3	2	0.33	0.2	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,994)	1:61:A:LYS:HE3	1:50:A:THR:HB	2	0.33	0.14	0.33
(1,749)	1:98:A:MET:H	1:96:A:ASP:HB3	2	0.32	0.01	0.32
(1,1252)	1:65:A:PRO:HB2	1:67:A:LEU:HD13	2	0.32	0.15	0.32
(1,1252)	1:65:A:PRO:HB2	1:67:A:LEU:HD12	2	0.32	0.15	0.32
(1,2724)	1:135:A:GLY:HA2	1:120:A:GLU:HB3	2	0.3	0.01	0.3
(1,303)	1:75:A:THR:HG21	1:13:A:HIS:HD2	2	0.3	0.0	0.3
(1,303)	1:75:A:THR:HG22	1:13:A:HIS:HD2	2	0.3	0.0	0.3
(1,760)	1:64:A:LYS:HE2	1:116:A:ASP:HB2	2	0.27	0.16	0.27
(1,2378)	1:87:A:GLN:HE21	1:87:A:GLN:HB3	2	0.27	0.01	0.27
(1,81)	1:91:A:TYR:HA	1:91:A:TYR:HD2	2	0.24	0.04	0.24
(1,89)	1:51:A:TYR:HD1	1:51:A:TYR:HA	2	0.24	0.14	0.24
(1,419)	1:111:A:ALA:HB1	1:156:A:PHE:HZ	2	0.23	0.03	0.23
(1,932)	1:16:A:ASN:HD22	1:16:A:ASN:HB3	2	0.22	0.11	0.22
(1,2957)	1:86:A:GLU:HB2	1:151:A:SER:HB2	2	0.22	0.02	0.22
(1,1258)	1:86:A:GLU:HB2	1:151:A:SER:HB2	2	0.22	0.02	0.22
(1,24)	1:140:A:ALA:HB1	1:141:A:PHE:HD2	2	0.22	0.02	0.22
(1,3130)	1:60:A:VAL:H	1:23:A:THR:HG22	2	0.21	0.03	0.21
(1,2731)	1:45:A:GLY:HA2	1:44:A:ASP:HB3	2	0.2	0.02	0.2
(1,2829)	1:58:A:CYS:HB2	1:51:A:TYR:HD1	2	0.19	0.08	0.19
(1,327)	1:101:A:MET:H	1:100:A:ALA:HB1	2	0.18	0.01	0.18
(1,327)	1:101:A:MET:H	1:100:A:ALA:HB3	2	0.18	0.01	0.18
(1,536)	1:27:A:PRO:HD3	1:23:A:THR:HG21	2	0.18	0.06	0.18
(1,119)	1:52:A:ASN:HA	1:50:A:THR:HG23	2	0.18	0.02	0.18
(1,3046)	1:65:A:PRO:HG3	1:108:A:ASP:HA	2	0.18	0.0	0.18
(1,3110)	1:56:A:LYS:HG2	1:56:A:LYS:H	2	0.17	0.01	0.17
(1,2311)	1:112:A:ALA:H	1:65:A:PRO:HD2	2	0.16	0.02	0.16
(1,739)	1:131:A:CYS:HB2	1:100:A:ALA:HB3	2	0.15	0.03	0.15
(1,739)	1:131:A:CYS:HB2	1:100:A:ALA:HB2	2	0.15	0.03	0.15
(1,2933)	1:57:A:MET:HG3	1:27:A:PRO:HB3	2	0.15	0.0	0.15
(1,2833)	1:125:A:ASN:HB2	1:130:A:LYS:HG2	2	0.15	0.0	0.15
(1,2730)	1:45:A:GLY:HA3	1:44:A:ASP:HB3	2	0.14	0.03	0.14
(1,2588)	1:75:A:THR:HG21	1:76:A:ALA:HA	2	0.14	0.03	0.14
(1,2588)	1:75:A:THR:HG23	1:76:A:ALA:HA	2	0.14	0.03	0.14
(1,607)	1:24:A:ILE:HG22	1:25:A:GLY:HA3	2	0.14	0.02	0.14
(1,607)	1:24:A:ILE:HG23	1:25:A:GLY:HA3	2	0.14	0.02	0.14
(1,2763)	1:136:A:ARG:HD3	1:136:A:ARG:HG3	2	0.14	0.01	0.14
(1,2857)	1:16:A:ASN:HB3	1:71:A:THR:HA	2	0.14	0.01	0.14
(1,938)	1:16:A:ASN:HD22	1:16:A:ASN:HB2	2	0.13	0.0	0.13
(1,1130)	1:39:A:GLN:HE22	1:39:A:GLN:HG2	2	0.12	0.0	0.12
(1,1799)	1:120:A:GLU:H	1:120:A:GLU:HG3	2	0.12	0.01	0.12
(1,894)	1:102:A:VAL:H	1:101:A:MET:HB2	2	0.12	0.0	0.12
(1,1207)	1:57:A:MET:HG3	1:27:A:PRO:HB3	2	0.12	0.0	0.12

Continued on next page...

Continued from previous page...

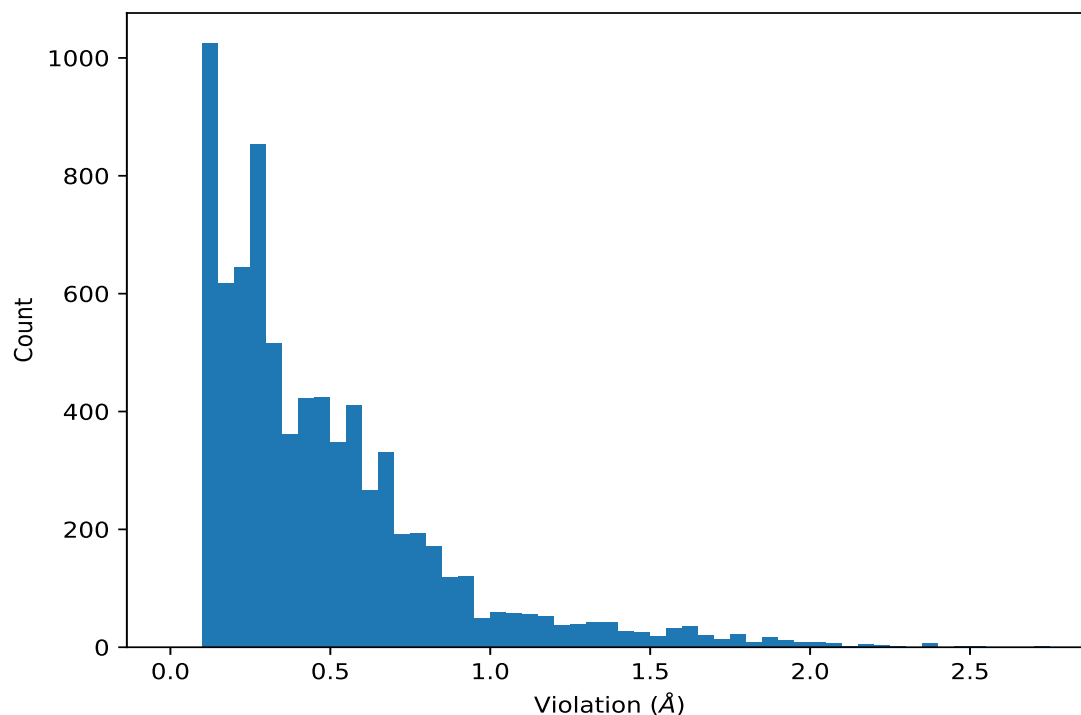
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,537)	1:22:A:PRO:HD3	1:21:A:ALA:HB3	2	0.11	0.0	0.11
(1,537)	1:22:A:PRO:HD3	1:21:A:ALA:HB2	2	0.11	0.0	0.11
(1,2233)	1:98:A:MET:H	1:96:A:ASP:HA	2	0.11	0.01	0.11
(1,2968)	1:159:A:GLU:HB3	1:159:A:GLU:HG3	2	0.11	0.01	0.11
(1,383)	1:36:A:CYS:HA	1:58:A:CYS:HB3	2	0.11	0.0	0.11
(1,1656)	1:60:A:VAL:HG13	1:49:A:PHE:HA	2	0.11	0.0	0.11
(1,413)	1:21:A:ALA:HB2	1:21:A:ALA:HA	2	0.1	0.0	0.1
(1,413)	1:21:A:ALA:HB3	1:21:A:ALA:HA	2	0.1	0.0	0.1
(1,828)	1:55:A:SER:H	1:52:A:ASN:HB2	2	0.1	0.0	0.1
(1,3199)	1:52:A:ASN:H	1:57:A:MET:HB2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



9.5.2 Table : All distance violations

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	10	2.72
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG12	7	2.52
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	1	2.45
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	1	2.4
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG12	9	2.39
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	2	2.37
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	8	2.37
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	4	2.35
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	6	2.35
(1,2927)	1:31:A:VAL:HG23	1:57:A:MET:HG3	5	2.25
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG12	3	2.23
(1,2927)	1:31:A:VAL:HG22	1:57:A:MET:HG3	1	2.23
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG13	5	2.2
(1,2927)	1:31:A:VAL:HG21	1:57:A:MET:HG3	4	2.19
(1,2927)	1:31:A:VAL:HG22	1:57:A:MET:HG3	8	2.19
(1,2927)	1:31:A:VAL:HG22	1:57:A:MET:HG3	2	2.18
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	3	2.18
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	6	2.17
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	8	2.14
(1,2927)	1:31:A:VAL:HG21	1:57:A:MET:HG3	9	2.12
(1,2927)	1:31:A:VAL:HG21	1:57:A:MET:HG3	7	2.09
(1,3018)	1:35:A:GLN:HB2	1:28:A:VAL:HG12	10	2.07
(1,2788)	1:142:A:LYS:HE2	1:142:A:LYS:H	4	2.07
(1,2788)	1:142:A:LYS:HE2	1:142:A:LYS:H	5	2.07
(1,1476)	1:33:A:LEU:HD13	1:14:A:SER:HB2	8	2.07
(1,2976)	1:26:A:GLU:HB2	1:23:A:THR:HG23	2	2.06
(1,2927)	1:31:A:VAL:HG21	1:57:A:MET:HG3	3	2.05
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	3	2.04
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	8	2.03
(1,2698)	1:73:A:GLY:HA3	1:74:A:LYS:HB3	4	2.03
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD2	2	2.02
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD2	9	2.02
(1,2788)	1:142:A:LYS:HE2	1:142:A:LYS:H	7	2.0
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	5	2.0
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	8	1.99
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	4	1.99
(1,2927)	1:31:A:VAL:HG22	1:57:A:MET:HG3	10	1.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	5	1.98
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	9	1.98
(1,2788)	1:142:A:LYS:HE2	1:142:A:LYS:H	10	1.97
(1,2747)	1:49:A:PHE:HB3	1:59:A:HIS:HB3	3	1.97
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	5	1.97
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	6	1.96
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	10	1.95
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	4	1.95
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	3	1.95
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	2	1.95
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	2	1.95
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	4	1.95
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	2	1.94
(1,2927)	1:31:A:VAL:HG23	1:57:A:MET:HG3	6	1.93
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	1	1.92
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	9	1.92
(1,2604)	1:149:A:VAL:HG21	1:92:A:GLU:HG3	4	1.91
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	4	1.91
(1,2747)	1:49:A:PHE:HB3	1:59:A:HIS:HB3	8	1.9
(1,2723)	1:152:A:GLY:HA3	1:153:A:PRO:HG2	2	1.9
(1,2604)	1:149:A:VAL:HG23	1:92:A:GLU:HG3	7	1.9
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	5	1.9
(1,2976)	1:26:A:GLU:HB2	1:23:A:THR:HG23	4	1.89
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD2	6	1.89
(1,2976)	1:112:A:ALA:HB3	1:98:A:MET:HG2	5	1.88
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	5	1.88
(1,2604)	1:149:A:VAL:HG23	1:92:A:GLU:HG3	5	1.88
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	9	1.87
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	9	1.87
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	8	1.86
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	10	1.86
(1,2604)	1:149:A:VAL:HG21	1:92:A:GLU:HG3	9	1.86
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	3	1.86
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG23	6	1.85
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD2	3	1.85
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG22	3	1.84
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	7	1.84
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB1	9	1.84
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	7	1.83
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	4	1.83
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD12	9	1.81
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	7	1.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	6	1.8
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	4	1.79
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	8	1.79
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD11	10	1.79
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	5	1.79
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG21	7	1.78
(1,2976)	1:26:A:GLU:HB2	1:23:A:THR:HG22	8	1.78
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD2	1	1.78
(1,2604)	1:149:A:VAL:HG23	1:92:A:GLU:HG3	6	1.78
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	3	1.78
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB2	1	1.78
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD11	10	1.77
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	3	1.77
(1,2698)	1:73:A:GLY:HA3	1:52:A:ASN:HB2	1	1.77
(1,2604)	1:149:A:VAL:HG21	1:92:A:GLU:HG3	1	1.77
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	1	1.77
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	6	1.77
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	5	1.76
(1,3274)	1:67:A:LEU:H	1:68:A:TYR:HB2	6	1.75
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD11	2	1.75
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD12	5	1.75
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB3	3	1.75
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD11	5	1.75
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	9	1.74
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	1	1.74
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB3	2	1.74
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	8	1.74
(1,3274)	1:67:A:LEU:H	1:68:A:TYR:HB2	10	1.73
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	4	1.73
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	9	1.73
(1,3274)	1:67:A:LEU:H	1:68:A:TYR:HB2	1	1.72
(1,3274)	1:67:A:LEU:H	1:68:A:TYR:HB2	7	1.72
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD11	3	1.72
(1,2604)	1:149:A:VAL:HG21	1:92:A:GLU:HG3	10	1.72
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	7	1.72
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB3	8	1.71
(1,2976)	1:26:A:GLU:HB2	1:23:A:THR:HG23	9	1.7
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	6	1.7
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	5	1.7
(1,3142)	1:47:A:THR:HG21	1:62:A:GLU:HB2	3	1.69
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	7	1.69
(1,3142)	1:47:A:THR:HG21	1:62:A:GLU:HG2	1	1.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HB2	8	1.68
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	8	1.68
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	3	1.68
(1,329)	1:100:A:ALA:HB2	1:130:A:LYS:HE2	7	1.68
(1,1405)	1:88:A:HIS:HB2	1:145:A:GLY:HA3	10	1.67
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	2	1.67
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	10	1.67
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HG2	10	1.66
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD11	6	1.66
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD11	7	1.66
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB1	6	1.66
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB1	7	1.66
(1,800)	1:128:A:ASP:HB2	1:130:A:LYS:HB3	9	1.66
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD21	10	1.66
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HG2	2	1.65
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	8	1.65
(1,329)	1:100:A:ALA:HB2	1:130:A:LYS:HE2	2	1.65
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HB2	7	1.64
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	2	1.64
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	9	1.64
(1,2604)	1:149:A:VAL:HG22	1:92:A:GLU:HG3	3	1.64
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	7	1.64
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD12	3	1.64
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	9	1.63
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	7	1.63
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	8	1.63
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	10	1.63
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB3	10	1.63
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	2	1.62
(1,3142)	1:47:A:THR:HG22	1:62:A:GLU:HB2	5	1.62
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	2	1.62
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	8	1.62
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB3	9	1.62
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	6	1.62
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD12	4	1.62
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD11	9	1.62
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	5	1.62
(1,3142)	1:47:A:THR:HG22	1:62:A:GLU:HB2	4	1.61
(1,3142)	1:47:A:THR:HG22	1:62:A:GLU:HG2	6	1.61
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	2	1.61
(1,2894)	1:36:A:CYS:HB3	1:28:A:VAL:HB	4	1.61
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	4	1.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	10	1.61
(1,3142)	1:47:A:THR:HG23	1:62:A:GLU:HG2	9	1.6
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	5	1.6
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB2	5	1.6
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	2	1.6
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	10	1.6
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	8	1.6
(1,2976)	1:112:A:ALA:HB3	1:98:A:MET:HG2	1	1.59
(1,2747)	1:49:A:PHE:HB3	1:59:A:HIS:HB3	4	1.59
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	10	1.59
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	5	1.59
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD13	8	1.58
(1,2894)	1:80:A:CYS:HB2	1:9:A:LEU:HB3	3	1.58
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	9	1.58
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD11	6	1.58
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	3	1.58
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	4	1.58
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	6	1.58
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	2	1.58
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	4	1.58
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD13	1	1.57
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	3	1.57
(1,2894)	1:80:A:CYS:HB2	1:9:A:LEU:HB3	1	1.57
(1,2604)	1:149:A:VAL:HG21	1:92:A:GLU:HG3	8	1.57
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	2	1.57
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	3	1.57
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB3	4	1.57
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	7	1.57
(1,2981)	1:41:A:LYS:HD3	1:38:A:ALA:H	6	1.56
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	1	1.56
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	7	1.56
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	3	1.56
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	3	1.55
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB2	2	1.55
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG21	9	1.55
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	1	1.55
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	9	1.55
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	5	1.55
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	9	1.55
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	4	1.54
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD12	2	1.54
(1,770)	1:81:A:ASP:HB2	1:79:A:SER:HB2	4	1.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2894)	1:36:A:CYS:HB3	1:35:A:GLN:HB2	6	1.53
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB2	5	1.53
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	3	1.53
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	2	1.53
(1,1131)	1:57:A:MET:HG3	1:59:A:HIS:HB3	8	1.53
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD12	8	1.52
(1,535)	1:4:A:PRO:HD3	1:35:A:GLN:HB3	9	1.52
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	9	1.51
(1,2976)	1:26:A:GLU:HB3	1:23:A:THR:HG22	10	1.51
(1,1318)	1:127:A:HIS:HB2	1:128:A:ASP:HB2	1	1.51
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	5	1.51
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	7	1.51
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	7	1.5
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD12	7	1.5
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	8	1.5
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	9	1.49
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	6	1.49
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	10	1.49
(1,2634)	1:112:A:ALA:HB3	1:111:A:ALA:HB2	9	1.49
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	2	1.49
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	7	1.49
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	9	1.49
(1,2923)	1:39:A:GLN:HG2	1:42:A:ALA:H	8	1.48
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	1	1.48
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	4	1.48
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	7	1.48
(1,329)	1:100:A:ALA:HB1	1:130:A:LYS:HE2	9	1.48
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	9	1.47
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB3	5	1.47
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	6	1.47
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	7	1.47
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	2	1.47
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	10	1.47
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB2	6	1.46
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB2	8	1.46
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB2	10	1.46
(1,2634)	1:112:A:ALA:HB3	1:111:A:ALA:HB2	6	1.46
(1,2604)	1:149:A:VAL:HG23	1:92:A:GLU:HG3	2	1.46
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	10	1.46
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	6	1.46
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	3	1.46
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG21	10	1.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB3	2	1.45
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB2	3	1.45
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB2	7	1.45
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB1	9	1.45
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	9	1.45
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	3	1.45
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	8	1.44
(1,3019)	1:34:A:GLU:HB2	1:9:A:LEU:HD13	4	1.44
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB3	1	1.44
(1,2661)	1:37:A:ALA:HA	1:38:A:ALA:HB1	4	1.44
(1,2634)	1:112:A:ALA:HB3	1:111:A:ALA:HB2	4	1.44
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	2	1.44
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	6	1.44
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	5	1.43
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	5	1.43
(1,1279)	1:105:A:GLN:HG3	1:67:A:LEU:HD13	1	1.43
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	9	1.43
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	6	1.43
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	6	1.42
(1,2894)	1:80:A:CYS:HB2	1:9:A:LEU:HB3	5	1.42
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	7	1.42
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	8	1.42
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	2	1.42
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	6	1.42
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	8	1.41
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	9	1.41
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG23	8	1.4
(1,3195)	1:125:A:ASN:H	1:128:A:ASP:HB2	9	1.4
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	5	1.4
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	8	1.4
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	1	1.4
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	6	1.4
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	2	1.4
(1,3494)	1:55:A:SER:H	1:57:A:MET:HB2	8	1.39
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	3	1.39
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG21	10	1.39
(1,1297)	1:105:A:GLN:HG2	1:76:A:ALA:HB1	10	1.39
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	2	1.39
(1,3494)	1:55:A:SER:H	1:57:A:MET:HB2	5	1.38
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG22	2	1.38
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	2	1.38
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	9	1.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	4	1.38
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	1	1.38
(1,339)	1:149:A:VAL:HG22	1:88:A:HIS:HB2	1	1.38
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	3	1.38
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	2	1.37
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	3	1.37
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	9	1.37
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	3	1.37
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	6	1.37
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	3	1.37
(1,339)	1:149:A:VAL:HG22	1:88:A:HIS:HB2	8	1.37
(1,339)	1:149:A:VAL:HG22	1:88:A:HIS:HB2	10	1.37
(1,3494)	1:55:A:SER:H	1:57:A:MET:HB2	4	1.36
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG21	3	1.36
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	7	1.36
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	4	1.36
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	8	1.35
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	6	1.35
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	1	1.35
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	3	1.35
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	5	1.35
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	8	1.35
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	10	1.35
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	5	1.35
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	4	1.35
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	5	1.35
(1,339)	1:149:A:VAL:HG21	1:88:A:HIS:HB2	7	1.35
(1,3494)	1:55:A:SER:H	1:6:A:LYS:HD2	6	1.34
(1,2936)	1:59:A:HIS:HB2	1:61:A:LYS:HD2	9	1.34
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	8	1.34
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	2	1.34
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	4	1.34
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	8	1.34
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	1	1.34
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	2	1.34
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	9	1.34
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	3	1.34
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB2	1	1.33
(1,2275)	1:40:A:CYS:H	1:41:A:LYS:HB3	6	1.33
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	7	1.33
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	10	1.33
(1,339)	1:149:A:VAL:HG21	1:88:A:HIS:HB2	2	1.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	1	1.33
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	3	1.33
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	6	1.33
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	4	1.33
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	9	1.32
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG22	5	1.32
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	9	1.32
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	4	1.32
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	1	1.32
(1,797)	1:130:A:LYS:H	1:128:A:ASP:HB2	9	1.32
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	4	1.32
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	5	1.32
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	9	1.32
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	10	1.32
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	10	1.31
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG21	8	1.31
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	6	1.31
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	7	1.31
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	2	1.31
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG22	4	1.31
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	10	1.31
(1,339)	1:149:A:VAL:HG22	1:88:A:HIS:HB2	9	1.31
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	3	1.3
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG23	4	1.3
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	10	1.3
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG21	3	1.3
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG21	1	1.3
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	10	1.3
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	6	1.29
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	9	1.29
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	3	1.29
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	9	1.29
(1,973)	1:85:A:PHE:HB3	1:82:A:ARG:HB2	1	1.29
(1,339)	1:149:A:VAL:HG23	1:88:A:HIS:HB2	3	1.29
(1,3368)	1:129:A:GLN:H	1:149:A:VAL:HG11	1	1.28
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG22	4	1.28
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	1	1.28
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	10	1.28
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	10	1.28
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	1	1.28
(1,1191)	1:59:A:HIS:HB2	1:61:A:LYS:HG2	4	1.28
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	8	1.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	5	1.27
(1,2960)	1:78:A:ARG:HB2	1:77:A:SER:HA	10	1.27
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	10	1.27
(1,1852)	1:60:A:VAL:H	1:27:A:PRO:HG2	1	1.27
(1,1611)	1:7:A:LEU:HD12	1:4:A:PRO:HD3	9	1.27
(1,171)	1:12:A:VAL:HG21	1:74:A:LYS:HB2	5	1.27
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	7	1.27
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG23	2	1.26
(1,2960)	1:78:A:ARG:HB2	1:77:A:SER:HA	9	1.26
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG22	1	1.26
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG23	7	1.26
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG21	10	1.26
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	4	1.26
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	5	1.26
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	1	1.26
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	7	1.26
(1,339)	1:149:A:VAL:HG21	1:88:A:HIS:HB2	6	1.26
(1,3368)	1:129:A:GLN:H	1:149:A:VAL:HG12	3	1.25
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	5	1.25
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG23	7	1.25
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG23	2	1.25
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG23	5	1.25
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG21	8	1.25
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	8	1.25
(1,152)	1:40:A:CYS:HA	1:39:A:GLN:HG2	8	1.25
(1,2936)	1:59:A:HIS:HB2	1:23:A:THR:HG22	6	1.24
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG21	8	1.24
(1,2494)	1:49:A:PHE:HD2	1:37:A:ALA:HB3	4	1.24
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	3	1.24
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	2	1.24
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	7	1.24
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	1	1.24
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	5	1.24
(1,339)	1:149:A:VAL:HG22	1:88:A:HIS:HB2	4	1.24
(1,171)	1:12:A:VAL:HG23	1:74:A:LYS:HB2	2	1.24
(1,171)	1:12:A:VAL:HG21	1:74:A:LYS:HB2	3	1.24
(1,171)	1:12:A:VAL:HG23	1:74:A:LYS:HB2	8	1.24
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	4	1.23
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	7	1.23
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	7	1.23
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	9	1.23
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	4	1.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	9	1.23
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	3	1.22
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	2	1.22
(1,2960)	1:78:A:ARG:HB2	1:77:A:SER:HA	6	1.22
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	2	1.22
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	4	1.22
(1,339)	1:149:A:VAL:HG21	1:88:A:HIS:HB2	5	1.22
(1,171)	1:12:A:VAL:HG23	1:74:A:LYS:HB2	6	1.22
(1,171)	1:12:A:VAL:HG21	1:74:A:LYS:HB2	7	1.22
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG21	9	1.21
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	4	1.21
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	7	1.21
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	4	1.21
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG21	3	1.21
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG21	6	1.21
(1,2761)	1:49:A:PHE:HB2	1:39:A:GLN:HG3	3	1.21
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	6	1.21
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	4	1.21
(1,1611)	1:7:A:LEU:HD11	1:4:A:PRO:HD3	10	1.21
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	10	1.21
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	3	1.21
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	1	1.2
(1,3368)	1:129:A:GLN:H	1:149:A:VAL:HG12	7	1.2
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG23	2	1.2
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG23	7	1.2
(1,3320)	1:39:A:GLN:H	1:60:A:VAL:HG12	9	1.2
(1,2785)	1:130:A:LYS:HE3	1:125:A:ASN:HD21	8	1.2
(1,2595)	1:75:A:THR:HG21	1:13:A:HIS:HB2	9	1.2
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	2	1.2
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	1	1.2
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	1	1.2
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	2	1.2
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	7	1.2
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	8	1.2
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	9	1.2
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB1	5	1.19
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG23	7	1.19
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD21	5	1.19
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	5	1.19
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	6	1.19
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	10	1.19
(1,171)	1:12:A:VAL:HG21	1:74:A:LYS:HB2	1	1.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:12:A:VAL:HG23	1:74:A:LYS:HB2	4	1.19
(1,171)	1:12:A:VAL:HG21	1:74:A:LYS:HB2	10	1.19
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	3	1.19
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG23	5	1.18
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG21	8	1.18
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	5	1.18
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG23	1	1.18
(1,2595)	1:75:A:THR:HG21	1:13:A:HIS:HB2	5	1.18
(1,1624)	1:59:A:HIS:HB2	1:23:A:THR:HG22	6	1.18
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	7	1.18
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	6	1.18
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB2	5	1.18
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	7	1.18
(1,1183)	1:59:A:HIS:HB3	1:58:A:CYS:HA	4	1.18
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	2	1.18
(1,437)	1:38:A:ALA:HA	1:41:A:LYS:HB3	6	1.18
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	2	1.18
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	8	1.17
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	10	1.17
(1,1190)	1:59:A:HIS:HB2	1:61:A:LYS:HE3	4	1.17
(1,3412)	1:115:A:ALA:H	1:112:A:ALA:HB2	9	1.16
(1,3274)	1:67:A:LEU:H	1:17:A:LYS:HE2	4	1.16
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	8	1.16
(1,2929)	1:135:A:GLY:H	1:97:A:VAL:HB	8	1.16
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	9	1.16
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	9	1.16
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	2	1.16
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	8	1.16
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG21	3	1.16
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG23	5	1.16
(1,171)	1:12:A:VAL:HG23	1:74:A:LYS:HB2	9	1.16
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	9	1.16
(1,3092)	1:49:A:PHE:H	1:76:A:ALA:HB3	7	1.15
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	5	1.15
(1,2629)	1:111:A:ALA:HB1	1:110:A:GLN:H	3	1.15
(1,1190)	1:59:A:HIS:HB2	1:61:A:LYS:HE3	3	1.15
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB3	2	1.15
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	1	1.14
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	6	1.14
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB3	10	1.14
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	3	1.14
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	6	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	10	1.14
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG21	5	1.13
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG22	10	1.13
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG23	1	1.13
(1,3092)	1:49:A:PHE:H	1:76:A:ALA:HB3	6	1.13
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB1	8	1.13
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	1	1.13
(1,2788)	1:142:A:LYS:HE2	1:91:A:TYR:HD1	8	1.13
(1,2556)	1:71:A:THR:HG22	1:54:A:ASP:HB2	6	1.13
(1,2494)	1:49:A:PHE:HD2	1:37:A:ALA:HB1	3	1.13
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	5	1.13
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	6	1.13
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	5	1.13
(1,3412)	1:115:A:ALA:H	1:112:A:ALA:HB3	2	1.12
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG23	4	1.12
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB2	10	1.12
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	1	1.12
(1,2634)	1:112:A:ALA:HB1	1:111:A:ALA:HB1	2	1.12
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	5	1.12
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	7	1.12
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	5	1.12
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	5	1.12
(1,3320)	1:39:A:GLN:H	1:60:A:VAL:HG12	6	1.11
(1,3093)	1:76:A:ALA:HB3	1:80:A:CYS:HA	3	1.11
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB3	1	1.11
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB3	5	1.11
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	7	1.11
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	4	1.11
(1,2898)	1:36:A:CYS:HB2	1:28:A:VAL:HG21	9	1.11
(1,2747)	1:82:A:ARG:HD3	1:85:A:PHE:HB3	1	1.11
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	1	1.11
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	6	1.11
(1,1374)	1:27:A:PRO:HG2	1:23:A:THR:HB	9	1.11
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	4	1.11
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG23	2	1.11
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG21	8	1.11
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG22	10	1.11
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	2	1.1
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	1	1.1
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG21	10	1.1
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	10	1.1
(1,2634)	1:112:A:ALA:HB1	1:111:A:ALA:HB1	8	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2629)	1:111:A:ALA:HB1	1:110:A:GLN:H	2	1.1
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	4	1.1
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD23	1	1.1
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	6	1.1
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	10	1.09
(1,2629)	1:111:A:ALA:HB3	1:110:A:GLN:H	10	1.09
(1,2595)	1:75:A:THR:HG21	1:48:A:HIS:HB3	8	1.09
(1,2595)	1:75:A:THR:HG21	1:48:A:HIS:HB3	10	1.09
(1,1819)	1:53:A:ASP:H	1:74:A:LYS:HB3	7	1.09
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	5	1.09
(1,1278)	1:105:A:GLN:HG2	1:77:A:SER:H	10	1.09
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG23	7	1.09
(1,1081)	1:4:A:PRO:HB3	1:32:A:SER:HB3	4	1.09
(1,3412)	1:16:A:ASN:HD22	1:71:A:THR:HG21	3	1.08
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG23	6	1.08
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB1	2	1.08
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	7	1.08
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	7	1.08
(1,2629)	1:111:A:ALA:HB1	1:110:A:GLN:H	8	1.08
(1,2595)	1:75:A:THR:HG21	1:48:A:HIS:HB3	7	1.08
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	1	1.08
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	10	1.08
(1,3412)	1:115:A:ALA:H	1:112:A:ALA:HB2	4	1.07
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG22	10	1.07
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	5	1.07
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	7	1.07
(1,2851)	1:100:A:ALA:HB1	1:101:A:MET:HB2	9	1.07
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	2	1.07
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	7	1.07
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	9	1.07
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	6	1.07
(1,3449)	1:130:A:LYS:H	1:129:A:GLN:HB2	9	1.06
(1,2944)	1:60:A:VAL:HB	1:23:A:THR:HG22	4	1.06
(1,2595)	1:75:A:THR:HG22	1:48:A:HIS:HB3	2	1.06
(1,2595)	1:75:A:THR:HG22	1:48:A:HIS:HB3	6	1.06
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	8	1.06
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB1	9	1.06
(1,2357)	1:97:A:VAL:H	1:134:A:LYS:HG3	10	1.06
(1,1863)	1:21:A:ALA:H	1:61:A:LYS:HE2	4	1.06
(1,1663)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	8	1.06
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	10	1.06
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	3	1.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	4	1.06
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	1	1.06
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	8	1.06
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB2	9	1.05
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	3	1.05
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	1	1.05
(1,2667)	1:94:A:ALA:HB3	1:121:A:ILE:HG12	3	1.05
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB2	7	1.05
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	2	1.05
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	5	1.05
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	6	1.05
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB1	1	1.05
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	9	1.05
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	8	1.05
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	9	1.05
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	2	1.05
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	6	1.05
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	8	1.05
(1,118)	1:73:A:GLY:HA3	1:52:A:ASN:HA	7	1.05
(1,3320)	1:39:A:GLN:H	1:28:A:VAL:HG21	3	1.04
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	6	1.04
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	1	1.04
(1,2583)	1:146:A:VAL:HG13	1:143:A:GLU:HB3	5	1.04
(1,2556)	1:71:A:THR:HG23	1:54:A:ASP:HB2	5	1.04
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	1	1.04
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	3	1.04
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	2	1.04
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	1	1.04
(1,1186)	1:59:A:HIS:HB3	1:50:A:THR:HG21	6	1.04
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	2	1.03
(1,2859)	1:71:A:THR:HG22	1:16:A:ASN:HB2	8	1.03
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	1	1.03
(1,2667)	1:94:A:ALA:HB2	1:121:A:ILE:HG12	10	1.03
(1,2634)	1:112:A:ALA:HB2	1:111:A:ALA:HB1	3	1.03
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	4	1.03
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	9	1.03
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	10	1.03
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB3	6	1.03
(1,1414)	1:134:A:LYS:HG3	1:96:A:ASP:HB2	1	1.03
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	5	1.03
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	7	1.03
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	6	1.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB1	8	1.02
(1,2851)	1:100:A:ALA:HB3	1:101:A:MET:HB2	5	1.02
(1,2713)	1:148:A:GLY:HA2	1:147:A:LEU:HB2	5	1.02
(1,2583)	1:146:A:VAL:HG13	1:143:A:GLU:HB3	4	1.02
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	5	1.02
(1,2494)	1:49:A:PHE:HD2	1:37:A:ALA:HB1	7	1.02
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD23	1	1.02
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD22	2	1.02
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD21	6	1.02
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD21	8	1.02
(1,1233)	1:146:A:VAL:HB	1:88:A:HIS:HB2	9	1.02
(1,3092)	1:11:A:CYS:H	1:76:A:ALA:HB1	4	1.01
(1,2929)	1:62:A:GLU:HB3	1:47:A:THR:H	5	1.01
(1,2822)	1:52:A:ASN:HB3	1:57:A:MET:HB2	3	1.01
(1,2713)	1:148:A:GLY:HA2	1:147:A:LEU:HB2	8	1.01
(1,2667)	1:94:A:ALA:HB3	1:121:A:ILE:HG12	6	1.01
(1,2636)	1:37:A:ALA:HB3	1:33:A:LEU:HA	4	1.01
(1,2636)	1:37:A:ALA:HB1	1:33:A:LEU:HA	5	1.01
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	2	1.01
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB2	10	1.01
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD21	4	1.01
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD22	5	1.01
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD22	7	1.01
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD22	9	1.01
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	10	1.01
(1,3368)	1:129:A:GLN:H	1:149:A:VAL:HG11	8	1.0
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	2	1.0
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	4	1.0
(1,2892)	1:80:A:CYS:HB2	1:11:A:CYS:HB2	5	1.0
(1,2852)	1:112:A:ALA:HB3	1:101:A:MET:HB2	9	1.0
(1,2851)	1:100:A:ALA:HB3	1:101:A:MET:HB2	4	1.0
(1,2667)	1:94:A:ALA:HB3	1:121:A:ILE:HG12	4	1.0
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	4	1.0
(1,2509)	1:130:A:LYS:HB3	1:102:A:VAL:HA	7	1.0
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD22	3	1.0
(1,1672)	1:147:A:LEU:HB2	1:147:A:LEU:HD23	10	1.0
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	9	1.0
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	9	0.99
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG23	1	0.99
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG23	8	0.99
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD13	4	0.99
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	10	0.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2852)	1:112:A:ALA:HB2	1:101:A:MET:HB2	8	0.99
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG21	7	0.99
(1,2822)	1:52:A:ASN:HB3	1:57:A:MET:HB2	1	0.99
(1,2636)	1:37:A:ALA:HB1	1:33:A:LEU:HA	6	0.99
(1,2583)	1:146:A:VAL:HG12	1:143:A:GLU:HB3	2	0.99
(1,2583)	1:146:A:VAL:HG12	1:143:A:GLU:HB3	7	0.99
(1,2568)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	6	0.99
(1,2568)	1:43:A:VAL:HG22	1:60:A:VAL:HB	8	0.99
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD23	6	0.99
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	4	0.98
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	9	0.98
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG23	5	0.98
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	4	0.98
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	5	0.98
(1,2974)	1:98:A:MET:HG2	1:119:A:CYS:HB3	8	0.98
(1,2944)	1:60:A:VAL:HB	1:23:A:THR:HG21	8	0.98
(1,2713)	1:148:A:GLY:HA2	1:147:A:LEU:HB2	10	0.98
(1,2636)	1:37:A:ALA:HB1	1:33:A:LEU:HA	9	0.98
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	6	0.98
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB3	2	0.98
(1,1863)	1:21:A:ALA:H	1:61:A:LYS:HE2	3	0.98
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	3	0.98
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	5	0.98
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD21	9	0.98
(1,3461)	1:155:A:GLN:HE22	1:154:A:LYS:HA	10	0.97
(1,3092)	1:49:A:PHE:H	1:76:A:ALA:HB1	3	0.97
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	7	0.97
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB3	3	0.97
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD12	10	0.97
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	9	0.97
(1,2569)	1:97:A:VAL:HG11	1:120:A:GLU:HB2	2	0.97
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	1	0.97
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	9	0.97
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	8	0.97
(1,3520)	1:39:A:GLN:HE22	1:60:A:VAL:HG11	9	0.96
(1,3456)	1:125:A:ASN:HD21	1:92:A:GLU:HG2	9	0.96
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	5	0.96
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	3	0.96
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD11	6	0.96
(1,2859)	1:71:A:THR:HG22	1:16:A:ASN:HB2	10	0.96
(1,2667)	1:94:A:ALA:HB1	1:121:A:ILE:HG12	5	0.96
(1,2667)	1:94:A:ALA:HB1	1:121:A:ILE:HG12	7	0.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2636)	1:37:A:ALA:HB2	1:33:A:LEU:HA	8	0.96
(1,2568)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	3	0.96
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD23	4	0.96
(1,3459)	1:118:A:SER:H	1:118:A:SER:HB2	9	0.95
(1,3327)	1:90:A:SER:H	1:89:A:VAL:HG11	6	0.95
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	1	0.95
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	10	0.95
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD13	1	0.95
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD11	2	0.95
(1,2974)	1:98:A:MET:HG2	1:119:A:CYS:HB3	9	0.95
(1,2962)	1:65:A:PRO:HB3	1:67:A:LEU:HG	4	0.95
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	3	0.95
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	8	0.95
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	2	0.95
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB3	5	0.95
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB2	7	0.95
(1,2859)	1:71:A:THR:HG21	1:16:A:ASN:HB2	1	0.95
(1,2667)	1:94:A:ALA:HB1	1:121:A:ILE:HG12	8	0.95
(1,2636)	1:37:A:ALA:HB2	1:33:A:LEU:HA	10	0.95
(1,2629)	1:111:A:ALA:HB2	1:110:A:GLN:H	5	0.95
(1,2585)	1:97:A:VAL:HG12	1:134:A:LYS:HB2	10	0.95
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG22	3	0.95
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	7	0.95
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	4	0.95
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	2	0.95
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	10	0.95
(1,3494)	1:55:A:SER:H	1:56:A:LYS:HD3	7	0.94
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	8	0.94
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG22	5	0.94
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB2	7	0.94
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	3	0.94
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB2	10	0.94
(1,2852)	1:112:A:ALA:HB2	1:101:A:MET:HB2	2	0.94
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG21	3	0.94
(1,2822)	1:52:A:ASN:HB3	1:57:A:MET:HB2	2	0.94
(1,2568)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	5	0.94
(1,1584)	1:74:A:LYS:HG2	1:14:A:SER:HB2	3	0.94
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	2	0.94
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	3	0.94
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	10	0.94
(1,396)	1:107:A:ALA:HB1	1:77:A:SER:HB2	5	0.94
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	1	0.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	9	0.94
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG22	10	0.93
(1,3461)	1:110:A:GLN:HE22	1:157:A:CYS:HB3	5	0.93
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	1	0.93
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	3	0.93
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	4	0.93
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD11	5	0.93
(1,2974)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	6	0.93
(1,2960)	1:78:A:ARG:HB2	1:40:A:CYS:HA	1	0.93
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	3	0.93
(1,2892)	1:80:A:CYS:HB2	1:11:A:CYS:HB2	6	0.93
(1,2852)	1:112:A:ALA:HB3	1:101:A:MET:HB2	10	0.93
(1,2747)	1:82:A:ARG:HD3	1:85:A:PHE:HB3	7	0.93
(1,2583)	1:146:A:VAL:HG11	1:143:A:GLU:HB3	6	0.93
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	2	0.93
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	6	0.93
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	10	0.93
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB1	7	0.93
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD21	6	0.92
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD22	8	0.92
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB2	2	0.92
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	6	0.92
(1,3093)	1:76:A:ALA:HB3	1:80:A:CYS:HA	1	0.92
(1,3093)	1:76:A:ALA:HB2	1:80:A:CYS:HA	7	0.92
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD11	7	0.92
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	2	0.92
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	9	0.92
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD13	1	0.92
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG23	1	0.92
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB3	9	0.92
(1,2822)	1:108:A:ASP:HB3	1:67:A:LEU:HG	10	0.92
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	2	0.92
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB3	1	0.92
(1,2667)	1:94:A:ALA:HB2	1:121:A:ILE:HG12	1	0.92
(1,2636)	1:37:A:ALA:HB2	1:33:A:LEU:HA	2	0.92
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	8	0.92
(1,2568)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	7	0.92
(1,1663)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	4	0.92
(1,1181)	1:64:A:LYS:HE2	1:64:A:LYS:HB2	6	0.92
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	1	0.92
(1,218)	1:89:A:VAL:HG22	1:151:A:SER:HB2	3	0.92
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD23	2	0.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD22	5	0.91
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG3	3	0.91
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG22	10	0.91
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	4	0.91
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	8	0.91
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE2	9	0.91
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG22	6	0.91
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	4	0.91
(1,2822)	1:52:A:ASN:HB3	1:57:A:MET:HB2	4	0.91
(1,2822)	1:108:A:ASP:HB3	1:67:A:LEU:HG	6	0.91
(1,2822)	1:108:A:ASP:HB3	1:67:A:LEU:HG	8	0.91
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB2	3	0.91
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	1	0.91
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG12	9	0.91
(1,1663)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	6	0.91
(1,1611)	1:7:A:LEU:HD12	1:4:A:PRO:HD3	5	0.91
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	5	0.91
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	6	0.91
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	1	0.91
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	10	0.91
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	4	0.91
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	5	0.91
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD23	3	0.9
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD21	4	0.9
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD21	9	0.9
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	4	0.9
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG23	3	0.9
(1,3132)	1:23:A:THR:HG23	1:59:A:HIS:HD2	3	0.9
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB1	8	0.9
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	9	0.9
(1,2852)	1:112:A:ALA:HB2	1:101:A:MET:HB2	5	0.9
(1,2852)	1:112:A:ALA:HB3	1:101:A:MET:HB2	6	0.9
(1,2822)	1:108:A:ASP:HB3	1:67:A:LEU:HG	5	0.9
(1,2636)	1:37:A:ALA:HB2	1:33:A:LEU:HA	1	0.9
(1,2583)	1:146:A:VAL:HG12	1:143:A:GLU:HB3	9	0.9
(1,2568)	1:149:A:VAL:HG13	1:125:A:ASN:HB2	2	0.9
(1,2556)	1:71:A:THR:HG22	1:54:A:ASP:HB2	3	0.9
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	1	0.9
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	1	0.9
(1,295)	1:28:A:VAL:HG23	1:39:A:GLN:HG3	2	0.9
(1,3461)	1:110:A:GLN:HE22	1:157:A:CYS:HB3	3	0.89
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD21	7	0.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3327)	1:90:A:SER:H	1:89:A:VAL:HG13	7	0.89
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG21	9	0.89
(1,3185)	1:76:A:ALA:H	1:78:A:ARG:H	4	0.89
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD13	10	0.89
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB2	6	0.89
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	8	0.89
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	3	0.89
(1,2944)	1:60:A:VAL:HB	1:23:A:THR:HG22	9	0.89
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB2	6	0.89
(1,2859)	1:71:A:THR:HG23	1:16:A:ASN:HB2	7	0.89
(1,2852)	1:112:A:ALA:HB3	1:101:A:MET:HB2	3	0.89
(1,2852)	1:112:A:ALA:HB3	1:101:A:MET:HB2	4	0.89
(1,2852)	1:112:A:ALA:HB2	1:101:A:MET:HB2	7	0.89
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG22	2	0.89
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB3	3	0.89
(1,2824)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	8	0.89
(1,2822)	1:52:A:ASN:HB3	1:57:A:MET:HB2	9	0.89
(1,2592)	1:75:A:THR:HG22	1:13:A:HIS:H	8	0.89
(1,2589)	1:60:A:VAL:HG23	1:24:A:ILE:HA	4	0.89
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG22	6	0.89
(1,2549)	1:67:A:LEU:HD23	1:17:A:LYS:HE3	9	0.89
(1,2494)	1:138:A:PHE:HD1	1:94:A:ALA:HB3	8	0.89
(1,1663)	1:149:A:VAL:HG12	1:148:A:GLY:HA2	2	0.89
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG21	2	0.89
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG23	4	0.89
(1,1642)	1:47:A:THR:HG23	1:111:A:ALA:HB3	3	0.89
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB3	8	0.89
(1,1181)	1:64:A:LYS:HE3	1:64:A:LYS:HB2	7	0.89
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	4	0.89
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG23	7	0.89
(1,295)	1:28:A:VAL:HG23	1:39:A:GLN:HG3	1	0.89
(1,295)	1:28:A:VAL:HG21	1:39:A:GLN:HG3	6	0.89
(1,3327)	1:90:A:SER:H	1:89:A:VAL:HG13	5	0.88
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG3	10	0.88
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG23	7	0.88
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG21	2	0.88
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD21	1	0.88
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD11	3	0.88
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD13	8	0.88
(1,3088)	1:9:A:LEU:H	1:9:A:LEU:HD12	9	0.88
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	5	0.88
(1,2958)	1:86:A:GLU:HB2	1:89:A:VAL:H	2	0.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB3	1	0.88
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	8	0.88
(1,2655)	1:97:A:VAL:HG23	1:134:A:LYS:HB2	9	0.88
(1,2636)	1:37:A:ALA:HB3	1:33:A:LEU:HA	3	0.88
(1,2549)	1:67:A:LEU:HD23	1:17:A:LYS:HE3	3	0.88
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG12	1	0.88
(1,1663)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	7	0.88
(1,1663)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	9	0.88
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	1	0.88
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	8	0.88
(1,1181)	1:64:A:LYS:HE2	1:64:A:LYS:HB2	1	0.88
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	5	0.88
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	5	0.88
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	6	0.88
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	5	0.88
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	6	0.88
(1,468)	1:97:A:VAL:HG23	1:98:A:MET:HG3	3	0.88
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG23	6	0.88
(1,218)	1:89:A:VAL:HG21	1:151:A:SER:HB2	9	0.88
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB2	6	0.87
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD23	10	0.87
(1,3176)	1:74:A:LYS:H	1:12:A:VAL:HG23	9	0.87
(1,3098)	1:67:A:LEU:HD13	1:67:A:LEU:HA	7	0.87
(1,3093)	1:76:A:ALA:HB2	1:80:A:CYS:HA	10	0.87
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB1	8	0.87
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	8	0.87
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB3	5	0.87
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	6	0.87
(1,2662)	1:24:A:ILE:HG21	1:62:A:GLU:HG3	4	0.87
(1,2549)	1:67:A:LEU:HD21	1:17:A:LYS:HE3	4	0.87
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	10	0.87
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	7	0.87
(1,1253)	1:67:A:LEU:HD23	1:65:A:PRO:HB2	1	0.87
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	9	0.87
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	9	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	1	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	2	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	3	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	4	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	7	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	8	0.87
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	9	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG23	2	0.87
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG23	5	0.87
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG21	10	0.87
(1,3520)	1:39:A:GLN:HE22	1:60:A:VAL:HG13	2	0.86
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	10	0.86
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB2	5	0.86
(1,3264)	1:96:A:ASP:H	1:95:A:PRO:HG2	7	0.86
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB3	5	0.86
(1,3191)	1:102:A:VAL:H	1:100:A:ALA:HB1	9	0.86
(1,3098)	1:67:A:LEU:HD13	1:67:A:LEU:HA	2	0.86
(1,3098)	1:67:A:LEU:HD12	1:67:A:LEU:HA	6	0.86
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB1	9	0.86
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB2	10	0.86
(1,2944)	1:60:A:VAL:HB	1:23:A:THR:HG21	10	0.86
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB1	2	0.86
(1,2859)	1:71:A:THR:HG21	1:16:A:ASN:HB2	3	0.86
(1,2859)	1:71:A:THR:HG21	1:16:A:ASN:HB2	6	0.86
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	1	0.86
(1,2667)	1:94:A:ALA:HB2	1:121:A:ILE:HG12	9	0.86
(1,2636)	1:37:A:ALA:HB3	1:33:A:LEU:HA	7	0.86
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	1	0.86
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	3	0.86
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG11	5	0.86
(1,1611)	1:7:A:LEU:HD11	1:4:A:PRO:HD3	1	0.86
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	3	0.86
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	3	0.86
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	8	0.86
(1,780)	1:147:A:LEU:H	1:147:A:LEU:HB3	10	0.86
(1,468)	1:97:A:VAL:HG22	1:98:A:MET:HG3	5	0.86
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG21	4	0.86
(1,295)	1:28:A:VAL:HG21	1:39:A:GLN:HG3	3	0.86
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	8	0.86
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG21	6	0.85
(1,3185)	1:76:A:ALA:H	1:78:A:ARG:H	1	0.85
(1,3115)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	1	0.85
(1,3115)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	4	0.85
(1,3098)	1:67:A:LEU:HD11	1:67:A:LEU:HA	1	0.85
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	5	0.85
(1,2974)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	5	0.85
(1,2892)	1:36:A:CYS:HB3	1:6:A:LYS:HE3	1	0.85
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB2	9	0.85
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	3	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD12	7	0.85
(1,2822)	1:108:A:ASP:HB3	1:67:A:LEU:HG	7	0.85
(1,2594)	1:28:A:VAL:HG21	1:39:A:GLN:HA	9	0.85
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE2	1	0.85
(1,2583)	1:146:A:VAL:HG12	1:143:A:GLU:HB3	1	0.85
(1,2583)	1:146:A:VAL:HG13	1:143:A:GLU:HB3	8	0.85
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	4	0.85
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	7	0.85
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	9	0.85
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	1	0.85
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	6	0.85
(1,1663)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	5	0.85
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG22	9	0.85
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	6	0.85
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	2	0.85
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	8	0.85
(1,1129)	1:39:A:GLN:HG2	1:40:A:CYS:H	7	0.85
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB1	4	0.84
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	8	0.84
(1,3132)	1:23:A:THR:HG23	1:59:A:HIS:HD2	8	0.84
(1,3115)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	5	0.84
(1,3098)	1:67:A:LEU:HD12	1:67:A:LEU:HA	10	0.84
(1,3093)	1:76:A:ALA:HB2	1:80:A:CYS:HA	6	0.84
(1,3093)	1:76:A:ALA:HB1	1:80:A:CYS:HA	8	0.84
(1,2850)	1:100:A:ALA:HB1	1:101:A:MET:HB3	8	0.84
(1,2708)	1:116:A:ASP:HB3	1:115:A:ALA:HB1	1	0.84
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HB2	10	0.84
(1,2642)	1:24:A:ILE:HG22	1:46:A:CYS:H	6	0.84
(1,2592)	1:75:A:THR:HG21	1:13:A:HIS:H	1	0.84
(1,2589)	1:60:A:VAL:HG22	1:24:A:ILE:HA	9	0.84
(1,2583)	1:146:A:VAL:HG13	1:143:A:GLU:HB3	10	0.84
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	5	0.84
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG11	10	0.84
(1,1663)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	3	0.84
(1,1663)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	10	0.84
(1,1277)	1:89:A:VAL:HG21	1:142:A:LYS:HD2	1	0.84
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	6	0.84
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	5	0.84
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG21	1	0.84
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG22	3	0.84
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG21	9	0.84
(1,3392)	1:34:A:GLU:H	1:33:A:LEU:HD22	1	0.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3327)	1:90:A:SER:H	1:89:A:VAL:HG11	4	0.83
(1,3132)	1:23:A:THR:HG23	1:59:A:HIS:HD2	10	0.83
(1,3115)	1:56:A:LYS:HE3	1:56:A:LYS:HG2	8	0.83
(1,3093)	1:76:A:ALA:HB3	1:80:A:CYS:HA	5	0.83
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB3	2	0.83
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB3	5	0.83
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	7	0.83
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	10	0.83
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD12	8	0.83
(1,2836)	1:141:A:PHE:HB3	1:134:A:LYS:HG2	2	0.83
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	7	0.83
(1,2836)	1:141:A:PHE:HB3	1:140:A:ALA:HB1	10	0.83
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB2	4	0.83
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB3	8	0.83
(1,2589)	1:60:A:VAL:HG23	1:24:A:ILE:HA	10	0.83
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG13	9	0.83
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	5	0.83
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG22	10	0.83
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	2	0.83
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	4	0.83
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	6	0.83
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	1	0.83
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	4	0.83
(1,295)	1:28:A:VAL:HG21	1:39:A:GLN:HG3	8	0.83
(1,197)	1:99:A:THR:H	1:99:A:THR:HG21	9	0.83
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	6	0.82
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB1	5	0.82
(1,3427)	1:113:A:CYS:H	1:110:A:GLN:HG2	4	0.82
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG23	2	0.82
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD22	3	0.82
(1,3115)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	2	0.82
(1,3098)	1:67:A:LEU:HD13	1:67:A:LEU:HA	3	0.82
(1,3098)	1:67:A:LEU:HD12	1:67:A:LEU:HA	5	0.82
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB3	1	0.82
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB2	7	0.82
(1,2974)	1:98:A:MET:HG2	1:113:A:CYS:HA	1	0.82
(1,2974)	1:98:A:MET:HG2	1:119:A:CYS:HB3	2	0.82
(1,2974)	1:98:A:MET:HG2	1:113:A:CYS:HA	10	0.82
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	2	0.82
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	10	0.82
(1,2662)	1:24:A:ILE:HG23	1:62:A:GLU:HG3	3	0.82
(1,2662)	1:24:A:ILE:HG22	1:62:A:GLU:HG3	8	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2642)	1:24:A:ILE:HG22	1:46:A:CYS:H	1	0.82
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB3	4	0.82
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	3	0.82
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	5	0.82
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	7	0.82
(1,1663)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	1	0.82
(1,1642)	1:47:A:THR:HG23	1:111:A:ALA:HB1	1	0.82
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	3	0.82
(1,1476)	1:33:A:LEU:HD13	1:14:A:SER:HB2	10	0.82
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	1	0.82
(1,1277)	1:89:A:VAL:HG23	1:142:A:LYS:HD2	3	0.82
(1,1181)	1:64:A:LYS:HE2	1:64:A:LYS:HB2	10	0.82
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	10	0.82
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	8	0.82
(1,468)	1:97:A:VAL:HG23	1:98:A:MET:HG3	8	0.82
(1,295)	1:28:A:VAL:HG21	1:39:A:GLN:HG3	10	0.82
(1,218)	1:89:A:VAL:HG23	1:151:A:SER:HB2	4	0.82
(1,218)	1:89:A:VAL:HG23	1:151:A:SER:HB2	5	0.82
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	7	0.82
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB2	1	0.81
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG12	8	0.81
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB2	9	0.81
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG21	4	0.81
(1,3073)	1:33:A:LEU:HD13	1:9:A:LEU:HB3	9	0.81
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	10	0.81
(1,2982)	1:105:A:GLN:HG2	1:108:A:ASP:HA	3	0.81
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	7	0.81
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	7	0.81
(1,2884)	1:80:A:CYS:HB3	1:76:A:ALA:HB1	4	0.81
(1,2594)	1:28:A:VAL:HG23	1:39:A:GLN:HA	2	0.81
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	8	0.81
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	7	0.81
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	3	0.81
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	8	0.81
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB3	2	0.81
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB1	7	0.81
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB2	10	0.81
(1,1476)	1:33:A:LEU:HD11	1:14:A:SER:HB2	1	0.81
(1,1447)	1:97:A:VAL:HB	1:118:A:SER:HB2	5	0.81
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	4	0.81
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	1	0.81
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	10	0.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	6	0.81
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	4	0.81
(1,218)	1:89:A:VAL:HG23	1:151:A:SER:HB2	6	0.81
(1,197)	1:99:A:THR:H	1:99:A:THR:HG22	2	0.81
(1,197)	1:99:A:THR:H	1:99:A:THR:HG21	7	0.81
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG21	3	0.8
(1,3093)	1:76:A:ALA:HB1	1:80:A:CYS:HA	2	0.8
(1,3073)	1:33:A:LEU:HD11	1:9:A:LEU:HB3	10	0.8
(1,3008)	1:130:A:LYS:HD3	1:130:A:LYS:HA	7	0.8
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	2	0.8
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	4	0.8
(1,2859)	1:71:A:THR:HG22	1:16:A:ASN:HB2	5	0.8
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	3	0.8
(1,2662)	1:24:A:ILE:HG23	1:62:A:GLU:HG3	6	0.8
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB3	4	0.8
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB3	6	0.8
(1,2589)	1:60:A:VAL:HG21	1:24:A:ILE:HA	1	0.8
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	6	0.8
(1,2556)	1:71:A:THR:HG21	1:54:A:ASP:HB2	7	0.8
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB2	1	0.8
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	2	0.8
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	4	0.8
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	9	0.8
(1,1869)	1:7:A:LEU:H	1:7:A:LEU:HB3	10	0.8
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG22	8	0.8
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	7	0.8
(1,1277)	1:89:A:VAL:HG21	1:142:A:LYS:HD2	6	0.8
(1,1173)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	7	0.8
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	3	0.8
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	7	0.8
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	9	0.8
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	3	0.8
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB3	3	0.8
(1,295)	1:28:A:VAL:HG23	1:39:A:GLN:HG3	5	0.8
(1,197)	1:99:A:THR:H	1:99:A:THR:HG22	5	0.8
(1,197)	1:99:A:THR:H	1:99:A:THR:HG22	6	0.8
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG23	1	0.79
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB1	9	0.79
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB3	2	0.79
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB3	5	0.79
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	2	0.79
(1,3226)	1:85:A:PHE:H	1:150:A:THR:HG22	7	0.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3098)	1:67:A:LEU:HD12	1:67:A:LEU:HA	9	0.79
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB2	3	0.79
(1,3070)	1:39:A:GLN:HB3	1:38:A:ALA:HB1	4	0.79
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	1	0.79
(1,2974)	1:98:A:MET:HG2	1:119:A:CYS:HB3	4	0.79
(1,2974)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	7	0.79
(1,2962)	1:65:A:PRO:HB3	1:67:A:LEU:HG	9	0.79
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	5	0.79
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB3	2	0.79
(1,2662)	1:24:A:ILE:HG22	1:62:A:GLU:HG3	7	0.79
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB2	2	0.79
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB1	7	0.79
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE2	9	0.79
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	1	0.79
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	5	0.79
(1,2583)	1:146:A:VAL:HG11	1:143:A:GLU:HB3	3	0.79
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	7	0.79
(1,2569)	1:97:A:VAL:HG11	1:120:A:GLU:HB2	10	0.79
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG22	5	0.79
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG23	2	0.79
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG22	2	0.79
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG23	4	0.79
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	1	0.79
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG23	10	0.79
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG13	2	0.79
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	2	0.79
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	4	0.79
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	5	0.79
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	6	0.79
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	7	0.79
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	9	0.79
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	1	0.79
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	8	0.79
(1,468)	1:97:A:VAL:HG22	1:98:A:MET:HG3	7	0.79
(1,218)	1:89:A:VAL:HG23	1:151:A:SER:HB2	1	0.79
(1,197)	1:99:A:THR:H	1:99:A:THR:HG23	1	0.79
(1,108)	1:31:A:VAL:HG22	1:58:A:CYS:HA	2	0.79
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB2	7	0.78
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB1	8	0.78
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB1	10	0.78
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG12	2	0.78
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	5	0.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD23	6	0.78
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	9	0.78
(1,3098)	1:67:A:LEU:HD13	1:67:A:LEU:HA	4	0.78
(1,3098)	1:67:A:LEU:HD13	1:67:A:LEU:HA	8	0.78
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	2	0.78
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	10	0.78
(1,2662)	1:24:A:ILE:HG23	1:62:A:GLU:HG3	1	0.78
(1,2585)	1:97:A:VAL:HG11	1:134:A:LYS:HG3	9	0.78
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB1	7	0.78
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	6	0.78
(1,2511)	1:107:A:ALA:HB1	1:85:A:PHE:HZ	9	0.78
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	4	0.78
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	2	0.78
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	4	0.78
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	9	0.78
(1,1476)	1:33:A:LEU:HD13	1:14:A:SER:HB2	7	0.78
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	8	0.78
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	9	0.78
(1,704)	1:21:A:ALA:HB1	1:61:A:LYS:HE2	3	0.78
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	7	0.78
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	2	0.78
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	4	0.78
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	4	0.78
(1,295)	1:28:A:VAL:HG23	1:39:A:GLN:HG3	4	0.78
(1,108)	1:31:A:VAL:HG22	1:58:A:CYS:HA	3	0.78
(1,108)	1:31:A:VAL:HG23	1:58:A:CYS:HA	5	0.78
(1,3461)	1:110:A:GLN:HE22	1:157:A:CYS:HB3	1	0.77
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB3	1	0.77
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB3	2	0.77
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB3	5	0.77
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB2	10	0.77
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	3	0.77
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB1	9	0.77
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB1	2	0.77
(1,3427)	1:113:A:CYS:H	1:110:A:GLN:HG2	6	0.77
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG12	7	0.77
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB1	4	0.77
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB2	7	0.77
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB1	8	0.77
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	1	0.77
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD23	2	0.77
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	1	0.77

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3132)	1:23:A:THR:HG22	1:59:A:HIS:HD2	7	0.77
(1,3093)	1:76:A:ALA:HB2	1:80:A:CYS:HA	9	0.77
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	2	0.77
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG23	10	0.77
(1,2671)	1:24:A:ILE:HD12	1:60:A:VAL:HA	3	0.77
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB1	8	0.77
(1,2613)	1:53:A:ASP:HA	1:33:A:LEU:HD22	3	0.77
(1,2592)	1:75:A:THR:HG21	1:13:A:HIS:H	5	0.77
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG22	6	0.77
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	3	0.77
(1,2556)	1:71:A:THR:HG22	1:54:A:ASP:HB2	1	0.77
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	5	0.77
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	6	0.77
(1,1396)	1:95:A:PRO:HG2	1:95:A:PRO:HA	3	0.77
(1,1277)	1:89:A:VAL:HG22	1:142:A:LYS:HD2	10	0.77
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	4	0.77
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	8	0.77
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	10	0.77
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	5	0.77
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	6	0.77
(1,495)	1:94:A:ALA:HB2	1:134:A:LYS:HA	5	0.77
(1,295)	1:28:A:VAL:HG23	1:39:A:GLN:HG3	7	0.77
(1,197)	1:99:A:THR:H	1:99:A:THR:HG23	4	0.77
(1,197)	1:99:A:THR:H	1:99:A:THR:HG21	8	0.77
(1,108)	1:31:A:VAL:HG21	1:58:A:CYS:HA	9	0.77
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	2	0.76
(1,3427)	1:113:A:CYS:H	1:110:A:GLN:HG2	9	0.76
(1,3380)	1:16:A:ASN:HD21	1:71:A:THR:HG23	2	0.76
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB2	6	0.76
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG3	9	0.76
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG21	1	0.76
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	3	0.76
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG11	10	0.76
(1,3133)	1:123:A:THR:HG21	1:150:A:THR:HA	2	0.76
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	6	0.76
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HG	5	0.76
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	9	0.76
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	2	0.76
(1,2850)	1:100:A:ALA:HB2	1:101:A:MET:HB3	2	0.76
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	5	0.76
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB1	6	0.76
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB2	9	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2662)	1:24:A:ILE:HG23	1:62:A:GLU:HG3	9	0.76
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB1	3	0.76
(1,2614)	1:42:A:ALA:HB3	1:39:A:GLN:HG3	4	0.76
(1,2568)	1:43:A:VAL:HG21	1:60:A:VAL:HB	10	0.76
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	1	0.76
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD11	5	0.76
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	5	0.76
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG21	7	0.76
(1,1642)	1:47:A:THR:HG21	1:111:A:ALA:HB1	4	0.76
(1,1604)	1:33:A:LEU:HD23	1:51:A:TYR:HA	1	0.76
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	2	0.76
(1,1277)	1:89:A:VAL:HG23	1:142:A:LYS:HD2	7	0.76
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	2	0.76
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	9	0.76
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	2	0.76
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	10	0.76
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	9	0.76
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	2	0.76
(1,108)	1:31:A:VAL:HG23	1:58:A:CYS:HA	8	0.76
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG12	1	0.75
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB2	10	0.75
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	8	0.75
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG2	8	0.75
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD22	8	0.75
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	4	0.75
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	9	0.75
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD13	8	0.75
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	4	0.75
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	5	0.75
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	6	0.75
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	8	0.75
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	10	0.75
(1,2982)	1:105:A:GLN:HG2	1:108:A:ASP:HA	4	0.75
(1,2962)	1:65:A:PRO:HB3	1:67:A:LEU:HG	8	0.75
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG22	5	0.75
(1,2861)	1:34:A:GLU:HG3	1:33:A:LEU:HD11	6	0.75
(1,2851)	1:101:A:MET:HB2	1:99:A:THR:HG21	8	0.75
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB2	6	0.75
(1,2675)	1:24:A:ILE:HD11	1:61:A:LYS:HB3	9	0.75
(1,2613)	1:53:A:ASP:HA	1:33:A:LEU:HD23	7	0.75
(1,2590)	1:102:A:VAL:HG13	1:17:A:LYS:HE2	4	0.75
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE3	6	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2589)	1:60:A:VAL:HG23	1:24:A:ILE:HA	6	0.75
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	7	0.75
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	4	0.75
(1,2568)	1:43:A:VAL:HG22	1:60:A:VAL:HB	1	0.75
(1,2560)	1:151:A:SER:H	1:89:A:VAL:HG21	9	0.75
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB2	5	0.75
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	8	0.75
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	9	0.75
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	4	0.75
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG21	5	0.75
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	2	0.75
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	4	0.75
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	10	0.75
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD11	7	0.75
(1,468)	1:97:A:VAL:HG21	1:98:A:MET:HG3	4	0.75
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB3	2	0.75
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	7	0.75
(1,295)	1:28:A:VAL:HG21	1:39:A:GLN:HG3	9	0.75
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG22	9	0.75
(1,197)	1:99:A:THR:H	1:99:A:THR:HG21	3	0.75
(1,3443)	1:40:A:CYS:H	1:38:A:ALA:HB2	3	0.74
(1,3441)	1:40:A:CYS:H	1:49:A:PHE:HB2	7	0.74
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB3	6	0.74
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB2	1	0.74
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB3	10	0.74
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB2	3	0.74
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	6	0.74
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG3	1	0.74
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	6	0.74
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD23	1	0.74
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD22	5	0.74
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	10	0.74
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	10	0.74
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	3	0.74
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	10	0.74
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	3	0.74
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	8	0.74
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	6	0.74
(1,2675)	1:24:A:ILE:HD13	1:61:A:LYS:HB3	5	0.74
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD12	3	0.74
(1,2667)	1:94:A:ALA:HB1	1:121:A:ILE:HG12	2	0.74
(1,2662)	1:24:A:ILE:HG22	1:62:A:GLU:HG3	5	0.74

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG23	9	0.74
(1,2592)	1:75:A:THR:HG22	1:13:A:HIS:H	10	0.74
(1,2589)	1:60:A:VAL:HG21	1:24:A:ILE:HA	3	0.74
(1,2589)	1:60:A:VAL:HG22	1:24:A:ILE:HA	7	0.74
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	3	0.74
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG21	3	0.74
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG22	6	0.74
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG13	10	0.74
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	8	0.74
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	8	0.74
(1,1642)	1:47:A:THR:HG21	1:111:A:ALA:HB1	5	0.74
(1,1437)	1:7:A:LEU:HG	1:32:A:SER:HB3	1	0.74
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	10	0.74
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG13	8	0.74
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG11	10	0.74
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	10	0.74
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	3	0.74
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	7	0.74
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	10	0.74
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	9	0.74
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	2	0.74
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	3	0.74
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	5	0.74
(1,468)	1:97:A:VAL:HG23	1:98:A:MET:HG3	6	0.74
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	1	0.74
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB3	9	0.74
(1,108)	1:31:A:VAL:HG23	1:58:A:CYS:HA	1	0.74
(1,108)	1:31:A:VAL:HG21	1:58:A:CYS:HA	6	0.74
(1,3461)	1:110:A:GLN:HE22	1:157:A:CYS:HB3	7	0.73
(1,3461)	1:110:A:GLN:HE22	1:157:A:CYS:HB3	8	0.73
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG11	10	0.73
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG23	8	0.73
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	8	0.73
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG11	4	0.73
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	6	0.73
(1,3138)	1:12:A:VAL:HG13	1:51:A:TYR:HE2	1	0.73
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD12	4	0.73
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	3	0.73
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	4	0.73
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	7	0.73
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	6	0.73
(1,2824)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	6	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2603)	1:149:A:VAL:HG22	1:147:A:LEU:HA	6	0.73
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG22	2	0.73
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	8	0.73
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG12	6	0.73
(1,2269)	1:141:A:PHE:H	1:142:A:LYS:HB3	8	0.73
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	1	0.73
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD13	7	0.73
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD12	10	0.73
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	5	0.73
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG22	6	0.73
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	5	0.73
(1,1277)	1:89:A:VAL:HG21	1:142:A:LYS:HD2	4	0.73
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	5	0.73
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	9	0.73
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG22	1	0.73
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG21	2	0.73
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG22	4	0.73
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	4	0.73
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	9	0.73
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	10	0.73
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	7	0.73
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	10	0.73
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	5	0.73
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD12	6	0.73
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD13	10	0.73
(1,468)	1:97:A:VAL:HG22	1:98:A:MET:HG3	1	0.73
(1,468)	1:97:A:VAL:HG23	1:98:A:MET:HG3	2	0.73
(1,468)	1:97:A:VAL:HG22	1:98:A:MET:HG3	9	0.73
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	4	0.73
(1,218)	1:89:A:VAL:HG22	1:151:A:SER:HB2	7	0.73
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG22	7	0.73
(1,108)	1:31:A:VAL:HG23	1:58:A:CYS:HA	10	0.73
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG11	5	0.72
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB3	1	0.72
(1,3345)	1:150:A:THR:H	1:126:A:GLU:HB2	10	0.72
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	3	0.72
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	5	0.72
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	10	0.72
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG21	6	0.72
(1,3264)	1:96:A:ASP:H	1:134:A:LYS:HB3	10	0.72
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD21	7	0.72
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	2	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	3	0.72
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	7	0.72
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD23	1	0.72
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD21	3	0.72
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD12	2	0.72
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD12	5	0.72
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD13	7	0.72
(1,3012)	1:34:A:GLU:HB3	1:35:A:GLN:HA	1	0.72
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	6	0.72
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG21	8	0.72
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	1	0.72
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	8	0.72
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	1	0.72
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	2	0.72
(1,2671)	1:24:A:ILE:HD11	1:60:A:VAL:HA	4	0.72
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB3	3	0.72
(1,2662)	1:24:A:ILE:HG21	1:62:A:GLU:HG3	10	0.72
(1,2653)	1:97:A:VAL:HG22	1:121:A:ILE:H	6	0.72
(1,2653)	1:97:A:VAL:HG22	1:121:A:ILE:H	8	0.72
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG23	4	0.72
(1,2614)	1:42:A:ALA:HB2	1:39:A:GLN:HG3	5	0.72
(1,2594)	1:28:A:VAL:HG23	1:39:A:GLN:HA	1	0.72
(1,2594)	1:28:A:VAL:HG23	1:39:A:GLN:HA	5	0.72
(1,2592)	1:50:A:THR:H	1:75:A:THR:HG21	7	0.72
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	5	0.72
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG13	4	0.72
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG11	8	0.72
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	4	0.72
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	3	0.72
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD13	2	0.72
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD11	3	0.72
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	1	0.72
(1,1642)	1:47:A:THR:HG22	1:111:A:ALA:HB1	9	0.72
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	6	0.72
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG11	7	0.72
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG23	7	0.72
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	8	0.72
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	8	0.72
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	6	0.72
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	1	0.72
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	6	0.72
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	1	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD13	8	0.72
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG21	1	0.72
(1,197)	1:99:A:THR:H	1:99:A:THR:HG23	10	0.72
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	1	0.71
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB3	4	0.71
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD23	9	0.71
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD21	9	0.71
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD23	10	0.71
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	9	0.71
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	2	0.71
(1,3008)	1:130:A:LYS:HD3	1:130:A:LYS:HA	6	0.71
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	9	0.71
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG23	4	0.71
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	3	0.71
(1,2675)	1:24:A:ILE:HD12	1:61:A:LYS:HB3	2	0.71
(1,2675)	1:24:A:ILE:HD11	1:61:A:LYS:HB3	10	0.71
(1,2671)	1:24:A:ILE:HD11	1:60:A:VAL:HA	6	0.71
(1,2671)	1:24:A:ILE:HD11	1:60:A:VAL:HA	8	0.71
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD11	4	0.71
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB2	10	0.71
(1,2614)	1:42:A:ALA:HB2	1:39:A:GLN:HG3	2	0.71
(1,2603)	1:149:A:VAL:HG22	1:147:A:LEU:HA	5	0.71
(1,2589)	1:60:A:VAL:HG22	1:24:A:ILE:HA	8	0.71
(1,2568)	1:43:A:VAL:HG22	1:60:A:VAL:HB	9	0.71
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG22	4	0.71
(1,2560)	1:151:A:SER:H	1:89:A:VAL:HG22	7	0.71
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	3	0.71
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG11	2	0.71
(1,2488)	1:142:A:LYS:HB3	1:91:A:TYR:HD2	1	0.71
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	2	0.71
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	7	0.71
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD13	6	0.71
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD12	9	0.71
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	6	0.71
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	1	0.71
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	4	0.71
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	3	0.71
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG22	9	0.71
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	5	0.71
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	9	0.71
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	10	0.71
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	2	0.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:149:A:VAL:HG11	1:123:A:THR:HG23	2	0.71
(1,108)	1:31:A:VAL:HG22	1:58:A:CYS:HA	4	0.71
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	3	0.7
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG13	6	0.7
(1,3339)	1:156:A:PHE:H	1:155:A:GLN:HG3	9	0.7
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	2	0.7
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	4	0.7
(1,3331)	1:38:A:ALA:H	1:35:A:GLN:HB2	7	0.7
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	10	0.7
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	5	0.7
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	8	0.7
(1,3138)	1:12:A:VAL:HG12	1:51:A:TYR:HE2	2	0.7
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD12	6	0.7
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	3	0.7
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG22	1	0.7
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	9	0.7
(1,2824)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	3	0.7
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG22	6	0.7
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	7	0.7
(1,2675)	1:24:A:ILE:HD12	1:61:A:LYS:HB3	7	0.7
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD11	6	0.7
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD13	9	0.7
(1,2662)	1:24:A:ILE:HG22	1:62:A:GLU:HG3	2	0.7
(1,2655)	1:97:A:VAL:HG23	1:134:A:LYS:HB2	5	0.7
(1,2653)	1:97:A:VAL:HG21	1:121:A:ILE:H	1	0.7
(1,2653)	1:97:A:VAL:HG22	1:121:A:ILE:H	3	0.7
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG23	9	0.7
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB2	1	0.7
(1,2628)	1:79:A:SER:H	1:107:A:ALA:HB1	3	0.7
(1,2603)	1:149:A:VAL:HG23	1:147:A:LEU:HA	1	0.7
(1,2594)	1:28:A:VAL:HG23	1:39:A:GLN:HA	7	0.7
(1,2589)	1:60:A:VAL:HG22	1:24:A:ILE:HA	2	0.7
(1,2589)	1:60:A:VAL:HG21	1:24:A:ILE:HA	5	0.7
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	4	0.7
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG11	2	0.7
(1,2569)	1:97:A:VAL:HG13	1:120:A:GLU:HB2	9	0.7
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	7	0.7
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG22	8	0.7
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	3	0.7
(1,2234)	1:98:A:MET:H	1:98:A:MET:HG3	9	0.7
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD11	1	0.7
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD13	8	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	7	0.7
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	2	0.7
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	3	0.7
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	4	0.7
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	5	0.7
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	6	0.7
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	9	0.7
(1,1611)	1:7:A:LEU:HD13	1:4:A:PRO:HD3	8	0.7
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	8	0.7
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	9	0.7
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG12	3	0.7
(1,1277)	1:89:A:VAL:HG22	1:142:A:LYS:HD2	2	0.7
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	5	0.7
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG23	3	0.7
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG22	5	0.7
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG21	7	0.7
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	9	0.7
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	6	0.7
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	4	0.7
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD13	1	0.7
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	1	0.7
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	9	0.7
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	1	0.7
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	6	0.7
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG21	9	0.7
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG22	4	0.7
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB2	7	0.69
(1,3360)	1:35:A:GLN:H	1:38:A:ALA:HB1	9	0.69
(1,3327)	1:90:A:SER:H	1:142:A:LYS:HG3	2	0.69
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD22	10	0.69
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD23	10	0.69
(1,3138)	1:12:A:VAL:HG11	1:51:A:TYR:HE2	8	0.69
(1,3138)	1:12:A:VAL:HG11	1:51:A:TYR:HE2	9	0.69
(1,3138)	1:12:A:VAL:HG13	1:51:A:TYR:HE2	10	0.69
(1,3133)	1:123:A:THR:HG23	1:150:A:THR:HA	4	0.69
(1,3133)	1:123:A:THR:HG23	1:150:A:THR:HA	9	0.69
(1,3122)	1:7:A:LEU:HD23	1:5:A:ALA:H	5	0.69
(1,3073)	1:6:A:LYS:HB3	1:33:A:LEU:HD12	3	0.69
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	6	0.69
(1,2850)	1:100:A:ALA:HB1	1:101:A:MET:HB3	9	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	3	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	4	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	6	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	7	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	8	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	9	0.69
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	10	0.69
(1,2675)	1:24:A:ILE:HD13	1:61:A:LYS:HB3	3	0.69
(1,2675)	1:24:A:ILE:HD12	1:61:A:LYS:HB3	6	0.69
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD11	8	0.69
(1,2653)	1:97:A:VAL:HG21	1:121:A:ILE:H	7	0.69
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB1	7	0.69
(1,2640)	1:114:A:ALA:HB1	1:113:A:CYS:HB3	6	0.69
(1,2614)	1:42:A:ALA:HB3	1:39:A:GLN:HG3	1	0.69
(1,2595)	1:75:A:THR:HG21	1:13:A:HIS:HB2	3	0.69
(1,2594)	1:28:A:VAL:HG21	1:39:A:GLN:HA	8	0.69
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE2	2	0.69
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG22	1	0.69
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG21	3	0.69
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB3	10	0.69
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG12	3	0.69
(1,2537)	1:50:A:THR:H	1:60:A:VAL:HG11	7	0.69
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	8	0.69
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG22	3	0.69
(1,2175)	1:25:A:GLY:H	1:24:A:ILE:HD13	4	0.69
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	1	0.69
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	7	0.69
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	8	0.69
(1,1703)	1:27:A:PRO:HA	1:27:A:PRO:HG2	10	0.69
(1,1642)	1:47:A:THR:HG21	1:111:A:ALA:HB1	6	0.69
(1,1604)	1:33:A:LEU:HD21	1:51:A:TYR:HA	2	0.69
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	5	0.69
(1,1277)	1:89:A:VAL:HG22	1:142:A:LYS:HD2	9	0.69
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG22	6	0.69
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG21	5	0.69
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	5	0.69
(1,801)	1:128:A:ASP:HB2	1:130:A:LYS:HB2	9	0.69
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	2	0.69
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	2	0.69
(1,438)	1:38:A:ALA:HA	1:41:A:LYS:HD3	7	0.69
(1,3331)	1:38:A:ALA:H	1:34:A:GLU:HB2	1	0.68
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	9	0.68
(1,3149)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	1	0.68
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	7	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3138)	1:12:A:VAL:HG12	1:51:A:TYR:HE2	3	0.68
(1,3138)	1:12:A:VAL:HG12	1:51:A:TYR:HE2	5	0.68
(1,3132)	1:23:A:THR:HG21	1:59:A:HIS:HD2	5	0.68
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	9	0.68
(1,2824)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	5	0.68
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	5	0.68
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	2	0.68
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	5	0.68
(1,2671)	1:24:A:ILE:HD12	1:60:A:VAL:HA	1	0.68
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG21	2	0.68
(1,2556)	1:71:A:THR:HG23	1:54:A:ASP:HB2	10	0.68
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	9	0.68
(1,2529)	1:115:A:ALA:HB2	1:116:A:ASP:HA	3	0.68
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB2	5	0.68
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	4	0.68
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	10	0.68
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG22	6	0.68
(1,1604)	1:33:A:LEU:HD21	1:51:A:TYR:HA	3	0.68
(1,1476)	1:33:A:LEU:HD12	1:14:A:SER:HB2	6	0.68
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	10	0.68
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	2	0.68
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	1	0.68
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG22	7	0.68
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG23	8	0.68
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG22	9	0.68
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG22	10	0.68
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	1	0.68
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	9	0.68
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	4	0.68
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	6	0.68
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	7	0.68
(1,416)	1:21:A:ALA:HB3	1:62:A:GLU:HB3	2	0.68
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	6	0.68
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG22	6	0.68
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB1	2	0.67
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB1	8	0.67
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG13	3	0.67
(1,3339)	1:156:A:PHE:H	1:155:A:GLN:HG3	4	0.67
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD23	10	0.67
(1,3138)	1:12:A:VAL:HG12	1:51:A:TYR:HE2	4	0.67
(1,3138)	1:12:A:VAL:HG13	1:51:A:TYR:HE2	6	0.67
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG21	6	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3094)	1:76:A:ALA:HB3	1:77:A:SER:HB3	3	0.67
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG21	2	0.67
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	4	0.67
(1,2848)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	2	0.67
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	7	0.67
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	2	0.67
(1,2679)	1:22:A:PRO:HD3	1:22:A:PRO:HB3	1	0.67
(1,2675)	1:24:A:ILE:HD13	1:61:A:LYS:HB3	1	0.67
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD12	1	0.67
(1,2655)	1:97:A:VAL:HG22	1:134:A:LYS:HB2	4	0.67
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG21	8	0.67
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG21	10	0.67
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB3	5	0.67
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG21	5	0.67
(1,2603)	1:149:A:VAL:HG23	1:147:A:LEU:HA	10	0.67
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG22	1	0.67
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	6	0.67
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG23	10	0.67
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	9	0.67
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG21	5	0.67
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	1	0.67
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	6	0.67
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	8	0.67
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	5	0.67
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	3	0.67
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	8	0.67
(1,1604)	1:33:A:LEU:HD23	1:51:A:TYR:HA	5	0.67
(1,1604)	1:33:A:LEU:HD22	1:51:A:TYR:HA	6	0.67
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG12	1	0.67
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	7	0.67
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	1	0.67
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG23	10	0.67
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG22	6	0.67
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	2	0.67
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	6	0.67
(1,678)	1:20:A:ARG:HD2	1:20:A:ARG:HA	5	0.67
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	7	0.67
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	5	0.67
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	6	0.67
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	2	0.67
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	6	0.67
(1,416)	1:21:A:ALA:HB3	1:62:A:GLU:HB3	1	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,416)	1:21:A:ALA:HB1	1:62:A:GLU:HB3	4	0.67
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB1	8	0.67
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD12	8	0.67
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD13	6	0.67
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD12	8	0.67
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG22	5	0.67
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	8	0.67
(1,108)	1:31:A:VAL:HG22	1:58:A:CYS:HA	7	0.67
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	3	0.67
(1,74)	1:35:A:GLN:HB2	1:31:A:VAL:HA	6	0.67
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	6	0.66
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD22	2	0.66
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD22	1	0.66
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD22	9	0.66
(1,3133)	1:123:A:THR:HG21	1:150:A:THR:HA	10	0.66
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG22	10	0.66
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	6	0.66
(1,2824)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	7	0.66
(1,2747)	1:82:A:ARG:HD3	1:85:A:PHE:HB3	2	0.66
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	7	0.66
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG23	4	0.66
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD11	2	0.66
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD12	5	0.66
(1,2653)	1:97:A:VAL:HG22	1:121:A:ILE:H	2	0.66
(1,2614)	1:42:A:ALA:HB1	1:39:A:GLN:HG3	7	0.66
(1,2614)	1:42:A:ALA:HB3	1:39:A:GLN:HG3	9	0.66
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG23	10	0.66
(1,2603)	1:149:A:VAL:HG21	1:147:A:LEU:HA	3	0.66
(1,2590)	1:102:A:VAL:HG13	1:17:A:LYS:HE2	3	0.66
(1,2581)	1:119:A:CYS:H	1:97:A:VAL:HG12	1	0.66
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	7	0.66
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	3	0.66
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	2	0.66
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	3	0.66
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	4	0.66
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	5	0.66
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	7	0.66
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	7	0.66
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG11	8	0.66
(1,1604)	1:33:A:LEU:HD22	1:51:A:TYR:HA	4	0.66
(1,1545)	1:61:A:LYS:HG2	1:60:A:VAL:HA	4	0.66
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	3	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG12	9	0.66
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	6	0.66
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	6	0.66
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG21	1	0.66
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG22	3	0.66
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD2	3	0.66
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	7	0.66
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	8	0.66
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	9	0.66
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	1	0.66
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD12	5	0.66
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	8	0.66
(1,487)	1:24:A:ILE:HG23	1:43:A:VAL:HB	4	0.66
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD12	1	0.66
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD12	9	0.66
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	5	0.65
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	10	0.65
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	10	0.65
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB3	3	0.65
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	2	0.65
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	6	0.65
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	7	0.65
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG3	3	0.65
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	6	0.65
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG22	2	0.65
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD21	2	0.65
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD23	5	0.65
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD22	6	0.65
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	2	0.65
(1,2974)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	3	0.65
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	4	0.65
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG21	6	0.65
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	3	0.65
(1,2850)	1:100:A:ALA:HB3	1:101:A:MET:HB3	5	0.65
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	8	0.65
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	9	0.65
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD2	7	0.65
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG22	7	0.65
(1,2671)	1:24:A:ILE:HD13	1:60:A:VAL:HA	9	0.65
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD11	7	0.65
(1,2669)	1:24:A:ILE:H	1:24:A:ILE:HD13	10	0.65
(1,2665)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	2	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB3	4	0.65
(1,2655)	1:97:A:VAL:HG23	1:134:A:LYS:HB2	7	0.65
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB3	2	0.65
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG23	3	0.65
(1,2628)	1:79:A:SER:H	1:111:A:ALA:HB3	9	0.65
(1,2614)	1:42:A:ALA:HB2	1:39:A:GLN:HG3	3	0.65
(1,2594)	1:28:A:VAL:HG21	1:39:A:GLN:HA	3	0.65
(1,2585)	1:97:A:VAL:HG12	1:134:A:LYS:HG3	2	0.65
(1,2569)	1:97:A:VAL:HG12	1:120:A:GLU:HB2	6	0.65
(1,2560)	1:151:A:SER:H	1:89:A:VAL:HG23	8	0.65
(1,2539)	1:70:A:LEU:HD11	1:70:A:LEU:H	2	0.65
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB2	7	0.65
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	3	0.65
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	5	0.65
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	10	0.65
(1,2288)	1:41:A:LYS:H	1:41:A:LYS:HB3	9	0.65
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	2	0.65
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	2	0.65
(1,1664)	1:89:A:VAL:HG12	1:123:A:THR:HG21	2	0.65
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG12	6	0.65
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	3	0.65
(1,1245)	1:146:A:VAL:HB	1:123:A:THR:HG23	2	0.65
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG21	4	0.65
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	1	0.65
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	8	0.65
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	4	0.65
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	2	0.65
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	3	0.65
(1,677)	1:20:A:ARG:HD2	1:68:A:TYR:HE1	5	0.65
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	3	0.65
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	7	0.65
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG21	4	0.65
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	3	0.65
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	7	0.65
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD13	3	0.65
(1,328)	1:100:A:ALA:HB1	1:101:A:MET:HA	8	0.65
(1,288)	1:146:A:VAL:HG23	1:143:A:GLU:HG3	7	0.65
(1,284)	1:146:A:VAL:HG21	1:143:A:GLU:HA	4	0.65
(1,269)	1:75:A:THR:HG22	1:77:A:SER:H	4	0.65
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG21	9	0.64
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	7	0.64
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	2	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB1	3	0.64
(1,3368)	1:108:A:ASP:H	1:75:A:THR:HG22	4	0.64
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG22	4	0.64
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	6	0.64
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	5	0.64
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	8	0.64
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD23	2	0.64
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	1	0.64
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	8	0.64
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	8	0.64
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	7	0.64
(1,2866)	1:159:A:GLU:HG3	1:156:A:PHE:HD2	2	0.64
(1,2858)	1:16:A:ASN:HB3	1:71:A:THR:HG23	2	0.64
(1,2824)	1:149:A:VAL:HG13	1:125:A:ASN:HB2	2	0.64
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	4	0.64
(1,2786)	1:41:A:LYS:HE2	1:41:A:LYS:HG2	1	0.64
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB2	9	0.64
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG23	8	0.64
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HB2	6	0.64
(1,2640)	1:114:A:ALA:HB1	1:110:A:GLN:HA	8	0.64
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG21	2	0.64
(1,2590)	1:102:A:VAL:HG11	1:17:A:LYS:HE2	8	0.64
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG22	5	0.64
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG23	8	0.64
(1,2577)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	4	0.64
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG11	1	0.64
(1,2529)	1:115:A:ALA:HB2	1:116:A:ASP:HA	8	0.64
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	8	0.64
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	6	0.64
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	7	0.64
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	10	0.64
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	3	0.64
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	6	0.64
(1,1604)	1:33:A:LEU:HD21	1:51:A:TYR:HA	10	0.64
(1,1454)	1:78:A:ARG:HG3	1:156:A:PHE:HZ	8	0.64
(1,1404)	1:88:A:HIS:HB2	1:146:A:VAL:H	7	0.64
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG12	4	0.64
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	9	0.64
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG21	1	0.64
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG23	3	0.64
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	3	0.64
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	2	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	4	0.64
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	9	0.64
(1,704)	1:21:A:ALA:HB2	1:61:A:LYS:HE2	4	0.64
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	5	0.64
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	6	0.64
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	9	0.64
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	10	0.64
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG22	9	0.64
(1,416)	1:21:A:ALA:HB1	1:62:A:GLU:HB3	5	0.64
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	3	0.64
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD13	5	0.64
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	8	0.63
(1,3427)	1:113:A:CYS:H	1:111:A:ALA:HB2	7	0.63
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG13	1	0.63
(1,3209)	1:70:A:LEU:H	1:16:A:ASN:HB2	6	0.63
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	3	0.63
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	4	0.63
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD23	5	0.63
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG22	3	0.63
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD21	6	0.63
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB1	10	0.63
(1,2930)	1:22:A:PRO:HD2	1:62:A:GLU:HB3	5	0.63
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	6	0.63
(1,2859)	1:71:A:THR:HG22	1:16:A:ASN:HB2	4	0.63
(1,2824)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	4	0.63
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	9	0.63
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG22	2	0.63
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	3	0.63
(1,2675)	1:24:A:ILE:HD12	1:61:A:LYS:HB3	8	0.63
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB2	1	0.63
(1,2655)	1:97:A:VAL:HG23	1:134:A:LYS:HB2	1	0.63
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HB2	3	0.63
(1,2653)	1:97:A:VAL:HG21	1:121:A:ILE:H	5	0.63
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB3	8	0.63
(1,2603)	1:149:A:VAL:HG22	1:147:A:LEU:HA	2	0.63
(1,2603)	1:149:A:VAL:HG23	1:147:A:LEU:HA	4	0.63
(1,2603)	1:149:A:VAL:HG23	1:147:A:LEU:HA	8	0.63
(1,2603)	1:149:A:VAL:HG23	1:147:A:LEU:HA	9	0.63
(1,2592)	1:75:A:THR:HG22	1:13:A:HIS:H	4	0.63
(1,2577)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	10	0.63
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG11	9	0.63
(1,2530)	1:13:A:HIS:HD2	1:67:A:LEU:HG	1	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	6	0.63
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	10	0.63
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG21	1	0.63
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	6	0.63
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	4	0.63
(1,1389)	1:20:A:ARG:H	1:19:A:SER:HB2	5	0.63
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	5	0.63
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	3	0.63
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD3	7	0.63
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG21	2	0.63
(1,1215)	1:27:A:PRO:HB2	1:28:A:VAL:HG22	8	0.63
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	9	0.63
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	7	0.63
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG22	1	0.63
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	3	0.63
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	5	0.63
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	6	0.63
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	10	0.63
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	3	0.63
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	5	0.63
(1,703)	1:61:A:LYS:HE2	1:59:A:HIS:HB2	1	0.63
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	9	0.63
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	2	0.63
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	4	0.63
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	7	0.63
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	8	0.63
(1,416)	1:21:A:ALA:HB3	1:62:A:GLU:HB3	9	0.63
(1,404)	1:37:A:ALA:HB3	1:9:A:LEU:HD13	7	0.63
(1,396)	1:107:A:ALA:HB2	1:77:A:SER:HB2	1	0.63
(1,284)	1:146:A:VAL:HG21	1:143:A:GLU:HA	1	0.63
(1,284)	1:146:A:VAL:HG23	1:143:A:GLU:HA	2	0.63
(1,269)	1:75:A:THR:HG22	1:77:A:SER:H	10	0.63
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG22	7	0.62
(1,3496)	1:135:A:GLY:H	1:97:A:VAL:HB	5	0.62
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	8	0.62
(1,3306)	1:26:A:GLU:H	1:24:A:ILE:HG21	9	0.62
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	8	0.62
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	3	0.62
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	9	0.62
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG22	6	0.62
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	7	0.62
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD21	2	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG11	8	0.62
(1,3138)	1:12:A:VAL:HG12	1:51:A:TYR:HE2	7	0.62
(1,3133)	1:123:A:THR:HG23	1:150:A:THR:HA	5	0.62
(1,3133)	1:123:A:THR:HG23	1:150:A:THR:HA	7	0.62
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	2	0.62
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG21	7	0.62
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG21	9	0.62
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD23	3	0.62
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD22	7	0.62
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD21	10	0.62
(1,3073)	1:33:A:LEU:HD13	1:9:A:LEU:HB3	1	0.62
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	6	0.62
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG21	9	0.62
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	5	0.62
(1,2932)	1:146:A:VAL:H	1:143:A:GLU:HB3	7	0.62
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	9	0.62
(1,2824)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	1	0.62
(1,2824)	1:149:A:VAL:HG11	1:125:A:ASN:HB2	9	0.62
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	8	0.62
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG23	1	0.62
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG22	5	0.62
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	10	0.62
(1,2671)	1:24:A:ILE:HD12	1:60:A:VAL:HA	5	0.62
(1,2640)	1:114:A:ALA:HB1	1:110:A:GLN:HA	4	0.62
(1,2640)	1:114:A:ALA:HB2	1:110:A:GLN:HA	10	0.62
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB3	3	0.62
(1,2614)	1:42:A:ALA:HB3	1:39:A:GLN:HG3	10	0.62
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG23	6	0.62
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG23	3	0.62
(1,2594)	1:28:A:VAL:HG23	1:39:A:GLN:HA	4	0.62
(1,2594)	1:28:A:VAL:HG21	1:39:A:GLN:HA	6	0.62
(1,2585)	1:97:A:VAL:HG13	1:134:A:LYS:HG3	8	0.62
(1,2577)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	7	0.62
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG11	2	0.62
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG11	4	0.62
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG13	5	0.62
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG22	9	0.62
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG13	2	0.62
(1,2529)	1:115:A:ALA:HB3	1:116:A:ASP:HA	4	0.62
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	6	0.62
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	9	0.62
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	2	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG21	5	0.62
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	9	0.62
(1,1883)	1:94:A:ALA:H	1:134:A:LYS:HG2	10	0.62
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG23	4	0.62
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG23	6	0.62
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG22	4	0.62
(1,1401)	1:88:A:HIS:HB3	1:89:A:VAL:HG11	5	0.62
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	3	0.62
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	4	0.62
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	10	0.62
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	4	0.62
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD3	6	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	1	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	2	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	3	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	5	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	6	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	7	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	8	0.62
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	10	0.62
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	1	0.62
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	2	0.62
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	8	0.62
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	10	0.62
(1,615)	1:146:A:VAL:H	1:145:A:GLY:HA3	8	0.62
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD13	3	0.62
(1,550)	1:53:A:ASP:H	1:73:A:GLY:HA3	10	0.62
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	3	0.62
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD13	7	0.62
(1,284)	1:146:A:VAL:HG23	1:143:A:GLU:HA	9	0.62
(1,269)	1:75:A:THR:HG21	1:77:A:SER:H	1	0.62
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG23	3	0.62
(1,173)	1:35:A:GLN:HE21	1:31:A:VAL:HG13	2	0.62
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG12	5	0.61
(1,3339)	1:156:A:PHE:H	1:155:A:GLN:HG3	6	0.61
(1,3331)	1:38:A:ALA:H	1:34:A:GLU:HB2	9	0.61
(1,3323)	1:116:A:ASP:H	1:98:A:MET:HG2	10	0.61
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	7	0.61
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	8	0.61
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD21	5	0.61
(1,3176)	1:74:A:LYS:H	1:70:A:LEU:HB3	10	0.61
(1,3133)	1:123:A:THR:HG23	1:150:A:THR:HA	6	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG21	4	0.61
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD22	9	0.61
(1,2969)	1:92:A:GLU:HB2	1:93:A:GLY:HA2	2	0.61
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	3	0.61
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	3	0.61
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	4	0.61
(1,2719)	1:25:A:GLY:HA2	1:26:A:GLU:HB3	10	0.61
(1,2690)	1:94:A:ALA:HA	1:134:A:LYS:HB3	10	0.61
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB1	7	0.61
(1,2653)	1:97:A:VAL:HG21	1:121:A:ILE:H	9	0.61
(1,2640)	1:114:A:ALA:HB1	1:113:A:CYS:HB3	5	0.61
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG21	8	0.61
(1,2603)	1:149:A:VAL:HG22	1:147:A:LEU:HA	7	0.61
(1,2577)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	3	0.61
(1,2577)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	5	0.61
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG13	3	0.61
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG11	8	0.61
(1,2539)	1:70:A:LEU:HD12	1:70:A:LEU:H	1	0.61
(1,2539)	1:70:A:LEU:HD13	1:70:A:LEU:H	4	0.61
(1,2539)	1:70:A:LEU:HD11	1:70:A:LEU:H	6	0.61
(1,2539)	1:70:A:LEU:HD13	1:70:A:LEU:H	7	0.61
(1,2539)	1:70:A:LEU:HD13	1:70:A:LEU:H	9	0.61
(1,2529)	1:115:A:ALA:HB1	1:116:A:ASP:HA	1	0.61
(1,2529)	1:115:A:ALA:HB3	1:116:A:ASP:HA	6	0.61
(1,2503)	1:85:A:PHE:HE1	1:110:A:GLN:HG2	5	0.61
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	8	0.61
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG22	7	0.61
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	1	0.61
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	8	0.61
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD21	3	0.61
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD22	10	0.61
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	1	0.61
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	2	0.61
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	6	0.61
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	7	0.61
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	8	0.61
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	6	0.61
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	7	0.61
(1,1277)	1:89:A:VAL:HG21	1:142:A:LYS:HD2	5	0.61
(1,1270)	1:98:A:MET:HG2	1:133:A:PHE:HD1	8	0.61
(1,1187)	1:60:A:VAL:H	1:59:A:HIS:HB2	4	0.61
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	4	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD2	8	0.61
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG21	10	0.61
(1,548)	1:65:A:PRO:HD3	1:64:A:LYS:HB3	10	0.61
(1,487)	1:24:A:ILE:HG23	1:43:A:VAL:HB	7	0.61
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	9	0.61
(1,416)	1:21:A:ALA:HB3	1:62:A:GLU:HB3	7	0.61
(1,407)	1:142:A:LYS:H	1:140:A:ALA:HB3	5	0.61
(1,404)	1:37:A:ALA:HB1	1:9:A:LEU:HD13	6	0.61
(1,404)	1:37:A:ALA:HB1	1:9:A:LEU:HD11	9	0.61
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD13	1	0.61
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD13	4	0.61
(1,284)	1:146:A:VAL:HG23	1:143:A:GLU:HA	5	0.61
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	1	0.6
(1,3447)	1:50:A:THR:H	1:75:A:THR:HG23	9	0.6
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG13	10	0.6
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	7	0.6
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	8	0.6
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	9	0.6
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	2	0.6
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	5	0.6
(1,3209)	1:70:A:LEU:H	1:16:A:ASN:HB2	5	0.6
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD21	6	0.6
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	1	0.6
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG23	1	0.6
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG21	5	0.6
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG22	10	0.6
(1,3122)	1:7:A:LEU:HD22	1:5:A:ALA:H	8	0.6
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD21	10	0.6
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD21	6	0.6
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD22	8	0.6
(1,3008)	1:130:A:LYS:HD3	1:130:A:LYS:HA	10	0.6
(1,2950)	1:71:A:THR:HB	1:54:A:ASP:HB2	4	0.6
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	3	0.6
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	6	0.6
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	2	0.6
(1,2907)	1:84:A:CYS:HB3	1:154:A:LYS:HB3	9	0.6
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	8	0.6
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	1	0.6
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	10	0.6
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	5	0.6
(1,2716)	1:159:A:GLU:H	1:160:A:GLY:HA2	10	0.6
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG23	9	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	2	0.6
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	5	0.6
(1,2614)	1:42:A:ALA:HB2	1:39:A:GLN:HG3	6	0.6
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG22	8	0.6
(1,2594)	1:28:A:VAL:HG21	1:39:A:GLN:HA	10	0.6
(1,2577)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	2	0.6
(1,2577)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	6	0.6
(1,2539)	1:70:A:LEU:HD12	1:70:A:LEU:H	3	0.6
(1,2539)	1:70:A:LEU:HD11	1:70:A:LEU:H	5	0.6
(1,2539)	1:70:A:LEU:HD12	1:70:A:LEU:H	10	0.6
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG11	3	0.6
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	6	0.6
(1,2529)	1:115:A:ALA:HB3	1:116:A:ASP:HA	10	0.6
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB3	1	0.6
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	2	0.6
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG22	8	0.6
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG22	6	0.6
(1,1664)	1:89:A:VAL:HG13	1:123:A:THR:HG23	5	0.6
(1,1664)	1:89:A:VAL:HG13	1:123:A:THR:HG23	7	0.6
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	5	0.6
(1,1323)	1:34:A:GLU:H	1:34:A:GLU:HB3	9	0.6
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	3	0.6
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	4	0.6
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	6	0.6
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	7	0.6
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	2	0.6
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	3	0.6
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	10	0.6
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG21	6	0.6
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	6	0.6
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	2	0.6
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	3	0.6
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	2	0.6
(1,487)	1:24:A:ILE:HG23	1:43:A:VAL:HB	8	0.6
(1,487)	1:24:A:ILE:HG22	1:43:A:VAL:HB	10	0.6
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG12	4	0.6
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	10	0.6
(1,288)	1:146:A:VAL:HG23	1:143:A:GLU:HG3	3	0.6
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	1	0.6
(1,3496)	1:135:A:GLY:H	1:97:A:VAL:HB	3	0.59
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG12	6	0.59
(1,3428)	1:113:A:CYS:H	1:114:A:ALA:HB3	8	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG13	9	0.59
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	2	0.59
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	4	0.59
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD21	6	0.59
(1,3133)	1:123:A:THR:HG22	1:150:A:THR:HA	1	0.59
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD21	4	0.59
(1,3122)	1:8:A:ASP:H	1:7:A:LEU:HD23	7	0.59
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD23	1	0.59
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	4	0.59
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	7	0.59
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	2	0.59
(1,2907)	1:84:A:CYS:HB3	1:154:A:LYS:HB3	4	0.59
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD21	9	0.59
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	2	0.59
(1,2824)	1:149:A:VAL:HG12	1:125:A:ASN:HB2	10	0.59
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	2	0.59
(1,2749)	1:82:A:ARG:HD3	1:82:A:ARG:HB2	8	0.59
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG21	3	0.59
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	8	0.59
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	9	0.59
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	10	0.59
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	4	0.59
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	9	0.59
(1,2675)	1:24:A:ILE:HD12	1:61:A:LYS:HB3	4	0.59
(1,2671)	1:24:A:ILE:HD11	1:60:A:VAL:HA	7	0.59
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG23	7	0.59
(1,2640)	1:114:A:ALA:HB1	1:110:A:GLN:HA	9	0.59
(1,2624)	1:37:A:ALA:HB1	1:36:A:CYS:HB3	6	0.59
(1,2614)	1:42:A:ALA:HB3	1:39:A:GLN:HG3	8	0.59
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	3	0.59
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	6	0.59
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG23	10	0.59
(1,2577)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	8	0.59
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG11	10	0.59
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	5	0.59
(1,2539)	1:70:A:LEU:HD12	1:70:A:LEU:H	8	0.59
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG13	7	0.59
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	1	0.59
(1,2486)	1:68:A:TYR:HD2	1:68:A:TYR:HA	8	0.59
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	6	0.59
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG21	3	0.59
(1,1604)	1:33:A:LEU:HD22	1:51:A:TYR:HA	7	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	8	0.59
(1,1316)	1:127:A:HIS:H	1:127:A:HIS:HB3	9	0.59
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD2	10	0.59
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	6	0.59
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	8	0.59
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG21	2	0.59
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG21	5	0.59
(1,1015)	1:121:A:ILE:H	1:120:A:GLU:HG3	4	0.59
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	1	0.59
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	3	0.59
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	4	0.59
(1,638)	1:122:A:PHE:HB2	1:113:A:CYS:HB3	3	0.59
(1,495)	1:94:A:ALA:HB1	1:134:A:LYS:HA	7	0.59
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	5	0.59
(1,284)	1:146:A:VAL:HG22	1:143:A:GLU:HA	7	0.59
(1,269)	1:75:A:THR:HG22	1:77:A:SER:H	8	0.59
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG23	4	0.59
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	7	0.58
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG13	4	0.58
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG11	8	0.58
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	7	0.58
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	8	0.58
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG21	4	0.58
(1,3133)	1:123:A:THR:HG21	1:150:A:THR:HA	8	0.58
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	1	0.58
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD23	2	0.58
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD23	3	0.58
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD22	5	0.58
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	1	0.58
(1,2962)	1:65:A:PRO:HB3	1:67:A:LEU:HG	5	0.58
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	6	0.58
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	2	0.58
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	1	0.58
(1,2858)	1:16:A:ASN:HB3	1:71:A:THR:HG22	4	0.58
(1,2850)	1:100:A:ALA:HB2	1:101:A:MET:HB3	7	0.58
(1,2825)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	7	0.58
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	2	0.58
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	10	0.58
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB2	5	0.58
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB3	10	0.58
(1,2641)	1:114:A:ALA:HB3	1:110:A:GLN:HG2	5	0.58
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB3	8	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG21	9	0.58
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	1	0.58
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	4	0.58
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	5	0.58
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	7	0.58
(1,2606)	1:129:A:GLN:HA	1:129:A:GLN:HB2	8	0.58
(1,2577)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	1	0.58
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG12	1	0.58
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG11	6	0.58
(1,2556)	1:71:A:THR:HG21	1:54:A:ASP:HB2	9	0.58
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	10	0.58
(1,2543)	1:92:A:GLU:HA	1:132:A:THR:HG23	8	0.58
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG12	4	0.58
(1,2538)	1:41:A:LYS:H	1:60:A:VAL:HG13	5	0.58
(1,2212)	1:17:A:LYS:H	1:17:A:LYS:HG3	7	0.58
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	7	0.58
(1,1645)	1:73:A:GLY:HA3	1:50:A:THR:HG22	1	0.58
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD21	7	0.58
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	2	0.58
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	4	0.58
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	5	0.58
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG22	4	0.58
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE2	3	0.58
(1,724)	1:8:A:ASP:H	1:7:A:LEU:HB2	1	0.58
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG22	1	0.58
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD11	3	0.58
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	6	0.58
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG12	7	0.58
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD13	2	0.58
(1,284)	1:146:A:VAL:HG22	1:143:A:GLU:HA	3	0.58
(1,210)	1:149:A:VAL:HG12	1:123:A:THR:HG23	8	0.58
(1,210)	1:149:A:VAL:HG13	1:123:A:THR:HG23	10	0.58
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG21	2	0.58
(1,167)	1:150:A:THR:HG23	1:85:A:PHE:HB2	1	0.58
(1,167)	1:150:A:THR:HG23	1:85:A:PHE:HB2	8	0.58
(1,3538)	1:152:A:GLY:H	1:151:A:SER:HB2	2	0.57
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	3	0.57
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG11	2	0.57
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG21	2	0.57
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	10	0.57
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	1	0.57
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	1	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	6	0.57
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG23	9	0.57
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD21	8	0.57
(1,3202)	1:100:A:ALA:H	1:133:A:PHE:HB2	2	0.57
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	9	0.57
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD21	1	0.57
(1,3155)	1:70:A:LEU:HD22	1:17:A:LYS:H	9	0.57
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD21	4	0.57
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD21	7	0.57
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD21	9	0.57
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB1	7	0.57
(1,3008)	1:130:A:LYS:HD3	1:130:A:LYS:HA	1	0.57
(1,2969)	1:92:A:GLU:HB2	1:93:A:GLY:HA2	3	0.57
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	7	0.57
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	10	0.57
(1,2907)	1:84:A:CYS:HB3	1:154:A:LYS:HB3	6	0.57
(1,2907)	1:84:A:CYS:HB3	1:154:A:LYS:HB3	10	0.57
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	3	0.57
(1,2848)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	6	0.57
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	5	0.57
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	9	0.57
(1,2771)	1:154:A:LYS:HE3	1:154:A:LYS:HG3	5	0.57
(1,2749)	1:82:A:ARG:HD3	1:82:A:ARG:HB2	3	0.57
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	1	0.57
(1,2671)	1:24:A:ILE:HD13	1:60:A:VAL:HA	10	0.57
(1,2653)	1:97:A:VAL:HG23	1:121:A:ILE:H	4	0.57
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB2	6	0.57
(1,2640)	1:114:A:ALA:HB3	1:110:A:GLN:HA	7	0.57
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG22	4	0.57
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG22	10	0.57
(1,2592)	1:75:A:THR:HG21	1:13:A:HIS:H	3	0.57
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG21	9	0.57
(1,2568)	1:43:A:VAL:HG21	1:60:A:VAL:HB	4	0.57
(1,2566)	1:103:A:THR:HG22	1:102:A:VAL:HA	1	0.57
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	1	0.57
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	5	0.57
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	10	0.57
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG22	3	0.57
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB1	10	0.57
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB1	2	0.57
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	2	0.57
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	6	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1640)	1:47:A:THR:HG23	1:156:A:PHE:HE2	5	0.57
(1,1604)	1:33:A:LEU:HD23	1:51:A:TYR:HA	8	0.57
(1,1604)	1:33:A:LEU:HD22	1:51:A:TYR:HA	9	0.57
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	6	0.57
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD23	8	0.57
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	10	0.57
(1,1277)	1:89:A:VAL:HG22	1:142:A:LYS:HD3	8	0.57
(1,1276)	1:143:A:GLU:H	1:142:A:LYS:HD3	8	0.57
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	4	0.57
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	2	0.57
(1,1018)	1:121:A:ILE:HG21	1:120:A:GLU:HG3	10	0.57
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	6	0.57
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD12	7	0.57
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD12	8	0.57
(1,495)	1:94:A:ALA:HB2	1:134:A:LYS:HA	1	0.57
(1,396)	1:107:A:ALA:HB2	1:77:A:SER:HB2	9	0.57
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG13	9	0.57
(1,335)	1:149:A:VAL:HG21	1:149:A:VAL:HA	3	0.57
(1,288)	1:146:A:VAL:HG22	1:143:A:GLU:HG3	6	0.57
(1,269)	1:75:A:THR:HG21	1:77:A:SER:H	5	0.57
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG23	5	0.57
(1,117)	1:134:A:LYS:HG3	1:134:A:LYS:HA	10	0.57
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	2	0.56
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	2	0.56
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG12	3	0.56
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG23	3	0.56
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	7	0.56
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	7	0.56
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	5	0.56
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG22	7	0.56
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	1	0.56
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	3	0.56
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD23	8	0.56
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD22	9	0.56
(1,3091)	1:94:A:ALA:HA	1:95:A:PRO:HA	7	0.56
(1,2982)	1:64:A:LYS:HA	1:64:A:LYS:HD3	10	0.56
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	5	0.56
(1,2907)	1:84:A:CYS:HB3	1:154:A:LYS:HB3	2	0.56
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	4	0.56
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	5	0.56
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	9	0.56
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	5	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2859)	1:71:A:THR:HG23	1:16:A:ASN:HB2	2	0.56
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	3	0.56
(1,2825)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	2	0.56
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	1	0.56
(1,2786)	1:41:A:LYS:HE2	1:41:A:LYS:HG2	5	0.56
(1,2713)	1:160:A:GLY:HA3	1:114:A:ALA:HB1	7	0.56
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	9	0.56
(1,2641)	1:114:A:ALA:HB1	1:110:A:GLN:HG2	1	0.56
(1,2560)	1:145:A:GLY:H	1:89:A:VAL:HG23	2	0.56
(1,2556)	1:71:A:THR:HG23	1:54:A:ASP:HB2	8	0.56
(1,2529)	1:115:A:ALA:HB3	1:116:A:ASP:HA	9	0.56
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	9	0.56
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG21	7	0.56
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG22	9	0.56
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	2	0.56
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB3	5	0.56
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	9	0.56
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG23	9	0.56
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG22	5	0.56
(1,1542)	1:76:A:ALA:HB3	1:75:A:THR:HA	9	0.56
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	1	0.56
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	8	0.56
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	10	0.56
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG21	7	0.56
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG22	9	0.56
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG22	10	0.56
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	5	0.56
(1,770)	1:81:A:ASP:HB2	1:79:A:SER:HB2	3	0.56
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE2	2	0.56
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD12	2	0.56
(1,416)	1:21:A:ALA:HB2	1:62:A:GLU:HB3	10	0.56
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD13	2	0.56
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD12	4	0.56
(1,404)	1:37:A:ALA:HB2	1:9:A:LEU:HD12	10	0.56
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG13	1	0.56
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG13	2	0.56
(1,335)	1:149:A:VAL:HG22	1:149:A:VAL:HA	2	0.56
(1,335)	1:149:A:VAL:HG23	1:149:A:VAL:HA	4	0.56
(1,335)	1:149:A:VAL:HG22	1:149:A:VAL:HA	5	0.56
(1,335)	1:149:A:VAL:HG22	1:149:A:VAL:HA	6	0.56
(1,335)	1:149:A:VAL:HG23	1:149:A:VAL:HA	8	0.56
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	1	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	6	0.56
(1,284)	1:146:A:VAL:HG22	1:143:A:GLU:HA	8	0.56
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG22	6	0.56
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG21	7	0.56
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG21	9	0.56
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG23	2	0.56
(1,44)	1:151:A:SER:HB3	1:123:A:THR:HA	2	0.56
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	1	0.55
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	5	0.55
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	9	0.55
(1,3447)	1:50:A:THR:H	1:60:A:VAL:HG11	7	0.55
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG23	9	0.55
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG21	10	0.55
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	7	0.55
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	5	0.55
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	3	0.55
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG22	2	0.55
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	8	0.55
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	3	0.55
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	4	0.55
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD23	10	0.55
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB2	5	0.55
(1,3094)	1:76:A:ALA:HB1	1:77:A:SER:HB3	4	0.55
(1,3055)	1:144:A:ARG:HG3	1:144:A:ARG:H	7	0.55
(1,2908)	1:110:A:GLN:HG2	1:79:A:SER:HB2	10	0.55
(1,2852)	1:101:A:MET:HB2	1:65:A:PRO:HB2	1	0.55
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	2	0.55
(1,2825)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	6	0.55
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	8	0.55
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	6	0.55
(1,2714)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	8	0.55
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	3	0.55
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	6	0.55
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	3	0.55
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	6	0.55
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	8	0.55
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	6	0.55
(1,2671)	1:24:A:ILE:HD11	1:60:A:VAL:HA	2	0.55
(1,2640)	1:114:A:ALA:HB1	1:110:A:GLN:HA	3	0.55
(1,2624)	1:37:A:ALA:HB2	1:36:A:CYS:HB3	1	0.55
(1,2624)	1:37:A:ALA:HB1	1:36:A:CYS:HB3	5	0.55
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG23	4	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG21	5	0.55
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG21	6	0.55
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG12	7	0.55
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	6	0.55
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG11	6	0.55
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG13	8	0.55
(1,2529)	1:115:A:ALA:HB1	1:116:A:ASP:HA	2	0.55
(1,2529)	1:115:A:ALA:HB1	1:116:A:ASP:HA	7	0.55
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	7	0.55
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	8	0.55
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	10	0.55
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	3	0.55
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD23	1	0.55
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB2	7	0.55
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB2	10	0.55
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	3	0.55
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	7	0.55
(1,1664)	1:89:A:VAL:HG11	1:123:A:THR:HG22	1	0.55
(1,1664)	1:89:A:VAL:HG12	1:123:A:THR:HG21	8	0.55
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG22	7	0.55
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	1	0.55
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	6	0.55
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	7	0.55
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	9	0.55
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	2	0.55
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG23	3	0.55
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	9	0.55
(1,495)	1:94:A:ALA:HB3	1:134:A:LYS:HA	4	0.55
(1,487)	1:24:A:ILE:HG21	1:43:A:VAL:HB	1	0.55
(1,486)	1:24:A:ILE:HG22	1:60:A:VAL:HB	1	0.55
(1,486)	1:24:A:ILE:HG21	1:60:A:VAL:HB	8	0.55
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	8	0.55
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG12	3	0.55
(1,349)	1:121:A:ILE:HG21	1:121:A:ILE:HD13	3	0.55
(1,335)	1:149:A:VAL:HG22	1:149:A:VAL:HA	7	0.55
(1,335)	1:149:A:VAL:HG23	1:149:A:VAL:HA	10	0.55
(1,331)	1:149:A:VAL:HG23	1:146:A:VAL:H	1	0.55
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	4	0.55
(1,284)	1:146:A:VAL:HG22	1:143:A:GLU:HA	10	0.55
(1,269)	1:75:A:THR:HG23	1:77:A:SER:H	2	0.55
(1,269)	1:75:A:THR:HG23	1:77:A:SER:H	6	0.55
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG22	3	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:35:A:GLN:HE21	1:31:A:VAL:HG13	9	0.55
(1,44)	1:151:A:SER:HB3	1:123:A:THR:HA	10	0.55
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG23	4	0.54
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	3	0.54
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	2	0.54
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	3	0.54
(1,3133)	1:123:A:THR:HG21	1:150:A:THR:HA	3	0.54
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB1	6	0.54
(1,3091)	1:94:A:ALA:HA	1:95:A:PRO:HA	6	0.54
(1,3091)	1:94:A:ALA:HA	1:95:A:PRO:HA	8	0.54
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	5	0.54
(1,2952)	1:101:A:MET:HG3	1:103:A:THR:HA	6	0.54
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	8	0.54
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	4	0.54
(1,2848)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	8	0.54
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	7	0.54
(1,2723)	1:63:A:GLY:HA3	1:64:A:LYS:HD2	7	0.54
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	7	0.54
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	8	0.54
(1,2665)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	6	0.54
(1,2643)	1:31:A:VAL:HG22	1:57:A:MET:HA	1	0.54
(1,2640)	1:114:A:ALA:HB2	1:113:A:CYS:HB3	1	0.54
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG21	7	0.54
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG22	9	0.54
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	1	0.54
(1,2543)	1:92:A:GLU:HA	1:94:A:ALA:HB1	2	0.54
(1,2488)	1:68:A:TYR:HD1	1:20:A:ARG:HB2	3	0.54
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG23	4	0.54
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB3	5	0.54
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	6	0.54
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB1	8	0.54
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG21	1	0.54
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG23	3	0.54
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB3	7	0.54
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB3	8	0.54
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB1	10	0.54
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	9	0.54
(1,1406)	1:88:A:HIS:HB2	1:147:A:LEU:HD21	2	0.54
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	3	0.54
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	8	0.54
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	3	0.54
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	5	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	3	0.54
(1,1154)	1:118:A:SER:H	1:117:A:PRO:HB3	9	0.54
(1,1095)	1:89:A:VAL:HB	1:149:A:VAL:HG22	8	0.54
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE2	5	0.54
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	5	0.54
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD11	9	0.54
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	4	0.54
(1,486)	1:24:A:ILE:HG22	1:60:A:VAL:HB	3	0.54
(1,486)	1:24:A:ILE:HG22	1:60:A:VAL:HB	6	0.54
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	6	0.54
(1,335)	1:149:A:VAL:HG23	1:149:A:VAL:HA	1	0.54
(1,335)	1:149:A:VAL:HG23	1:149:A:VAL:HA	9	0.54
(1,328)	1:100:A:ALA:HB2	1:101:A:MET:HA	2	0.54
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	3	0.54
(1,328)	1:100:A:ALA:HB2	1:101:A:MET:HA	7	0.54
(1,288)	1:146:A:VAL:HG21	1:143:A:GLU:HG3	2	0.54
(1,288)	1:146:A:VAL:HG21	1:143:A:GLU:HG3	5	0.54
(1,284)	1:146:A:VAL:HG21	1:143:A:GLU:HA	6	0.54
(1,269)	1:75:A:THR:HG21	1:77:A:SER:H	3	0.54
(1,269)	1:75:A:THR:HG22	1:77:A:SER:H	7	0.54
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	10	0.53
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG23	2	0.53
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG23	5	0.53
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG22	7	0.53
(1,3404)	1:48:A:HIS:H	1:60:A:VAL:HG11	4	0.53
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD11	5	0.53
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	9	0.53
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG22	5	0.53
(1,3209)	1:70:A:LEU:H	1:16:A:ASN:HB2	1	0.53
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	8	0.53
(1,3155)	1:70:A:LEU:HD22	1:17:A:LYS:H	5	0.53
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD22	7	0.53
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	9	0.53
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	6	0.53
(1,3115)	1:6:A:LYS:HE3	1:6:A:LYS:HG3	6	0.53
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB3	2	0.53
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB3	8	0.53
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB1	9	0.53
(1,3094)	1:76:A:ALA:HB2	1:77:A:SER:HB3	10	0.53
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	9	0.53
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	1	0.53
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	10	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	3	0.53
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	5	0.53
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	9	0.53
(1,2938)	1:101:A:MET:HG2	1:103:A:THR:HG22	3	0.53
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	8	0.53
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	10	0.53
(1,2798)	1:130:A:LYS:HE2	1:132:A:THR:HG21	8	0.53
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	5	0.53
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD3	1	0.53
(1,2716)	1:159:A:GLU:H	1:160:A:GLY:HA2	2	0.53
(1,2707)	1:148:A:GLY:HA3	1:149:A:VAL:HG23	10	0.53
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	1	0.53
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	4	0.53
(1,2642)	1:35:A:GLN:H	1:31:A:VAL:HG22	5	0.53
(1,2624)	1:37:A:ALA:HB2	1:36:A:CYS:HB3	2	0.53
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	9	0.53
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG22	9	0.53
(1,2538)	1:42:A:ALA:H	1:60:A:VAL:HG12	10	0.53
(1,2530)	1:88:A:HIS:HD2	1:147:A:LEU:HB3	4	0.53
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	7	0.53
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB2	4	0.53
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	10	0.53
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD21	5	0.53
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	7	0.53
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	10	0.53
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	5	0.53
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB3	4	0.53
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	5	0.53
(1,1253)	1:67:A:LEU:HD23	1:65:A:PRO:HB2	2	0.53
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	5	0.53
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	7	0.53
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	8	0.53
(1,1206)	1:27:A:PRO:HD2	1:27:A:PRO:HB3	2	0.53
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	10	0.53
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE2	8	0.53
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG21	7	0.53
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD12	2	0.53
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD13	5	0.53
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD11	10	0.53
(1,486)	1:24:A:ILE:HG23	1:60:A:VAL:HB	4	0.53
(1,486)	1:24:A:ILE:HG21	1:60:A:VAL:HB	7	0.53
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG22	10	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:37:A:ALA:HB1	1:9:A:LEU:HD13	5	0.53
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG13	6	0.53
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG12	10	0.53
(1,331)	1:149:A:VAL:HG23	1:146:A:VAL:H	9	0.53
(1,288)	1:146:A:VAL:HG22	1:143:A:GLU:HG3	4	0.53
(1,288)	1:146:A:VAL:HG23	1:143:A:GLU:HG3	10	0.53
(1,238)	1:103:A:THR:HG23	1:101:A:MET:HG3	7	0.53
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	5	0.52
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	5	0.52
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	6	0.52
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG22	10	0.52
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG23	1	0.52
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	7	0.52
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	7	0.52
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD22	3	0.52
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD23	4	0.52
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD23	6	0.52
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG23	5	0.52
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG22	10	0.52
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	2	0.52
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	5	0.52
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	6	0.52
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	7	0.52
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG22	5	0.52
(1,3055)	1:144:A:ARG:HG3	1:144:A:ARG:H	5	0.52
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	5	0.52
(1,2992)	1:16:A:ASN:H	1:13:A:HIS:HB3	3	0.52
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	10	0.52
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	5	0.52
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	3	0.52
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	1	0.52
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	2	0.52
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	6	0.52
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	7	0.52
(1,2932)	1:146:A:VAL:H	1:143:A:GLU:HB3	9	0.52
(1,2848)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	9	0.52
(1,2793)	1:40:A:CYS:HB2	1:46:A:CYS:HB3	2	0.52
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	1	0.52
(1,2716)	1:159:A:GLU:H	1:160:A:GLY:HA2	1	0.52
(1,2716)	1:159:A:GLU:H	1:160:A:GLY:HA2	8	0.52
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	7	0.52
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB3	10	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2624)	1:37:A:ALA:HB3	1:36:A:CYS:HB3	3	0.52
(1,2624)	1:37:A:ALA:HB3	1:36:A:CYS:HB3	7	0.52
(1,2624)	1:37:A:ALA:HB2	1:36:A:CYS:HB3	8	0.52
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	4	0.52
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD13	1	0.52
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB1	8	0.52
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	2	0.52
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	4	0.52
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG12	7	0.52
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG23	6	0.52
(1,1584)	1:74:A:LYS:HG2	1:14:A:SER:HB2	8	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	1	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	2	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	3	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	4	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	5	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	6	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	7	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	8	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	9	0.52
(1,1570)	1:74:A:LYS:HG2	1:74:A:LYS:HB2	10	0.52
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	1	0.52
(1,1018)	1:121:A:ILE:HG21	1:120:A:GLU:HG3	1	0.52
(1,918)	1:130:A:LYS:HB2	1:130:A:LYS:HE3	1	0.52
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	8	0.52
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	1	0.52
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG22	2	0.52
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD13	6	0.52
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD13	3	0.52
(1,495)	1:94:A:ALA:HB2	1:134:A:LYS:HA	9	0.52
(1,486)	1:24:A:ILE:HG21	1:60:A:VAL:HB	5	0.52
(1,486)	1:24:A:ILE:HG22	1:60:A:VAL:HB	9	0.52
(1,456)	1:38:A:ALA:HB2	1:35:A:GLN:HG3	7	0.52
(1,396)	1:107:A:ALA:HB2	1:77:A:SER:HB2	10	0.52
(1,329)	1:100:A:ALA:HB1	1:130:A:LYS:HE2	8	0.52
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	10	0.52
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG22	1	0.52
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG23	8	0.52
(1,167)	1:150:A:THR:HG22	1:85:A:PHE:HB2	5	0.52
(1,165)	1:150:A:THR:HG22	1:123:A:THR:HA	2	0.52
(1,21)	1:156:A:PHE:HD2	1:114:A:ALA:HB2	8	0.52
(1,3538)	1:152:A:GLY:H	1:151:A:SER:HB2	10	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	1	0.51
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	7	0.51
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	4	0.51
(1,3457)	1:125:A:ASN:HD22	1:126:A:GLU:H	4	0.51
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	2	0.51
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	4	0.51
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	8	0.51
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD11	3	0.51
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD13	10	0.51
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	1	0.51
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	8	0.51
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	10	0.51
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG21	6	0.51
(1,3202)	1:100:A:ALA:H	1:96:A:ASP:HB3	6	0.51
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	1	0.51
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	7	0.51
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	2	0.51
(1,3121)	1:34:A:GLU:H	1:33:A:LEU:HD22	1	0.51
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB2	3	0.51
(1,3094)	1:76:A:ALA:HB2	1:77:A:SER:HB3	6	0.51
(1,2952)	1:101:A:MET:HG3	1:103:A:THR:HA	4	0.51
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	8	0.51
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	10	0.51
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD21	4	0.51
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	1	0.51
(1,2848)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	3	0.51
(1,2825)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	5	0.51
(1,2825)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	8	0.51
(1,2825)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	9	0.51
(1,2825)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	10	0.51
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	8	0.51
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	3	0.51
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	6	0.51
(1,2793)	1:40:A:CYS:HB2	1:46:A:CYS:HB3	8	0.51
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD2	6	0.51
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	7	0.51
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	1	0.51
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	3	0.51
(1,2665)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	8	0.51
(1,2664)	1:94:A:ALA:HB1	1:95:A:PRO:HD2	5	0.51
(1,2643)	1:31:A:VAL:HG23	1:57:A:MET:HA	5	0.51
(1,2639)	1:114:A:ALA:HB3	1:156:A:PHE:HE2	10	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2624)	1:37:A:ALA:HB1	1:36:A:CYS:HB3	9	0.51
(1,2624)	1:37:A:ALA:HB2	1:36:A:CYS:HB3	10	0.51
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	8	0.51
(1,2582)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	4	0.51
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	2	0.51
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	8	0.51
(1,2529)	1:115:A:ALA:HB1	1:116:A:ASP:HA	5	0.51
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	2	0.51
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG13	2	0.51
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	2	0.51
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG21	7	0.51
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB3	9	0.51
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	6	0.51
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB3	1	0.51
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB2	6	0.51
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	3	0.51
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	6	0.51
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	8	0.51
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	4	0.51
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	8	0.51
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG13	2	0.51
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB2	1	0.51
(1,1542)	1:76:A:ALA:HB1	1:75:A:THR:HA	5	0.51
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	10	0.51
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	9	0.51
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG22	3	0.51
(1,1240)	1:78:A:ARG:HB2	1:47:A:THR:HA	1	0.51
(1,1018)	1:121:A:ILE:HG21	1:120:A:GLU:HG3	6	0.51
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD12	6	0.51
(1,486)	1:24:A:ILE:HG23	1:60:A:VAL:HB	10	0.51
(1,416)	1:21:A:ALA:HB1	1:62:A:GLU:HB3	6	0.51
(1,349)	1:121:A:ILE:HG23	1:121:A:ILE:HD12	10	0.51
(1,304)	1:75:A:THR:H	1:75:A:THR:HG21	9	0.51
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG23	6	0.51
(1,167)	1:150:A:THR:HG22	1:85:A:PHE:HB2	10	0.51
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	4	0.5
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	8	0.5
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG23	4	0.5
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	2	0.5
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	5	0.5
(1,3212)	1:53:A:ASP:H	1:33:A:LEU:HD23	7	0.5
(1,3202)	1:100:A:ALA:H	1:133:A:PHE:HB2	10	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	4	0.5
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD22	7	0.5
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	5	0.5
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	7	0.5
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	10	0.5
(1,2952)	1:101:A:MET:HG3	1:103:A:THR:HA	9	0.5
(1,2948)	1:27:A:PRO:HD3	1:27:A:PRO:HB3	4	0.5
(1,2848)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	10	0.5
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	8	0.5
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	4	0.5
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	5	0.5
(1,2716)	1:159:A:GLU:H	1:160:A:GLY:HA2	5	0.5
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	1	0.5
(1,2704)	1:117:A:PRO:HD3	1:116:A:ASP:HB2	4	0.5
(1,2700)	1:73:A:GLY:HA2	1:72:A:GLY:H	5	0.5
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB1	4	0.5
(1,2643)	1:31:A:VAL:HG22	1:57:A:MET:HA	8	0.5
(1,2641)	1:114:A:ALA:HB3	1:110:A:GLN:HG2	7	0.5
(1,2615)	1:42:A:ALA:HB3	1:43:A:VAL:HB	1	0.5
(1,2615)	1:42:A:ALA:HB3	1:43:A:VAL:HB	9	0.5
(1,2511)	1:107:A:ALA:HB1	1:85:A:PHE:HZ	10	0.5
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	7	0.5
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	4	0.5
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	4	0.5
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB3	6	0.5
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	1	0.5
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	1	0.5
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	9	0.5
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD13	4	0.5
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG12	5	0.5
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG21	5	0.5
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG23	8	0.5
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB3	2	0.5
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB1	6	0.5
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	4	0.5
(1,1320)	1:128:A:ASP:H	1:127:A:HIS:HB2	5	0.5
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	1	0.5
(1,1253)	1:67:A:LEU:HD23	1:65:A:PRO:HB2	7	0.5
(1,1018)	1:120:A:GLU:HG3	1:121:A:ILE:HG22	9	0.5
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG22	5	0.5
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG21	6	0.5
(1,594)	1:70:A:LEU:HB2	1:73:A:GLY:HA2	4	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,556)	1:73:A:GLY:HA2	1:70:A:LEU:HD11	4	0.5
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD13	4	0.5
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD13	1	0.5
(1,416)	1:21:A:ALA:HB3	1:62:A:GLU:HB3	3	0.5
(1,416)	1:21:A:ALA:HB1	1:62:A:GLU:HB3	8	0.5
(1,411)	1:21:A:ALA:HB1	1:48:A:HIS:HD2	1	0.5
(1,396)	1:107:A:ALA:HB3	1:77:A:SER:HB2	6	0.5
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	7	0.5
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG11	5	0.5
(1,282)	1:146:A:VAL:HG22	1:88:A:HIS:HA	8	0.5
(1,199)	1:73:A:GLY:H	1:71:A:THR:HG23	10	0.5
(1,188)	1:67:A:LEU:HD22	1:75:A:THR:HG22	9	0.5
(1,21)	1:156:A:PHE:HD2	1:114:A:ALA:HB2	3	0.5
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	10	0.49
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	5	0.49
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG22	3	0.49
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG22	7	0.49
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	1	0.49
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	4	0.49
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	5	0.49
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	10	0.49
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	1	0.49
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG22	2	0.49
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG23	3	0.49
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD23	3	0.49
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	10	0.49
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	4	0.49
(1,3127)	1:132:A:THR:HG23	1:92:A:GLU:HG2	2	0.49
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	3	0.49
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	5	0.49
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	9	0.49
(1,3097)	1:67:A:LEU:HD13	1:102:A:VAL:H	10	0.49
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	3	0.49
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	8	0.49
(1,2969)	1:92:A:GLU:HB3	1:93:A:GLY:HA2	9	0.49
(1,2811)	1:128:A:ASP:HB2	1:130:A:LYS:HG3	7	0.49
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	10	0.49
(1,2690)	1:94:A:ALA:HA	1:95:A:PRO:HG2	5	0.49
(1,2665)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	3	0.49
(1,2665)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	9	0.49
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HG3	8	0.49
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB3	1	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB2	9	0.49
(1,2615)	1:42:A:ALA:HB2	1:43:A:VAL:HB	6	0.49
(1,2615)	1:42:A:ALA:HB3	1:43:A:VAL:HB	10	0.49
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG21	8	0.49
(1,2577)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	9	0.49
(1,2570)	1:39:A:GLN:HA	1:43:A:VAL:HG12	9	0.49
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	4	0.49
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	3	0.49
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	4	0.49
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	1	0.49
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	3	0.49
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	8	0.49
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD13	2	0.49
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	6	0.49
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	8	0.49
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG11	8	0.49
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG21	9	0.49
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB1	2	0.49
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB2	3	0.49
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB3	7	0.49
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	2	0.49
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	5	0.49
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB2	8	0.49
(1,1825)	1:85:A:PHE:H	1:85:A:PHE:HB3	5	0.49
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	10	0.49
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG12	10	0.49
(1,1542)	1:76:A:ALA:HB2	1:75:A:THR:HA	2	0.49
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	3	0.49
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	7	0.49
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	3	0.49
(1,1018)	1:121:A:ILE:HG21	1:120:A:GLU:HG3	8	0.49
(1,606)	1:25:A:GLY:HA3	1:43:A:VAL:HG22	8	0.49
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD13	8	0.49
(1,495)	1:94:A:ALA:HB3	1:134:A:LYS:HA	3	0.49
(1,495)	1:94:A:ALA:HB3	1:134:A:LYS:HA	10	0.49
(1,328)	1:100:A:ALA:HB1	1:101:A:MET:HA	9	0.49
(1,282)	1:146:A:VAL:HG22	1:88:A:HIS:HA	7	0.49
(1,218)	1:89:A:VAL:HG23	1:151:A:SER:HB2	8	0.49
(1,167)	1:150:A:THR:HG21	1:85:A:PHE:HB2	9	0.49
(1,146)	1:9:A:LEU:HD21	1:37:A:ALA:HB2	2	0.49
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG2	1	0.48
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	4	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	3	0.48
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	3	0.48
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	7	0.48
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG2	8	0.48
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD11	2	0.48
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD13	8	0.48
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	8	0.48
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	7	0.48
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	9	0.48
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB2	5	0.48
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG23	4	0.48
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG23	10	0.48
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG23	7	0.48
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	3	0.48
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	6	0.48
(1,3155)	1:70:A:LEU:HD21	1:17:A:LYS:H	2	0.48
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD23	3	0.48
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	7	0.48
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	8	0.48
(1,3094)	1:76:A:ALA:HB1	1:77:A:SER:HB3	2	0.48
(1,3094)	1:76:A:ALA:HB1	1:77:A:SER:HB3	8	0.48
(1,3093)	1:76:A:ALA:HB1	1:80:A:CYS:HA	4	0.48
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	6	0.48
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	7	0.48
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	9	0.48
(1,3022)	1:79:A:SER:HB3	1:159:A:GLU:H	10	0.48
(1,3004)	1:56:A:LYS:H	1:56:A:LYS:HD3	7	0.48
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	2	0.48
(1,2952)	1:101:A:MET:HG3	1:103:A:THR:HA	1	0.48
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD22	8	0.48
(1,2866)	1:159:A:GLU:HG3	1:156:A:PHE:HD1	4	0.48
(1,2848)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	4	0.48
(1,2831)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	4	0.48
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	9	0.48
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	10	0.48
(1,2793)	1:64:A:LYS:HE2	1:117:A:PRO:HD3	9	0.48
(1,2773)	1:6:A:LYS:HE2	1:51:A:TYR:HD1	6	0.48
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD13	6	0.48
(1,2655)	1:97:A:VAL:HG21	1:134:A:LYS:HG3	2	0.48
(1,2641)	1:114:A:ALA:HB1	1:110:A:GLN:HG2	8	0.48
(1,2640)	1:114:A:ALA:HB2	1:110:A:GLN:HA	2	0.48
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG23	7	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	5	0.48
(1,2615)	1:42:A:ALA:HB2	1:43:A:VAL:HB	3	0.48
(1,2615)	1:42:A:ALA:HB1	1:43:A:VAL:HB	7	0.48
(1,2615)	1:42:A:ALA:HB3	1:43:A:VAL:HB	8	0.48
(1,2613)	1:44:A:ASP:HA	1:43:A:VAL:HG21	1	0.48
(1,2602)	1:151:A:SER:H	1:149:A:VAL:HG21	2	0.48
(1,2595)	1:75:A:THR:HG21	1:13:A:HIS:HB2	1	0.48
(1,2590)	1:102:A:VAL:HG13	1:17:A:LYS:HE3	7	0.48
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG21	2	0.48
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG21	4	0.48
(1,2544)	1:154:A:LYS:HA	1:121:A:ILE:HA	4	0.48
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	7	0.48
(1,2511)	1:110:A:GLN:HG2	1:85:A:PHE:HZ	4	0.48
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG21	1	0.48
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG23	9	0.48
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	9	0.48
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB2	6	0.48
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB2	9	0.48
(1,1803)	1:87:A:GLN:H	1:87:A:GLN:HB3	1	0.48
(1,1664)	1:89:A:VAL:HG13	1:123:A:THR:HG21	10	0.48
(1,1640)	1:47:A:THR:HG22	1:156:A:PHE:HE2	1	0.48
(1,1542)	1:76:A:ALA:HB3	1:75:A:THR:HA	10	0.48
(1,1295)	1:87:A:GLN:HE21	1:87:A:GLN:HB2	10	0.48
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	8	0.48
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	5	0.48
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	8	0.48
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD23	9	0.48
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD12	4	0.48
(1,486)	1:24:A:ILE:HG21	1:60:A:VAL:HB	2	0.48
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD23	10	0.48
(1,411)	1:21:A:ALA:HB2	1:48:A:HIS:HD2	5	0.48
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	10	0.48
(1,331)	1:149:A:VAL:HG21	1:146:A:VAL:H	3	0.48
(1,331)	1:149:A:VAL:HG23	1:146:A:VAL:H	10	0.48
(1,328)	1:100:A:ALA:HB3	1:101:A:MET:HA	5	0.48
(1,288)	1:146:A:VAL:HG21	1:143:A:GLU:HG3	9	0.48
(1,282)	1:146:A:VAL:HG22	1:88:A:HIS:HA	3	0.48
(1,282)	1:146:A:VAL:HG22	1:88:A:HIS:HA	10	0.48
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	5	0.48
(1,165)	1:150:A:THR:HG23	1:123:A:THR:HA	10	0.48
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB2	10	0.48
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG2	5	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG2	10	0.47
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	4	0.47
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	9	0.47
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG23	5	0.47
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	10	0.47
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	8	0.47
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	6	0.47
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG23	1	0.47
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG21	3	0.47
(1,3244)	1:126:A:GLU:H	1:149:A:VAL:HG23	8	0.47
(1,3166)	1:131:A:CYS:HA	1:130:A:LYS:HG2	1	0.47
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG22	5	0.47
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD22	9	0.47
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	10	0.47
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG11	9	0.47
(1,3139)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	10	0.47
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	1	0.47
(1,3113)	1:56:A:LYS:HG3	1:56:A:LYS:HE3	3	0.47
(1,3113)	1:56:A:LYS:HG3	1:56:A:LYS:HE2	7	0.47
(1,3113)	1:56:A:LYS:HG3	1:56:A:LYS:HE3	10	0.47
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	2	0.47
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	4	0.47
(1,3094)	1:76:A:ALA:HB2	1:77:A:SER:HB3	9	0.47
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	1	0.47
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	4	0.47
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	5	0.47
(1,3055)	1:144:A:ARG:HG3	1:144:A:ARG:H	10	0.47
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	1	0.47
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	2	0.47
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	7	0.47
(1,2907)	1:110:A:GLN:HG2	1:77:A:SER:HB2	1	0.47
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	9	0.47
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD13	1	0.47
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	9	0.47
(1,2848)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	1	0.47
(1,2848)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	7	0.47
(1,2831)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	10	0.47
(1,2825)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	1	0.47
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	3	0.47
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	6	0.47
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	5	0.47
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	6	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2665)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	10	0.47
(1,2641)	1:114:A:ALA:HB1	1:110:A:GLN:HG2	3	0.47
(1,2637)	1:140:A:ALA:HB1	1:137:A:GLY:HA2	8	0.47
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG23	2	0.47
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG22	1	0.47
(1,2566)	1:103:A:THR:HG23	1:102:A:VAL:HA	4	0.47
(1,2558)	1:149:A:VAL:HG13	1:126:A:GLU:H	2	0.47
(1,2546)	1:150:A:THR:HG23	1:106:A:SER:HB2	4	0.47
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB1	4	0.47
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB3	7	0.47
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG11	7	0.47
(1,2269)	1:141:A:PHE:H	1:142:A:LYS:HB3	5	0.47
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD12	10	0.47
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	5	0.47
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	7	0.47
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	10	0.47
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	2	0.47
(1,2097)	1:127:A:HIS:H	1:125:A:ASN:HD22	1	0.47
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG22	10	0.47
(1,1973)	1:36:A:CYS:H	1:37:A:ALA:HB1	1	0.47
(1,1954)	1:144:A:ARG:H	1:142:A:LYS:HG3	10	0.47
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD23	8	0.47
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD11	2	0.47
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD11	6	0.47
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB1	9	0.47
(1,1542)	1:76:A:ALA:HB1	1:75:A:THR:HA	1	0.47
(1,1542)	1:76:A:ALA:HB3	1:75:A:THR:HA	6	0.47
(1,1542)	1:76:A:ALA:HB2	1:75:A:THR:HA	8	0.47
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	1	0.47
(1,994)	1:61:A:LYS:HE3	1:50:A:THR:HB	4	0.47
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE3	7	0.47
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE2	9	0.47
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD21	4	0.47
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	6	0.47
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	7	0.47
(1,501)	1:94:A:ALA:HB3	1:121:A:ILE:HD11	10	0.47
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	2	0.47
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	8	0.47
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	8	0.47
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG22	1	0.47
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG23	4	0.47
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	9	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	6	0.46
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	7	0.46
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	10	0.46
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	9	0.46
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG22	6	0.46
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG22	8	0.46
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG23	6	0.46
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG21	9	0.46
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	9	0.46
(1,3345)	1:150:A:THR:H	1:126:A:GLU:HB2	1	0.46
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	10	0.46
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	10	0.46
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	3	0.46
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG23	4	0.46
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD22	5	0.46
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	7	0.46
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	5	0.46
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG23	1	0.46
(1,3113)	1:56:A:LYS:HG3	1:56:A:LYS:HE3	9	0.46
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	10	0.46
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG3	4	0.46
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG3	9	0.46
(1,3094)	1:76:A:ALA:HB2	1:77:A:SER:HB3	7	0.46
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	7	0.46
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	9	0.46
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	3	0.46
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	2	0.46
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	5	0.46
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	7	0.46
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	3	0.46
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	3	0.46
(1,2932)	1:146:A:VAL:H	1:143:A:GLU:HB3	1	0.46
(1,2932)	1:146:A:VAL:H	1:144:A:ARG:HB3	4	0.46
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	1	0.46
(1,2907)	1:110:A:GLN:HG2	1:77:A:SER:HB2	3	0.46
(1,2907)	1:110:A:GLN:HG2	1:77:A:SER:HB2	5	0.46
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD22	5	0.46
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD21	6	0.46
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	10	0.46
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	8	0.46
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	9	0.46
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	6	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2831)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	7	0.46
(1,2801)	1:41:A:LYS:H	1:40:A:CYS:HB2	8	0.46
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD3	4	0.46
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD12	7	0.46
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD12	9	0.46
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	4	0.46
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	7	0.46
(1,2615)	1:42:A:ALA:HB3	1:43:A:VAL:HB	4	0.46
(1,2558)	1:149:A:VAL:HG12	1:126:A:GLU:H	7	0.46
(1,2558)	1:149:A:VAL:HG12	1:126:A:GLU:H	10	0.46
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB2	2	0.46
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB3	9	0.46
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG23	5	0.46
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG11	10	0.46
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG21	4	0.46
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD12	6	0.46
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD13	7	0.46
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	3	0.46
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	1	0.46
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	8	0.46
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD23	2	0.46
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB1	4	0.46
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD13	1	0.46
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG12	3	0.46
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG23	2	0.46
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG21	10	0.46
(1,1542)	1:76:A:ALA:HB2	1:75:A:THR:HA	4	0.46
(1,1541)	1:76:A:ALA:HB2	1:51:A:TYR:HE2	4	0.46
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	2	0.46
(1,1324)	1:34:A:GLU:HB3	1:35:A:GLN:H	6	0.46
(1,1275)	1:161:A:GLY:HA2	1:155:A:GLN:HB2	2	0.46
(1,1252)	1:65:A:PRO:HB2	1:67:A:LEU:HD12	4	0.46
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG22	6	0.46
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG22	9	0.46
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	10	0.46
(1,1018)	1:120:A:GLU:HG3	1:121:A:ILE:HG22	2	0.46
(1,1018)	1:121:A:ILE:HG21	1:120:A:GLU:HG3	7	0.46
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	1	0.46
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	2	0.46
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD23	3	0.46
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD22	5	0.46
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	2	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	8	0.46
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD12	9	0.46
(1,522)	1:48:A:HIS:H	1:24:A:ILE:HD11	9	0.46
(1,495)	1:94:A:ALA:HB1	1:134:A:LYS:HA	6	0.46
(1,495)	1:94:A:ALA:HB1	1:134:A:LYS:HA	8	0.46
(1,488)	1:24:A:ILE:HG23	1:62:A:GLU:HG2	1	0.46
(1,386)	1:112:A:ALA:HB1	1:114:A:ALA:H	3	0.46
(1,386)	1:112:A:ALA:HB1	1:114:A:ALA:H	7	0.46
(1,380)	1:112:A:ALA:HB1	1:65:A:PRO:HG3	2	0.46
(1,354)	1:129:A:GLN:HA	1:102:A:VAL:HG13	8	0.46
(1,331)	1:149:A:VAL:HG22	1:146:A:VAL:H	2	0.46
(1,331)	1:149:A:VAL:HG22	1:146:A:VAL:H	5	0.46
(1,331)	1:149:A:VAL:HG22	1:146:A:VAL:H	7	0.46
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	8	0.46
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	3	0.46
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	9	0.46
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	5	0.46
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	6	0.46
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG23	6	0.46
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	6	0.45
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	2	0.45
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	3	0.45
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	7	0.45
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	4	0.45
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	2	0.45
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	4	0.45
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	9	0.45
(1,3493)	1:129:A:GLN:HE21	1:128:A:ASP:HB3	6	0.45
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	6	0.45
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	7	0.45
(1,3418)	1:122:A:PHE:H	1:121:A:ILE:HG22	1	0.45
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	10	0.45
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	5	0.45
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	1	0.45
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB2	6	0.45
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB2	8	0.45
(1,3208)	1:70:A:LEU:H	1:16:A:ASN:HB3	4	0.45
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	10	0.45
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG22	4	0.45
(1,3166)	1:131:A:CYS:HA	1:130:A:LYS:HG2	8	0.45
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	6	0.45
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG21	7	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3120)	1:51:A:TYR:H	1:33:A:LEU:HD22	4	0.45
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	5	0.45
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB1	8	0.45
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	2	0.45
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	6	0.45
(1,3055)	1:18:A:GLY:H	1:17:A:LYS:HD3	1	0.45
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	3	0.45
(1,3022)	1:79:A:SER:HB3	1:156:A:PHE:HD1	2	0.45
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	5	0.45
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	6	0.45
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	7	0.45
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	1	0.45
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	8	0.45
(1,2839)	1:30:A:ASP:HB3	1:29:A:PRO:HG2	4	0.45
(1,2831)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	3	0.45
(1,2831)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	5	0.45
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	1	0.45
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD3	2	0.45
(1,2747)	1:82:A:ARG:HD3	1:85:A:PHE:HB3	10	0.45
(1,2708)	1:116:A:ASP:HB3	1:64:A:LYS:HG2	2	0.45
(1,2665)	1:94:A:ALA:HB3	1:91:A:TYR:HB2	4	0.45
(1,2624)	1:37:A:ALA:HB3	1:36:A:CYS:HB3	4	0.45
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	10	0.45
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG22	3	0.45
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG22	5	0.45
(1,2548)	1:31:A:VAL:HG11	1:30:A:ASP:HA	6	0.45
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB1	1	0.45
(1,2503)	1:85:A:PHE:HE1	1:110:A:GLN:HG2	2	0.45
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG23	3	0.45
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG12	6	0.45
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	3	0.45
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD23	3	0.45
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD21	6	0.45
(1,1842)	1:78:A:ARG:H	1:76:A:ALA:HB1	3	0.45
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD11	5	0.45
(1,1542)	1:76:A:ALA:HB3	1:75:A:THR:HA	7	0.45
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG21	6	0.45
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	3	0.45
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	9	0.45
(1,1018)	1:120:A:GLU:HG3	1:121:A:ILE:HG22	3	0.45
(1,701)	1:67:A:LEU:HB2	1:67:A:LEU:HD21	10	0.45
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	2	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	4	0.45
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	7	0.45
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	6	0.45
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD12	10	0.45
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD22	1	0.45
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD22	9	0.45
(1,380)	1:112:A:ALA:HB2	1:65:A:PRO:HG3	3	0.45
(1,331)	1:149:A:VAL:HG23	1:146:A:VAL:H	4	0.45
(1,331)	1:149:A:VAL:HG23	1:146:A:VAL:H	8	0.45
(1,269)	1:75:A:THR:HG21	1:77:A:SER:H	9	0.45
(1,228)	1:89:A:VAL:HG22	1:142:A:LYS:HA	1	0.45
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	7	0.45
(1,165)	1:150:A:THR:HG22	1:123:A:THR:HA	9	0.45
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	3	0.45
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	6	0.45
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG22	8	0.45
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG23	9	0.45
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG21	10	0.45
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HB3	1	0.44
(1,3502)	1:87:A:GLN:HE21	1:88:A:HIS:HA	8	0.44
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	3	0.44
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	10	0.44
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	9	0.44
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	1	0.44
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	4	0.44
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	7	0.44
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	4	0.44
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB1	2	0.44
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB2	4	0.44
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD23	3	0.44
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG21	5	0.44
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG23	8	0.44
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG21	10	0.44
(1,3129)	1:34:A:GLU:HA	1:9:A:LEU:HB2	8	0.44
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	6	0.44
(1,3068)	1:119:A:CYS:H	1:118:A:SER:HB2	9	0.44
(1,3055)	1:144:A:ARG:HG3	1:144:A:ARG:H	2	0.44
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	10	0.44
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	1	0.44
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	8	0.44
(1,2952)	1:60:A:VAL:HB	1:46:A:CYS:HA	2	0.44
(1,2907)	1:110:A:GLN:HG2	1:77:A:SER:HB2	8	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	6	0.44
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	7	0.44
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD13	1	0.44
(1,2831)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	2	0.44
(1,2831)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	6	0.44
(1,2825)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	3	0.44
(1,2817)	1:56:A:LYS:H	1:54:A:ASP:HB3	2	0.44
(1,2817)	1:36:A:CYS:H	1:58:A:CYS:HB2	4	0.44
(1,2817)	1:56:A:LYS:H	1:54:A:ASP:HB3	5	0.44
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	3	0.44
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD3	3	0.44
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD2	8	0.44
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD2	9	0.44
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD11	10	0.44
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	8	0.44
(1,2665)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	1	0.44
(1,2665)	1:94:A:ALA:HB1	1:91:A:TYR:HB2	7	0.44
(1,2643)	1:31:A:VAL:HG21	1:57:A:MET:HA	9	0.44
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG23	5	0.44
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	1	0.44
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	10	0.44
(1,2615)	1:42:A:ALA:HB2	1:43:A:VAL:HB	5	0.44
(1,2558)	1:149:A:VAL:HG11	1:126:A:GLU:H	1	0.44
(1,2548)	1:31:A:VAL:HG11	1:30:A:ASP:HA	5	0.44
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	8	0.44
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB1	3	0.44
(1,2124)	1:68:A:TYR:H	1:67:A:LEU:HB2	1	0.44
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD13	4	0.44
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	2	0.44
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	4	0.44
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD11	7	0.44
(1,1584)	1:74:A:LYS:HG2	1:14:A:SER:HB2	2	0.44
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	4	0.44
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB1	1	0.44
(1,1185)	1:59:A:HIS:HB3	1:61:A:LYS:HE3	3	0.44
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	2	0.44
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	6	0.44
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	8	0.44
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	3	0.44
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	1	0.44
(1,411)	1:21:A:ALA:HB3	1:48:A:HIS:HD2	10	0.44
(1,386)	1:112:A:ALA:HB3	1:114:A:ALA:H	8	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,282)	1:146:A:VAL:HG23	1:88:A:HIS:HA	2	0.44
(1,235)	1:103:A:THR:HG21	1:124:A:TYR:HD2	1	0.44
(1,228)	1:89:A:VAL:HG23	1:142:A:LYS:HA	10	0.44
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	1	0.44
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD22	9	0.44
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	2	0.44
(1,167)	1:150:A:THR:HG23	1:85:A:PHE:HB2	3	0.44
(1,165)	1:150:A:THR:HG23	1:123:A:THR:HA	5	0.44
(1,146)	1:9:A:LEU:HD22	1:37:A:ALA:HB1	9	0.44
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	7	0.44
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	4	0.44
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	7	0.44
(1,3514)	1:145:A:GLY:H	1:144:A:ARG:HG3	9	0.43
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	2	0.43
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	5	0.43
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	6	0.43
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	8	0.43
(1,3345)	1:150:A:THR:H	1:126:A:GLU:HB2	8	0.43
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	2	0.43
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG11	2	0.43
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG21	9	0.43
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG3	1	0.43
(1,3055)	1:18:A:GLY:H	1:17:A:LYS:HD3	6	0.43
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	6	0.43
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	7	0.43
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	9	0.43
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD22	1	0.43
(1,2867)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	1	0.43
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	3	0.43
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	6	0.43
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD12	7	0.43
(1,2848)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	5	0.43
(1,2801)	1:41:A:LYS:H	1:40:A:CYS:HB2	2	0.43
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	7	0.43
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	2	0.43
(1,2652)	1:78:A:ARG:HA	1:37:A:ALA:HB2	5	0.43
(1,2643)	1:31:A:VAL:HG22	1:57:A:MET:HA	2	0.43
(1,2643)	1:31:A:VAL:HG21	1:57:A:MET:HA	4	0.43
(1,2627)	1:111:A:ALA:HB2	1:156:A:PHE:HD1	3	0.43
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	2	0.43
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	6	0.43
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB1	2	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG21	6	0.43
(1,2561)	1:89:A:VAL:HG22	1:91:A:TYR:HD1	3	0.43
(1,2561)	1:89:A:VAL:HG23	1:91:A:TYR:HD1	6	0.43
(1,2558)	1:149:A:VAL:HG12	1:126:A:GLU:H	3	0.43
(1,2558)	1:149:A:VAL:HG12	1:126:A:GLU:H	4	0.43
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB2	8	0.43
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG22	6	0.43
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG12	9	0.43
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG23	2	0.43
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG23	9	0.43
(1,1947)	1:69:A:ASP:H	1:68:A:TYR:HB3	9	0.43
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	3	0.43
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	10	0.43
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD22	9	0.43
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD21	10	0.43
(1,1637)	1:106:A:SER:HA	1:103:A:THR:HG23	9	0.43
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB2	5	0.43
(1,1541)	1:76:A:ALA:HB2	1:51:A:TYR:HE2	3	0.43
(1,1488)	1:41:A:LYS:H	1:41:A:LYS:HG2	8	0.43
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB1	7	0.43
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	6	0.43
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG21	4	0.43
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG21	7	0.43
(1,1185)	1:59:A:HIS:HB3	1:61:A:LYS:HE3	4	0.43
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	1	0.43
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	4	0.43
(1,1096)	1:154:A:LYS:HB2	1:154:A:LYS:HE2	7	0.43
(1,1018)	1:120:A:GLU:HG3	1:121:A:ILE:HG22	5	0.43
(1,760)	1:64:A:LYS:HE2	1:116:A:ASP:HB2	4	0.43
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	4	0.43
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	10	0.43
(1,411)	1:21:A:ALA:HB2	1:48:A:HIS:HD2	4	0.43
(1,411)	1:21:A:ALA:HB2	1:48:A:HIS:HD2	6	0.43
(1,396)	1:107:A:ALA:HB1	1:77:A:SER:HB2	7	0.43
(1,386)	1:112:A:ALA:HB1	1:114:A:ALA:H	1	0.43
(1,228)	1:89:A:VAL:HG21	1:142:A:LYS:HA	3	0.43
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	4	0.43
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG22	7	0.43
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD23	4	0.43
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	7	0.43
(1,165)	1:150:A:THR:HG21	1:123:A:THR:HA	1	0.43
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	1	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	3	0.43
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	10	0.43
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG22	3	0.43
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG21	7	0.43
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	6	0.42
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	4	0.42
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	7	0.42
(1,3377)	1:89:A:VAL:H	1:89:A:VAL:HG23	8	0.42
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	9	0.42
(1,3263)	1:96:A:ASP:H	1:95:A:PRO:HD2	10	0.42
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB1	1	0.42
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB1	7	0.42
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB1	9	0.42
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB3	10	0.42
(1,3236)	1:78:A:ARG:H	1:108:A:ASP:HA	1	0.42
(1,3201)	1:52:A:ASN:H	1:58:A:CYS:HB2	4	0.42
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	2	0.42
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG21	2	0.42
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG22	6	0.42
(1,3124)	1:125:A:ASN:H	1:123:A:THR:HG22	8	0.42
(1,3112)	1:6:A:LYS:HG2	1:6:A:LYS:HA	6	0.42
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	2	0.42
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	3	0.42
(1,3097)	1:67:A:LEU:HD13	1:102:A:VAL:H	5	0.42
(1,3094)	1:76:A:ALA:HB3	1:77:A:SER:HB3	1	0.42
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	5	0.42
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD23	2	0.42
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	5	0.42
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	9	0.42
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	10	0.42
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	6	0.42
(1,2831)	1:28:A:VAL:HG21	1:58:A:CYS:HB2	1	0.42
(1,2831)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	8	0.42
(1,2817)	1:56:A:LYS:H	1:54:A:ASP:HB3	1	0.42
(1,2793)	1:40:A:CYS:HB2	1:78:A:ARG:HA	3	0.42
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	9	0.42
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	7	0.42
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	9	0.42
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	4	0.42
(1,2746)	1:82:A:ARG:HD2	1:82:A:ARG:HB2	4	0.42
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	4	0.42
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	5	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	6	0.42
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	7	0.42
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB3	4	0.42
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB3	6	0.42
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB3	10	0.42
(1,2627)	1:111:A:ALA:HB2	1:156:A:PHE:HD1	8	0.42
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	6	0.42
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG22	10	0.42
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	2	0.42
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	3	0.42
(1,2548)	1:31:A:VAL:HG13	1:30:A:ASP:HA	4	0.42
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	9	0.42
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG12	4	0.42
(1,2326)	1:110:A:GLN:HE22	1:85:A:PHE:HE1	10	0.42
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG23	7	0.42
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG23	8	0.42
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD12	5	0.42
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	7	0.42
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG22	2	0.42
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD13	5	0.42
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	1	0.42
(1,1584)	1:74:A:LYS:HG2	1:14:A:SER:HB2	4	0.42
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG21	2	0.42
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG22	3	0.42
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG21	5	0.42
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	7	0.42
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	7	0.42
(1,692)	1:97:A:VAL:HG21	1:133:A:PHE:HB2	4	0.42
(1,499)	1:94:A:ALA:HB3	1:138:A:PHE:HB2	5	0.42
(1,499)	1:94:A:ALA:HB2	1:138:A:PHE:HB2	8	0.42
(1,488)	1:24:A:ILE:HG22	1:62:A:GLU:HG2	2	0.42
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD23	5	0.42
(1,411)	1:21:A:ALA:HB2	1:48:A:HIS:HD2	8	0.42
(1,380)	1:112:A:ALA:HB2	1:65:A:PRO:HG3	7	0.42
(1,380)	1:112:A:ALA:HB2	1:65:A:PRO:HG3	10	0.42
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	9	0.42
(1,331)	1:149:A:VAL:HG22	1:146:A:VAL:H	6	0.42
(1,288)	1:146:A:VAL:HG23	1:143:A:GLU:HG3	8	0.42
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	8	0.42
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	1	0.42
(1,165)	1:150:A:THR:HG22	1:123:A:THR:HA	4	0.42
(1,165)	1:150:A:THR:HG22	1:123:A:THR:HA	6	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	10	0.42
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	9	0.42
(1,21)	1:156:A:PHE:HD2	1:114:A:ALA:HB3	10	0.42
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG23	2	0.42
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	4	0.41
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG3	4	0.41
(1,3444)	1:40:A:CYS:H	1:41:A:LYS:HA	1	0.41
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	1	0.41
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	5	0.41
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	10	0.41
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	1	0.41
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	3	0.41
(1,3265)	1:12:A:VAL:H	1:105:A:GLN:HG2	10	0.41
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	5	0.41
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD23	8	0.41
(1,3146)	1:156:A:PHE:HA	1:159:A:GLU:HG2	4	0.41
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG22	3	0.41
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG21	2	0.41
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG23	9	0.41
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	7	0.41
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	8	0.41
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB2	6	0.41
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	2	0.41
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	4	0.41
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD12	3	0.41
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	2	0.41
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	8	0.41
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	8	0.41
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	4	0.41
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	5	0.41
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	1	0.41
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	9	0.41
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	10	0.41
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD23	3	0.41
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD23	10	0.41
(1,2867)	1:92:A:GLU:HG2	1:92:A:GLU:HB3	4	0.41
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	2	0.41
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD12	8	0.41
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD12	10	0.41
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	3	0.41
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	4	0.41
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	6	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2834)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	7	0.41
(1,2817)	1:56:A:LYS:H	1:54:A:ASP:HB3	7	0.41
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	2	0.41
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	9	0.41
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	2	0.41
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	7	0.41
(1,2719)	1:25:A:GLY:HA2	1:26:A:GLU:HB3	8	0.41
(1,2716)	1:160:A:GLY:HA2	1:156:A:PHE:HD2	3	0.41
(1,2714)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	4	0.41
(1,2710)	1:161:A:GLY:HA2	1:155:A:GLN:HG3	9	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB1	1	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB3	3	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB1	5	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB3	7	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB2	8	0.41
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB2	9	0.41
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG23	4	0.41
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG21	8	0.41
(1,2558)	1:149:A:VAL:HG11	1:126:A:GLU:H	9	0.41
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB3	3	0.41
(1,2436)	1:152:A:GLY:H	1:121:A:ILE:HG23	9	0.41
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD11	2	0.41
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG12	3	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG21	1	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG21	3	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG22	4	0.41
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG23	10	0.41
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG12	3	0.41
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD21	4	0.41
(1,1891)	1:8:A:ASP:H	1:7:A:LEU:HD23	7	0.41
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD13	10	0.41
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG11	6	0.41
(1,1640)	1:47:A:THR:HG21	1:156:A:PHE:HE2	2	0.41
(1,1640)	1:47:A:THR:HG21	1:156:A:PHE:HE2	7	0.41
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB1	9	0.41
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	3	0.41
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG22	2	0.41
(1,1141)	1:6:A:LYS:H	1:6:A:LYS:HB2	1	0.41
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB3	8	0.41
(1,1000)	1:112:A:ALA:HB1	1:109:A:CYS:HB2	1	0.41
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	6	0.41
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	6	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	6	0.41
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD13	7	0.41
(1,499)	1:94:A:ALA:HB1	1:138:A:PHE:HB2	4	0.41
(1,495)	1:94:A:ALA:HB1	1:134:A:LYS:HA	2	0.41
(1,494)	1:94:A:ALA:HB2	1:141:A:PHE:HD2	6	0.41
(1,488)	1:24:A:ILE:HG23	1:62:A:GLU:HG2	9	0.41
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD21	2	0.41
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG23	9	0.41
(1,456)	1:38:A:ALA:HB1	1:35:A:GLN:HG3	4	0.41
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG22	9	0.41
(1,282)	1:146:A:VAL:HG23	1:88:A:HIS:HA	9	0.41
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD22	9	0.41
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	6	0.41
(1,165)	1:150:A:THR:HG21	1:123:A:THR:HA	3	0.41
(1,123)	1:127:A:HIS:HD2	1:127:A:HIS:HB3	2	0.41
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	5	0.4
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	5	0.4
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	5	0.4
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG3	9	0.4
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG3	2	0.4
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD13	1	0.4
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	9	0.4
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	4	0.4
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	2	0.4
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG12	3	0.4
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG11	10	0.4
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG22	1	0.4
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG23	10	0.4
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG23	3	0.4
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG22	6	0.4
(1,3127)	1:132:A:THR:HG21	1:92:A:GLU:HG2	5	0.4
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	10	0.4
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG2	7	0.4
(1,3097)	1:67:A:LEU:HD11	1:102:A:VAL:H	4	0.4
(1,3074)	1:78:A:ARG:HA	1:78:A:ARG:HG2	10	0.4
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	9	0.4
(1,2983)	1:61:A:LYS:HD3	1:21:A:ALA:HA	10	0.4
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	2	0.4
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	4	0.4
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	5	0.4
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	8	0.4
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	1	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2801)	1:64:A:LYS:HE2	1:116:A:ASP:H	3	0.4
(1,2793)	1:64:A:LYS:HE2	1:117:A:PRO:HD3	5	0.4
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	4	0.4
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD11	8	0.4
(1,2719)	1:25:A:GLY:HA2	1:26:A:GLU:HB3	2	0.4
(1,2716)	1:160:A:GLY:HA2	1:156:A:PHE:HD2	4	0.4
(1,2714)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	6	0.4
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	3	0.4
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	4	0.4
(1,2665)	1:94:A:ALA:HB2	1:91:A:TYR:HB2	5	0.4
(1,2651)	1:38:A:ALA:HA	1:38:A:ALA:HB1	2	0.4
(1,2626)	1:30:A:ASP:HA	1:30:A:ASP:HB3	2	0.4
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG21	3	0.4
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG21	6	0.4
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG21	10	0.4
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	4	0.4
(1,2615)	1:42:A:ALA:HB2	1:43:A:VAL:HB	2	0.4
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	3	0.4
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	8	0.4
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG21	2	0.4
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG22	7	0.4
(1,2561)	1:89:A:VAL:HG23	1:91:A:TYR:HD1	4	0.4
(1,2548)	1:31:A:VAL:HG13	1:30:A:ASP:HA	10	0.4
(1,2503)	1:85:A:PHE:HE1	1:110:A:GLN:HG2	4	0.4
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD13	4	0.4
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB2	1	0.4
(1,2379)	1:35:A:GLN:HE22	1:31:A:VAL:HG13	3	0.4
(1,2318)	1:118:A:SER:H	1:97:A:VAL:HG23	10	0.4
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	2	0.4
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG23	3	0.4
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG23	8	0.4
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG21	10	0.4
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	5	0.4
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG12	7	0.4
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD13	10	0.4
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	7	0.4
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD13	8	0.4
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD12	9	0.4
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG11	8	0.4
(1,1542)	1:76:A:ALA:HB2	1:75:A:THR:HA	3	0.4
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	4	0.4
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG21	4	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG22	8	0.4
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	1	0.4
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	2	0.4
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	3	0.4
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	8	0.4
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	5	0.4
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	5	0.4
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	1	0.4
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	2	0.4
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	10	0.4
(1,488)	1:24:A:ILE:HG23	1:62:A:GLU:HG2	6	0.4
(1,396)	1:107:A:ALA:HB3	1:77:A:SER:HB2	8	0.4
(1,386)	1:112:A:ALA:HB1	1:114:A:ALA:H	5	0.4
(1,386)	1:112:A:ALA:HB1	1:114:A:ALA:H	10	0.4
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG22	4	0.4
(1,304)	1:75:A:THR:H	1:75:A:THR:HG23	2	0.4
(1,304)	1:75:A:THR:H	1:75:A:THR:HG22	7	0.4
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG13	5	0.4
(1,188)	1:67:A:LEU:HD22	1:75:A:THR:HG22	3	0.4
(1,165)	1:150:A:THR:HG21	1:123:A:THR:HA	8	0.4
(1,3503)	1:87:A:GLN:HE22	1:150:A:THR:HG21	4	0.39
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	7	0.39
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	4	0.39
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	6	0.39
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	9	0.39
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	5	0.39
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	6	0.39
(1,3279)	1:103:A:THR:H	1:130:A:LYS:HB3	4	0.39
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG22	1	0.39
(1,3166)	1:131:A:CYS:HA	1:130:A:LYS:HG2	7	0.39
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD23	8	0.39
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG21	5	0.39
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG22	8	0.39
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG22	9	0.39
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	3	0.39
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	2	0.39
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB2	10	0.39
(1,3048)	1:134:A:LYS:HG3	1:134:A:LYS:HA	10	0.39
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	1	0.39
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	2	0.39
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD13	4	0.39
(1,2992)	1:16:A:ASN:H	1:13:A:HIS:HB3	6	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2992)	1:16:A:ASN:H	1:13:A:HIS:HB3	8	0.39
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	6	0.39
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	3	0.39
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	2	0.39
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	1	0.39
(1,2907)	1:110:A:GLN:HG2	1:77:A:SER:HB2	7	0.39
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	5	0.39
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	3	0.39
(1,2834)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	2	0.39
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	4	0.39
(1,2825)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	4	0.39
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	4	0.39
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	10	0.39
(1,2754)	1:136:A:ARG:HD3	1:120:A:GLU:HG3	4	0.39
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD11	1	0.39
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	8	0.39
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	10	0.39
(1,2643)	1:31:A:VAL:HG22	1:57:A:MET:HA	10	0.39
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB3	9	0.39
(1,2561)	1:89:A:VAL:HG21	1:91:A:TYR:HD1	9	0.39
(1,2548)	1:31:A:VAL:HG12	1:30:A:ASP:HA	7	0.39
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	10	0.39
(1,2379)	1:35:A:GLN:HE22	1:31:A:VAL:HG12	6	0.39
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	4	0.39
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	10	0.39
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG22	6	0.39
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG11	1	0.39
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG12	5	0.39
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG11	6	0.39
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD12	9	0.39
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	4	0.39
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	5	0.39
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB3	9	0.39
(1,1759)	1:9:A:LEU:H	1:9:A:LEU:HD11	3	0.39
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG13	4	0.39
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG23	3	0.39
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG23	7	0.39
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG22	10	0.39
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	6	0.39
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	7	0.39
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	9	0.39
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	10	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1018)	1:120:A:GLU:HG3	1:121:A:ILE:HG22	4	0.39
(1,1000)	1:112:A:ALA:HB1	1:109:A:CYS:HB2	10	0.39
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	8	0.39
(1,761)	1:64:A:LYS:HE2	1:115:A:ALA:HB1	2	0.39
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD11	1	0.39
(1,488)	1:24:A:ILE:HG22	1:62:A:GLU:HG2	5	0.39
(1,488)	1:24:A:ILE:HG22	1:62:A:GLU:HG2	8	0.39
(1,386)	1:112:A:ALA:HB2	1:114:A:ALA:H	6	0.39
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG13	3	0.39
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD22	3	0.39
(1,167)	1:150:A:THR:HG21	1:85:A:PHE:HB2	2	0.39
(1,167)	1:150:A:THR:HG21	1:85:A:PHE:HB2	6	0.39
(1,11)	1:124:A:TYR:HD1	1:150:A:THR:HG21	5	0.39
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	4	0.38
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	9	0.38
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG3	1	0.38
(1,3366)	1:35:A:GLN:H	1:9:A:LEU:HD11	7	0.38
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	6	0.38
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	6	0.38
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	7	0.38
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	6	0.38
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	9	0.38
(1,3105)	1:130:A:LYS:H	1:130:A:LYS:HG3	10	0.38
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB3	5	0.38
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	4	0.38
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD13	9	0.38
(1,2992)	1:16:A:ASN:H	1:13:A:HIS:HB3	7	0.38
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	3	0.38
(1,2967)	1:159:A:GLU:HB3	1:156:A:PHE:HD2	2	0.38
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	4	0.38
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	5	0.38
(1,2896)	1:36:A:CYS:HB3	1:33:A:LEU:HD21	7	0.38
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	10	0.38
(1,2867)	1:92:A:GLU:HG3	1:92:A:GLU:HB2	2	0.38
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	7	0.38
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD11	5	0.38
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	8	0.38
(1,2847)	1:91:A:TYR:HB2	1:151:A:SER:HB2	4	0.38
(1,2834)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	6	0.38
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	5	0.38
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	7	0.38
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	8	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2786)	1:6:A:LYS:HE2	1:6:A:LYS:HG3	6	0.38
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	4	0.38
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	5	0.38
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	5	0.38
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	1	0.38
(1,2745)	1:82:A:ARG:HD2	1:85:A:PHE:HE2	4	0.38
(1,2719)	1:25:A:GLY:HA2	1:26:A:GLU:HB3	4	0.38
(1,2714)	1:149:A:VAL:HG12	1:148:A:GLY:HA2	2	0.38
(1,2653)	1:97:A:VAL:HG22	1:121:A:ILE:H	10	0.38
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB3	9	0.38
(1,2619)	1:38:A:ALA:H	1:36:A:CYS:HA	3	0.38
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB1	7	0.38
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	6	0.38
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG23	4	0.38
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD11	5	0.38
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG12	1	0.38
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG11	5	0.38
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG23	1	0.38
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG13	2	0.38
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD23	3	0.38
(1,1673)	1:147:A:LEU:HD22	1:147:A:LEU:HD12	1	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD11	2	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD12	3	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD11	7	0.38
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD11	9	0.38
(1,1640)	1:47:A:THR:HG23	1:156:A:PHE:HE2	4	0.38
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB1	2	0.38
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	1	0.38
(1,1210)	1:27:A:PRO:HB3	1:28:A:VAL:HG21	1	0.38
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	4	0.38
(1,1182)	1:59:A:HIS:H	1:59:A:HIS:HB3	5	0.38
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	1	0.38
(1,1000)	1:112:A:ALA:HB3	1:109:A:CYS:HB2	8	0.38
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	4	0.38
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	6	0.38
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD23	3	0.38
(1,728)	1:17:A:LYS:HE2	1:17:A:LYS:HD2	6	0.38
(1,728)	1:17:A:LYS:HE2	1:17:A:LYS:HD2	7	0.38
(1,728)	1:17:A:LYS:HE2	1:17:A:LYS:HD2	10	0.38
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	1	0.38
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG21	9	0.38
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	1	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:24:A:ILE:HG23	1:62:A:GLU:HG2	3	0.38
(1,488)	1:24:A:ILE:HG21	1:62:A:GLU:HG2	4	0.38
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD21	6	0.38
(1,456)	1:38:A:ALA:HB3	1:35:A:GLN:HG3	1	0.38
(1,411)	1:21:A:ALA:HB1	1:48:A:HIS:HD2	3	0.38
(1,411)	1:21:A:ALA:HB1	1:48:A:HIS:HD2	9	0.38
(1,380)	1:112:A:ALA:HB1	1:65:A:PRO:HG3	8	0.38
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG21	1	0.38
(1,304)	1:75:A:THR:H	1:75:A:THR:HG23	6	0.38
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	1	0.38
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	8	0.38
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	5	0.38
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	9	0.38
(1,184)	1:67:A:LEU:HD21	1:19:A:SER:HB3	1	0.38
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	5	0.38
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB1	5	0.38
(1,89)	1:51:A:TYR:HD1	1:51:A:TYR:HA	4	0.38
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	5	0.38
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	8	0.38
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	5	0.37
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	2	0.37
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	5	0.37
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	2	0.37
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	6	0.37
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD11	9	0.37
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	3	0.37
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	1	0.37
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	9	0.37
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	10	0.37
(1,3245)	1:21:A:ALA:H	1:21:A:ALA:HB1	3	0.37
(1,3220)	1:13:A:HIS:H	1:12:A:VAL:H	4	0.37
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	4	0.37
(1,3143)	1:51:A:TYR:H	1:50:A:THR:HG21	7	0.37
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	10	0.37
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	8	0.37
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	7	0.37
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	10	0.37
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	8	0.37
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	3	0.37
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	7	0.37
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	10	0.37
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	10	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	7	0.37
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	2	0.37
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	9	0.37
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD11	3	0.37
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD13	5	0.37
(1,2719)	1:25:A:GLY:HA2	1:26:A:GLU:HB3	1	0.37
(1,2714)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	7	0.37
(1,2714)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	9	0.37
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	1	0.37
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	2	0.37
(1,2663)	1:92:A:GLU:HA	1:94:A:ALA:HB1	2	0.37
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	5	0.37
(1,2656)	1:156:A:PHE:H	1:155:A:GLN:HA	2	0.37
(1,2656)	1:156:A:PHE:H	1:155:A:GLN:HA	7	0.37
(1,2643)	1:31:A:VAL:HG21	1:57:A:MET:HA	7	0.37
(1,2637)	1:140:A:ALA:HB1	1:137:A:GLY:HA2	1	0.37
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG23	1	0.37
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB3	8	0.37
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG21	6	0.37
(1,2558)	1:149:A:VAL:HG12	1:126:A:GLU:H	5	0.37
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	3	0.37
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD13	7	0.37
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD13	9	0.37
(1,2390)	1:145:A:GLY:H	1:89:A:VAL:HG13	8	0.37
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG12	4	0.37
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD13	8	0.37
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	5	0.37
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG13	9	0.37
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG11	10	0.37
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	5	0.37
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB3	5	0.37
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	1	0.37
(1,1673)	1:147:A:LEU:HD22	1:147:A:LEU:HD13	4	0.37
(1,1673)	1:147:A:LEU:HD23	1:147:A:LEU:HD13	5	0.37
(1,1673)	1:147:A:LEU:HD22	1:147:A:LEU:HD13	6	0.37
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB2	6	0.37
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG21	6	0.37
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	1	0.37
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	9	0.37
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	7	0.37
(1,1000)	1:112:A:ALA:HB1	1:109:A:CYS:HB2	5	0.37
(1,908)	1:130:A:LYS:HB3	1:129:A:GLN:H	7	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	9	0.37
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB3	8	0.37
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	2	0.37
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	5	0.37
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD21	4	0.37
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	2	0.37
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	8	0.37
(1,692)	1:97:A:VAL:HG22	1:133:A:PHE:HB2	5	0.37
(1,501)	1:94:A:ALA:HB2	1:121:A:ILE:HD12	1	0.37
(1,499)	1:94:A:ALA:HB1	1:138:A:PHE:HB2	3	0.37
(1,499)	1:94:A:ALA:HB2	1:138:A:PHE:HB2	7	0.37
(1,488)	1:24:A:ILE:HG22	1:62:A:GLU:HG2	7	0.37
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB2	4	0.37
(1,415)	1:21:A:ALA:HB3	1:66:A:ASP:HB2	5	0.37
(1,386)	1:112:A:ALA:HB2	1:114:A:ALA:H	9	0.37
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG21	8	0.37
(1,282)	1:146:A:VAL:HG23	1:88:A:HIS:HA	5	0.37
(1,235)	1:103:A:THR:HG23	1:124:A:TYR:HD2	2	0.37
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	6	0.37
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	7	0.37
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	6	0.37
(1,195)	1:126:A:GLU:HA	1:126:A:GLU:HG3	10	0.37
(1,184)	1:67:A:LEU:HD21	1:19:A:SER:HB3	5	0.37
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD23	10	0.37
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD23	10	0.37
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	2	0.37
(1,176)	1:31:A:VAL:HG13	1:58:A:CYS:HB2	5	0.37
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	9	0.37
(1,165)	1:150:A:THR:HG23	1:123:A:THR:HA	7	0.37
(1,146)	1:9:A:LEU:HD22	1:37:A:ALA:HB2	1	0.37
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	8	0.36
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	8	0.36
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	10	0.36
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	1	0.36
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	3	0.36
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	8	0.36
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	10	0.36
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	6	0.36
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	1	0.36
(1,3301)	1:37:A:ALA:H	1:34:A:GLU:HB2	4	0.36
(1,3220)	1:13:A:HIS:H	1:12:A:VAL:H	1	0.36
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	4	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3137)	1:12:A:VAL:HG13	1:11:A:CYS:H	9	0.36
(1,3097)	1:67:A:LEU:HD11	1:102:A:VAL:H	8	0.36
(1,3091)	1:83:A:SER:HB2	1:157:A:CYS:HB2	4	0.36
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB3	1	0.36
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB1	4	0.36
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	5	0.36
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	7	0.36
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	4	0.36
(1,3022)	1:79:A:SER:HB3	1:159:A:GLU:H	5	0.36
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	9	0.36
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	1	0.36
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	10	0.36
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	6	0.36
(1,2908)	1:142:A:LYS:HB2	1:139:A:SER:HB3	6	0.36
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	8	0.36
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	2	0.36
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	3	0.36
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	8	0.36
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	10	0.36
(1,2801)	1:64:A:LYS:HE2	1:116:A:ASP:H	5	0.36
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	3	0.36
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	5	0.36
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	1	0.36
(1,2702)	1:117:A:PRO:HD3	1:116:A:ASP:HB3	9	0.36
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	6	0.36
(1,2618)	1:6:A:LYS:HA	1:6:A:LYS:HD2	6	0.36
(1,2561)	1:89:A:VAL:HG23	1:91:A:TYR:HD1	1	0.36
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD12	1	0.36
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD12	3	0.36
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD11	6	0.36
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD12	8	0.36
(1,2422)	1:73:A:GLY:H	1:70:A:LEU:HD12	10	0.36
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	6	0.36
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG22	5	0.36
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG23	6	0.36
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG22	7	0.36
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB3	3	0.36
(1,2211)	1:17:A:LYS:H	1:73:A:GLY:HA2	3	0.36
(1,2201)	1:48:A:HIS:H	1:47:A:THR:HG22	5	0.36
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD11	3	0.36
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB1	10	0.36
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD21	6	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD12	7	0.36
(1,1673)	1:147:A:LEU:HD22	1:147:A:LEU:HD13	8	0.36
(1,1673)	1:147:A:LEU:HD21	1:147:A:LEU:HD13	10	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG12	1	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG11	2	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG11	5	0.36
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG11	7	0.36
(1,1605)	1:33:A:LEU:HD23	1:74:A:LYS:HB3	8	0.36
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	8	0.36
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG21	5	0.36
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	6	0.36
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	8	0.36
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	5	0.36
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	2	0.36
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	4	0.36
(1,1061)	1:35:A:GLN:HE22	1:35:A:GLN:HG3	9	0.36
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	7	0.36
(1,1000)	1:112:A:ALA:HB2	1:109:A:CYS:HB2	9	0.36
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	2	0.36
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	3	0.36
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	5	0.36
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	1	0.36
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	5	0.36
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	7	0.36
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	10	0.36
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB1	3	0.36
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	8	0.36
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	5	0.36
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	4	0.36
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	6	0.36
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	4	0.36
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	8	0.36
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	7	0.36
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD12	2	0.36
(1,499)	1:94:A:ALA:HB3	1:138:A:PHE:HB2	1	0.36
(1,499)	1:94:A:ALA:HB2	1:138:A:PHE:HB2	6	0.36
(1,456)	1:38:A:ALA:HB2	1:35:A:GLN:HG3	3	0.36
(1,415)	1:21:A:ALA:HB3	1:66:A:ASP:HB2	4	0.36
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG21	10	0.36
(1,288)	1:146:A:VAL:HG22	1:143:A:GLU:HG3	1	0.36
(1,282)	1:146:A:VAL:HG21	1:88:A:HIS:HA	1	0.36
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	4	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:67:A:LEU:HD21	1:19:A:SER:HB3	6	0.36
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD22	3	0.36
(1,167)	1:150:A:THR:HG22	1:85:A:PHE:HB2	7	0.36
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	1	0.36
(1,3486)	1:155:A:GLN:HE22	1:155:A:GLN:HG2	10	0.35
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	10	0.35
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG2	7	0.35
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG3	9	0.35
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	8	0.35
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	8	0.35
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	4	0.35
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	8	0.35
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG13	7	0.35
(1,3202)	1:100:A:ALA:H	1:96:A:ASP:HB3	9	0.35
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	8	0.35
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	9	0.35
(1,3157)	1:12:A:VAL:HB	1:9:A:LEU:HD23	4	0.35
(1,3137)	1:12:A:VAL:HG11	1:11:A:CYS:H	7	0.35
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	3	0.35
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	9	0.35
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB2	7	0.35
(1,3032)	1:27:A:PRO:HG2	1:28:A:VAL:H	8	0.35
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	2	0.35
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD12	5	0.35
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	9	0.35
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	10	0.35
(1,2958)	1:86:A:GLU:HB2	1:152:A:GLY:H	1	0.35
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	9	0.35
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	6	0.35
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	1	0.35
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	8	0.35
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	2	0.35
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD12	7	0.35
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	6	0.35
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	5	0.35
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	9	0.35
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	6	0.35
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	8	0.35
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	3	0.35
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	8	0.35
(1,2760)	1:18:A:GLY:HA2	1:19:A:SER:HA	9	0.35
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB3	9	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2656)	1:156:A:PHE:H	1:155:A:GLN:HA	5	0.35
(1,2641)	1:114:A:ALA:HB2	1:110:A:GLN:HG2	10	0.35
(1,2621)	1:36:A:CYS:HA	1:28:A:VAL:HG21	9	0.35
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	1	0.35
(1,2566)	1:103:A:THR:HG23	1:102:A:VAL:HA	7	0.35
(1,2561)	1:89:A:VAL:HG23	1:91:A:TYR:HD1	5	0.35
(1,2558)	1:149:A:VAL:HG11	1:126:A:GLU:H	6	0.35
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB2	8	0.35
(1,2278)	1:50:A:THR:H	1:50:A:THR:HG22	2	0.35
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	7	0.35
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD13	4	0.35
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB3	1	0.35
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB1	4	0.35
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD21	10	0.35
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG13	10	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	1	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	3	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	4	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	6	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	7	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	8	0.35
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	10	0.35
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	10	0.35
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	2	0.35
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	7	0.35
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG21	1	0.35
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	2	0.35
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	3	0.35
(1,1133)	1:39:A:GLN:HE21	1:39:A:GLN:HG2	2	0.35
(1,1133)	1:39:A:GLN:HE21	1:39:A:GLN:HG2	9	0.35
(1,1075)	1:31:A:VAL:HG23	1:36:A:CYS:HB3	4	0.35
(1,1000)	1:112:A:ALA:HB2	1:109:A:CYS:HB2	6	0.35
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	3	0.35
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	2	0.35
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	3	0.35
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	6	0.35
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE3	10	0.35
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB3	2	0.35
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	9	0.35
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	3	0.35
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	5	0.35
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	9	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	10	0.35
(1,692)	1:97:A:VAL:HG21	1:133:A:PHE:HB2	2	0.35
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	3	0.35
(1,581)	1:148:A:GLY:HA2	1:125:A:ASN:HA	10	0.35
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	9	0.35
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD11	5	0.35
(1,499)	1:94:A:ALA:HB2	1:138:A:PHE:HB2	2	0.35
(1,499)	1:94:A:ALA:HB1	1:138:A:PHE:HB2	10	0.35
(1,456)	1:38:A:ALA:HB1	1:35:A:GLN:HG3	9	0.35
(1,396)	1:107:A:ALA:HB1	1:77:A:SER:HB2	2	0.35
(1,396)	1:107:A:ALA:HB1	1:77:A:SER:HB2	3	0.35
(1,386)	1:112:A:ALA:HB2	1:114:A:ALA:H	4	0.35
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG21	6	0.35
(1,282)	1:146:A:VAL:HG21	1:88:A:HIS:HA	6	0.35
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	10	0.35
(1,184)	1:67:A:LEU:HD21	1:19:A:SER:HB3	7	0.35
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	7	0.35
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	8	0.35
(1,146)	1:9:A:LEU:HD21	1:37:A:ALA:HB1	6	0.35
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	9	0.34
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	1	0.34
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	7	0.34
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	8	0.34
(1,3520)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	7	0.34
(1,3496)	1:135:A:GLY:H	1:95:A:PRO:HB3	6	0.34
(1,3486)	1:155:A:GLN:HE22	1:155:A:GLN:HG2	7	0.34
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	8	0.34
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	7	0.34
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	3	0.34
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD12	4	0.34
(1,3366)	1:35:A:GLN:H	1:7:A:LEU:HD12	6	0.34
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	4	0.34
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	4	0.34
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	8	0.34
(1,3345)	1:150:A:THR:H	1:87:A:GLN:HG2	7	0.34
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	4	0.34
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB2	5	0.34
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	10	0.34
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG23	9	0.34
(1,3164)	1:75:A:THR:HG22	1:19:A:SER:HA	3	0.34
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	1	0.34
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	8	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3137)	1:12:A:VAL:HG11	1:11:A:CYS:H	2	0.34
(1,3137)	1:12:A:VAL:HG12	1:11:A:CYS:H	6	0.34
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	5	0.34
(1,3094)	1:76:A:ALA:HB3	1:77:A:SER:HB3	5	0.34
(1,3055)	1:18:A:GLY:H	1:17:A:LYS:HD3	3	0.34
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	6	0.34
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	7	0.34
(1,3004)	1:56:A:LYS:H	1:6:A:LYS:HD2	6	0.34
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	10	0.34
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	9	0.34
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	3	0.34
(1,2834)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	5	0.34
(1,2834)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	8	0.34
(1,2834)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	9	0.34
(1,2834)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	10	0.34
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	7	0.34
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	1	0.34
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	3	0.34
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	6	0.34
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	2	0.34
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	6	0.34
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	4	0.34
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	6	0.34
(1,2714)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	5	0.34
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	3	0.34
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	7	0.34
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	8	0.34
(1,2656)	1:156:A:PHE:H	1:155:A:GLN:HA	4	0.34
(1,2643)	1:31:A:VAL:HG21	1:57:A:MET:HA	3	0.34
(1,2639)	1:114:A:ALA:HB3	1:156:A:PHE:HE2	1	0.34
(1,2590)	1:102:A:VAL:HG12	1:17:A:LYS:HE2	5	0.34
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	5	0.34
(1,2510)	1:114:A:ALA:HB2	1:156:A:PHE:HE2	9	0.34
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	1	0.34
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	5	0.34
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	3	0.34
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	5	0.34
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG11	9	0.34
(1,2059)	1:150:A:THR:H	1:149:A:VAL:HG12	10	0.34
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD12	4	0.34
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	1	0.34
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	7	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	1:33:A:LEU:HD22	1:74:A:LYS:HB3	7	0.34
(1,1584)	1:74:A:LYS:HG2	1:14:A:SER:HB2	5	0.34
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	2	0.34
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	5	0.34
(1,1308)	1:87:A:GLN:HG2	1:87:A:GLN:HB2	9	0.34
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG22	10	0.34
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	5	0.34
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	6	0.34
(1,1000)	1:112:A:ALA:HB3	1:109:A:CYS:HB2	2	0.34
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	8	0.34
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE3	1	0.34
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	3	0.34
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	4	0.34
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	1	0.34
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	2	0.34
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	7	0.34
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	1	0.34
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD13	1	0.34
(1,488)	1:24:A:ILE:HG21	1:62:A:GLU:HG2	10	0.34
(1,356)	1:115:A:ALA:HB2	1:116:A:ASP:HA	3	0.34
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG22	3	0.34
(1,304)	1:75:A:THR:H	1:75:A:THR:HG21	1	0.34
(1,290)	1:102:A:VAL:HG23	1:131:A:CYS:H	3	0.34
(1,228)	1:89:A:VAL:HG22	1:142:A:LYS:HA	6	0.34
(1,228)	1:89:A:VAL:HG21	1:142:A:LYS:HA	7	0.34
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD23	4	0.34
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	3	0.34
(1,176)	1:31:A:VAL:HG12	1:58:A:CYS:HB2	4	0.34
(1,176)	1:31:A:VAL:HG13	1:58:A:CYS:HB2	6	0.34
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	8	0.34
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	2	0.34
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	8	0.34
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	4	0.33
(1,3493)	1:129:A:GLN:HE21	1:128:A:ASP:HB3	3	0.33
(1,3486)	1:155:A:GLN:HE22	1:155:A:GLN:HG3	8	0.33
(1,3478)	1:149:A:VAL:H	1:147:A:LEU:HB2	3	0.33
(1,3450)	1:130:A:LYS:H	1:130:A:LYS:HG3	10	0.33
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	3	0.33
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	5	0.33
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	8	0.33
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	9	0.33
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	7	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG3	10	0.33
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	6	0.33
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	7	0.33
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	6	0.33
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	5	0.33
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	1	0.33
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	8	0.33
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG11	8	0.33
(1,3187)	1:76:A:ALA:H	1:13:A:HIS:HB2	3	0.33
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	1	0.33
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	7	0.33
(1,3055)	1:18:A:GLY:H	1:17:A:LYS:HD3	9	0.33
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	6	0.33
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	3	0.33
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	6	0.33
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	5	0.33
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	2	0.33
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	2	0.33
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	5	0.33
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	6	0.33
(1,2831)	1:28:A:VAL:HG22	1:58:A:CYS:HB2	9	0.33
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	2	0.33
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HD3	10	0.33
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	4	0.33
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	7	0.33
(1,2753)	1:136:A:ARG:HA	1:136:A:ARG:HD3	5	0.33
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	3	0.33
(1,2714)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	3	0.33
(1,2714)	1:149:A:VAL:HG11	1:148:A:GLY:HA2	10	0.33
(1,2692)	1:153:A:PRO:HD3	1:152:A:GLY:HA3	7	0.33
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	3	0.33
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	4	0.33
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	5	0.33
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	6	0.33
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	9	0.33
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	1	0.33
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB1	3	0.33
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB3	8	0.33
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	4	0.33
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG23	7	0.33
(1,2506)	1:31:A:VAL:HG12	1:29:A:PRO:HA	2	0.33
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	5	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	3	0.33
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG21	6	0.33
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD12	9	0.33
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	7	0.33
(1,1925)	1:43:A:VAL:H	1:41:A:LYS:HB3	9	0.33
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	10	0.33
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD23	2	0.33
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD11	9	0.33
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	8	0.33
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG12	3	0.33
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG12	6	0.33
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG13	8	0.33
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	1	0.33
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	4	0.33
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	6	0.33
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	7	0.33
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	10	0.33
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	10	0.33
(1,1075)	1:31:A:VAL:HG22	1:36:A:CYS:HB3	5	0.33
(1,1075)	1:31:A:VAL:HG22	1:36:A:CYS:HB3	6	0.33
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB1	2	0.33
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	4	0.33
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB1	7	0.33
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB3	9	0.33
(1,932)	1:16:A:ASN:HD22	1:16:A:ASN:HB3	3	0.33
(1,761)	1:64:A:LYS:HE2	1:115:A:ALA:HB2	3	0.33
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB1	10	0.33
(1,749)	1:98:A:MET:H	1:96:A:ASP:HB3	9	0.33
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	8	0.33
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	4	0.33
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	9	0.33
(1,693)	1:67:A:LEU:H	1:67:A:LEU:HB3	6	0.33
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	9	0.33
(1,525)	1:46:A:CYS:H	1:24:A:ILE:HD13	2	0.33
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD13	5	0.33
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD11	10	0.33
(1,456)	1:38:A:ALA:HB2	1:35:A:GLN:HG3	10	0.33
(1,415)	1:21:A:ALA:HB3	1:66:A:ASP:HB2	6	0.33
(1,415)	1:21:A:ALA:HB2	1:66:A:ASP:HB2	7	0.33
(1,342)	1:149:A:VAL:HG23	1:123:A:THR:HG22	7	0.33
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	10	0.33
(1,235)	1:103:A:THR:HG23	1:124:A:TYR:HD2	6	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:67:A:LEU:HD21	1:19:A:SER:HB3	2	0.33
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	5	0.33
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	1	0.33
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	1	0.33
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	6	0.33
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	8	0.32
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	10	0.32
(1,3471)	1:57:A:MET:H	1:56:A:LYS:HG2	2	0.32
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	1	0.32
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	4	0.32
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	6	0.32
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	9	0.32
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	3	0.32
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	4	0.32
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	7	0.32
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	2	0.32
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	3	0.32
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	10	0.32
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	5	0.32
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG12	2	0.32
(1,3164)	1:75:A:THR:HG23	1:19:A:SER:HA	8	0.32
(1,3144)	1:75:A:THR:HB	1:50:A:THR:HG23	4	0.32
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	2	0.32
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	4	0.32
(1,3136)	1:52:A:ASN:H	1:50:A:THR:HG23	6	0.32
(1,3127)	1:132:A:THR:HG23	1:92:A:GLU:HG2	1	0.32
(1,3125)	1:123:A:THR:HG21	1:91:A:TYR:HD1	1	0.32
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	9	0.32
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB3	2	0.32
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB1	9	0.32
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	1	0.32
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	3	0.32
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	10	0.32
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD11	8	0.32
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD11	10	0.32
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	9	0.32
(1,2977)	1:26:A:GLU:HB3	1:26:A:GLU:H	10	0.32
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	1	0.32
(1,2937)	1:102:A:VAL:H	1:101:A:MET:HG2	3	0.32
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	9	0.32
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	10	0.32
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	7	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	1	0.32
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	9	0.32
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	1	0.32
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	9	0.32
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	2	0.32
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	7	0.32
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	10	0.32
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	1	0.32
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	1	0.32
(1,2777)	1:17:A:LYS:HE3	1:18:A:GLY:H	8	0.32
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	8	0.32
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	7	0.32
(1,2692)	1:153:A:PRO:HD3	1:152:A:GLY:HA3	1	0.32
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	1	0.32
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	2	0.32
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	7	0.32
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	8	0.32
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	10	0.32
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	9	0.32
(1,2549)	1:67:A:LEU:HD21	1:17:A:LYS:HE3	10	0.32
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	2	0.32
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	2	0.32
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD13	3	0.32
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD13	8	0.32
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG22	8	0.32
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD11	2	0.32
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD11	7	0.32
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG11	10	0.32
(1,1625)	1:132:A:THR:H	1:132:A:THR:HG21	8	0.32
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	2	0.32
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	3	0.32
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	8	0.32
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	8	0.32
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	7	0.32
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	1	0.32
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG21	1	0.32
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG23	3	0.32
(1,1075)	1:31:A:VAL:HG21	1:36:A:CYS:HB3	1	0.32
(1,1075)	1:31:A:VAL:HG21	1:36:A:CYS:HB3	8	0.32
(1,1075)	1:31:A:VAL:HG23	1:36:A:CYS:HB3	9	0.32
(1,1000)	1:112:A:ALA:HB1	1:109:A:CYS:HB2	3	0.32
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	7	0.32
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	8	0.32
(1,761)	1:64:A:LYS:HE2	1:115:A:ALA:HB1	5	0.32
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB1	1	0.32
(1,749)	1:98:A:MET:H	1:96:A:ASP:HB3	10	0.32
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD22	5	0.32
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	2	0.32
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	1	0.32
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	2	0.32
(1,680)	1:20:A:ARG:H	1:20:A:ARG:HD3	5	0.32
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	1	0.32
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	4	0.32
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	8	0.32
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD13	3	0.32
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD12	7	0.32
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD11	9	0.32
(1,456)	1:38:A:ALA:HB2	1:35:A:GLN:HG3	6	0.32
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG23	3	0.32
(1,415)	1:21:A:ALA:HB3	1:66:A:ASP:HB2	8	0.32
(1,415)	1:21:A:ALA:HB1	1:66:A:ASP:HB2	10	0.32
(1,408)	1:140:A:ALA:HB1	1:140:A:ALA:HA	9	0.32
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	1	0.32
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	6	0.32
(1,386)	1:112:A:ALA:HB3	1:114:A:ALA:H	2	0.32
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG23	2	0.32
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG23	5	0.32
(1,282)	1:146:A:VAL:HG21	1:88:A:HIS:HA	4	0.32
(1,218)	1:89:A:VAL:HG21	1:151:A:SER:HB2	2	0.32
(1,191)	1:127:A:HIS:HA	1:126:A:GLU:HB2	6	0.32
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	1	0.32
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	2	0.32
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	10	0.31
(1,3496)	1:135:A:GLY:H	1:95:A:PRO:HB3	9	0.31
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	5	0.31
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	10	0.31
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	7	0.31
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	10	0.31
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	3	0.31
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	2	0.31
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	1	0.31
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	8	0.31
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	9	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3280)	1:103:A:THR:H	1:129:A:GLN:HB2	7	0.31
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	2	0.31
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG12	6	0.31
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG23	6	0.31
(1,3164)	1:75:A:THR:HG23	1:19:A:SER:HA	10	0.31
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	2	0.31
(1,3137)	1:12:A:VAL:HG13	1:11:A:CYS:H	8	0.31
(1,3136)	1:52:A:ASN:H	1:50:A:THR:HG23	3	0.31
(1,3127)	1:132:A:THR:HG21	1:92:A:GLU:HG2	4	0.31
(1,3127)	1:132:A:THR:HG21	1:92:A:GLU:HG2	7	0.31
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	1	0.31
(1,3075)	1:39:A:GLN:HB2	1:38:A:ALA:HB2	3	0.31
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	8	0.31
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	9	0.31
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD11	1	0.31
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD12	6	0.31
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	1	0.31
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	10	0.31
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	3	0.31
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	3	0.31
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	9	0.31
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	4	0.31
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	5	0.31
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD11	9	0.31
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HD3	1	0.31
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	6	0.31
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	6	0.31
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	5	0.31
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	10	0.31
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	5	0.31
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	6	0.31
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	8	0.31
(1,2745)	1:82:A:ARG:HD2	1:85:A:PHE:HD2	1	0.31
(1,2724)	1:135:A:GLY:HA2	1:120:A:GLU:HB3	3	0.31
(1,2714)	1:149:A:VAL:HG13	1:148:A:GLY:HA2	1	0.31
(1,2684)	1:95:A:PRO:HD2	1:95:A:PRO:HB3	10	0.31
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	2	0.31
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	2	0.31
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB1	7	0.31
(1,2590)	1:102:A:VAL:HG13	1:17:A:LYS:HE3	10	0.31
(1,2584)	1:19:A:SER:H	1:75:A:THR:HG22	1	0.31
(1,2566)	1:103:A:THR:HG22	1:102:A:VAL:HA	5	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:150:A:THR:HG22	1:106:A:SER:HB2	3	0.31
(1,2517)	1:91:A:TYR:HA	1:94:A:ALA:HB1	10	0.31
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	6	0.31
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	4	0.31
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	10	0.31
(1,1918)	1:105:A:GLN:H	1:105:A:GLN:HE22	4	0.31
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD23	1	0.31
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	2	0.31
(1,1658)	1:39:A:GLN:HB3	1:60:A:VAL:HG12	9	0.31
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG13	5	0.31
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG23	6	0.31
(1,1606)	1:33:A:LEU:HD23	1:12:A:VAL:HB	8	0.31
(1,1605)	1:33:A:LEU:HD22	1:74:A:LYS:HB3	9	0.31
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB1	2	0.31
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	10	0.31
(1,1317)	1:127:A:HIS:HA	1:127:A:HIS:HB3	5	0.31
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	9	0.31
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	5	0.31
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG21	4	0.31
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG21	6	0.31
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG22	10	0.31
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	7	0.31
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	3	0.31
(1,1067)	1:132:A:THR:HB	1:100:A:ALA:HB2	10	0.31
(1,1000)	1:112:A:ALA:HB1	1:109:A:CYS:HB2	7	0.31
(1,964)	1:67:A:LEU:HD22	1:17:A:LYS:HB2	8	0.31
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	6	0.31
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	1	0.31
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	9	0.31
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	7	0.31
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	6	0.31
(1,717)	1:78:A:ARG:HD2	1:156:A:PHE:HD1	9	0.31
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	3	0.31
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	5	0.31
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	6	0.31
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG21	1	0.31
(1,415)	1:21:A:ALA:HB2	1:66:A:ASP:HB2	9	0.31
(1,411)	1:21:A:ALA:HB1	1:48:A:HIS:HD2	2	0.31
(1,408)	1:140:A:ALA:HB3	1:140:A:ALA:HA	1	0.31
(1,408)	1:140:A:ALA:HB1	1:140:A:ALA:HA	3	0.31
(1,408)	1:140:A:ALA:HB2	1:140:A:ALA:HA	4	0.31
(1,408)	1:140:A:ALA:HB2	1:140:A:ALA:HA	5	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,408)	1:140:A:ALA:HB3	1:140:A:ALA:HA	6	0.31
(1,408)	1:140:A:ALA:HB2	1:140:A:ALA:HA	8	0.31
(1,408)	1:140:A:ALA:HB2	1:140:A:ALA:HA	10	0.31
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB3	5	0.31
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB3	9	0.31
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG21	5	0.31
(1,329)	1:100:A:ALA:HB3	1:130:A:LYS:HE2	1	0.31
(1,304)	1:75:A:THR:H	1:75:A:THR:HG21	3	0.31
(1,304)	1:75:A:THR:H	1:75:A:THR:HG22	8	0.31
(1,304)	1:75:A:THR:H	1:75:A:THR:HG22	10	0.31
(1,290)	1:102:A:VAL:HG21	1:131:A:CYS:H	9	0.31
(1,228)	1:89:A:VAL:HG23	1:142:A:LYS:HA	2	0.31
(1,216)	1:89:A:VAL:HG21	1:143:A:GLU:HA	3	0.31
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD21	6	0.31
(1,180)	1:66:A:ASP:H	1:67:A:LEU:HD21	8	0.31
(1,167)	1:150:A:THR:HG21	1:85:A:PHE:HB2	4	0.31
(1,3509)	1:35:A:GLN:HE22	1:32:A:SER:HB2	10	0.3
(1,3496)	1:135:A:GLY:H	1:120:A:GLU:HG2	2	0.3
(1,3493)	1:55:A:SER:H	1:53:A:ASP:HB2	8	0.3
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	3	0.3
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	9	0.3
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	6	0.3
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	10	0.3
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	1	0.3
(1,3380)	1:16:A:ASN:HD21	1:71:A:THR:HG21	3	0.3
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	4	0.3
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	9	0.3
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG12	8	0.3
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	1	0.3
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	4	0.3
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	5	0.3
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG22	3	0.3
(1,3164)	1:75:A:THR:HG21	1:19:A:SER:HA	2	0.3
(1,3164)	1:75:A:THR:HG22	1:19:A:SER:HA	9	0.3
(1,3154)	1:18:A:GLY:H	1:70:A:LEU:HD21	1	0.3
(1,3137)	1:12:A:VAL:HG12	1:11:A:CYS:H	10	0.3
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	4	0.3
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	1	0.3
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	3	0.3
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	5	0.3
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	3	0.3
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	2	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	10	0.3
(1,2844)	1:156:A:PHE:HB3	1:159:A:GLU:HB3	2	0.3
(1,2834)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	1	0.3
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	3	0.3
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	1	0.3
(1,2808)	1:33:A:LEU:HB2	1:51:A:TYR:HE2	3	0.3
(1,2805)	1:34:A:GLU:H	1:33:A:LEU:HB3	9	0.3
(1,2801)	1:64:A:LYS:HE3	1:116:A:ASP:H	4	0.3
(1,2800)	1:51:A:TYR:HB3	1:6:A:LYS:HE3	4	0.3
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HD3	6	0.3
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	2	0.3
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	3	0.3
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	9	0.3
(1,2745)	1:82:A:ARG:HD2	1:85:A:PHE:HD2	2	0.3
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	9	0.3
(1,2724)	1:135:A:GLY:HA2	1:120:A:GLU:HB3	1	0.3
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	1	0.3
(1,2673)	1:24:A:ILE:HD13	1:62:A:GLU:HG3	3	0.3
(1,2672)	1:24:A:ILE:HD11	1:46:A:CYS:HB3	8	0.3
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	3	0.3
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB2	7	0.3
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	10	0.3
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	4	0.3
(1,2566)	1:103:A:THR:HG21	1:102:A:VAL:HA	8	0.3
(1,2566)	1:103:A:THR:HG22	1:102:A:VAL:HA	10	0.3
(1,2531)	1:75:A:THR:HG22	1:13:A:HIS:HD2	7	0.3
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB2	10	0.3
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	2	0.3
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	6	0.3
(1,2125)	1:68:A:TYR:H	1:67:A:LEU:HD11	1	0.3
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	1	0.3
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB2	7	0.3
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD22	5	0.3
(1,1991)	1:37:A:ALA:H	1:9:A:LEU:HD11	6	0.3
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	1	0.3
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	10	0.3
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG11	1	0.3
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG13	2	0.3
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG11	9	0.3
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG11	3	0.3
(1,1606)	1:33:A:LEU:HD22	1:12:A:VAL:HB	9	0.3
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB1	3	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB2	6	0.3
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	3	0.3
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD11	5	0.3
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	8	0.3
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	10	0.3
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	1	0.3
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	3	0.3
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	6	0.3
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	7	0.3
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	10	0.3
(1,1075)	1:31:A:VAL:HG23	1:36:A:CYS:HB3	3	0.3
(1,1075)	1:31:A:VAL:HG21	1:36:A:CYS:HB3	10	0.3
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	3	0.3
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	1	0.3
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG11	5	0.3
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	3	0.3
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG11	10	0.3
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB2	4	0.3
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB1	5	0.3
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB1	7	0.3
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB2	9	0.3
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	1	0.3
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	3	0.3
(1,729)	1:17:A:LYS:HE2	1:67:A:LEU:HD23	9	0.3
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	3	0.3
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG23	6	0.3
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD12	8	0.3
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD22	7	0.3
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB1	1	0.3
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB3	4	0.3
(1,408)	1:140:A:ALA:HB1	1:140:A:ALA:HA	2	0.3
(1,408)	1:140:A:ALA:HB2	1:140:A:ALA:HA	7	0.3
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	4	0.3
(1,380)	1:112:A:ALA:HB2	1:65:A:PRO:HG3	1	0.3
(1,342)	1:149:A:VAL:HG23	1:123:A:THR:HG23	2	0.3
(1,342)	1:149:A:VAL:HG23	1:123:A:THR:HG22	5	0.3
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG21	4	0.3
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG22	9	0.3
(1,303)	1:75:A:THR:HG21	1:13:A:HIS:HD2	1	0.3
(1,303)	1:75:A:THR:HG22	1:13:A:HIS:HD2	4	0.3
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	1	0.3
(1,290)	1:102:A:VAL:HG21	1:131:A:CYS:H	5	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:103:A:THR:HG23	1:124:A:TYR:HD2	9	0.3
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG23	4	0.3
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG22	10	0.3
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD22	9	0.3
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	10	0.3
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	1	0.29
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	4	0.29
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	7	0.29
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	8	0.29
(1,3429)	1:24:A:ILE:H	1:62:A:GLU:H	2	0.29
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	9	0.29
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	2	0.29
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	8	0.29
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	1	0.29
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	2	0.29
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	3	0.29
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	4	0.29
(1,3250)	1:91:A:TYR:H	1:92:A:GLU:HB2	1	0.29
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	1	0.29
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	3	0.29
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	6	0.29
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	7	0.29
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	8	0.29
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	3	0.29
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG12	4	0.29
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG21	2	0.29
(1,3164)	1:75:A:THR:HG22	1:19:A:SER:HA	5	0.29
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	7	0.29
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	8	0.29
(1,3137)	1:12:A:VAL:HG12	1:11:A:CYS:H	1	0.29
(1,3137)	1:12:A:VAL:HG11	1:11:A:CYS:H	3	0.29
(1,3127)	1:132:A:THR:HG23	1:92:A:GLU:HG2	10	0.29
(1,3125)	1:123:A:THR:HG21	1:91:A:TYR:HD1	8	0.29
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	2	0.29
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	2	0.29
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	1	0.29
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	3	0.29
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	8	0.29
(1,3000)	1:64:A:LYS:HD2	1:116:A:ASP:HA	10	0.29
(1,2945)	1:102:A:VAL:HB	1:130:A:LYS:HG3	10	0.29
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	2	0.29
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	4	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	7	0.29
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	7	0.29
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	7	0.29
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	7	0.29
(1,2757)	1:133:A:PHE:H	1:133:A:PHE:HB3	2	0.29
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD13	2	0.29
(1,2742)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	10	0.29
(1,2673)	1:24:A:ILE:HD12	1:62:A:GLU:HG3	4	0.29
(1,2672)	1:24:A:ILE:HD11	1:46:A:CYS:HB3	4	0.29
(1,2664)	1:94:A:ALA:HB2	1:95:A:PRO:HD2	3	0.29
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	9	0.29
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	5	0.29
(1,2566)	1:103:A:THR:HG21	1:102:A:VAL:HA	9	0.29
(1,2546)	1:150:A:THR:HG22	1:106:A:SER:HB2	1	0.29
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	5	0.29
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	9	0.29
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	1	0.29
(1,2506)	1:31:A:VAL:HG12	1:29:A:PRO:HA	3	0.29
(1,2506)	1:31:A:VAL:HG11	1:29:A:PRO:HA	6	0.29
(1,2269)	1:141:A:PHE:H	1:142:A:LYS:HB3	7	0.29
(1,2166)	1:10:A:SER:H	1:10:A:SER:HB3	8	0.29
(1,2106)	1:42:A:ALA:H	1:41:A:LYS:HB3	9	0.29
(1,1916)	1:104:A:SER:H	1:67:A:LEU:HD13	3	0.29
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	3	0.29
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	7	0.29
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	4	0.29
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	6	0.29
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG11	6	0.29
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG12	1	0.29
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG11	4	0.29
(1,1625)	1:132:A:THR:H	1:132:A:THR:HG21	1	0.29
(1,1540)	1:76:A:ALA:H	1:76:A:ALA:HB1	3	0.29
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD12	1	0.29
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD11	6	0.29
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	7	0.29
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	9	0.29
(1,1421)	1:108:A:ASP:HA	1:65:A:PRO:HG2	4	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	2	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	3	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	4	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	5	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	6	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	7	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	8	0.29
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	9	0.29
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	4	0.29
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	5	0.29
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	8	0.29
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	9	0.29
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	4	0.29
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	5	0.29
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	3	0.29
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG21	5	0.29
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG23	7	0.29
(1,1211)	1:27:A:PRO:HB2	1:59:A:HIS:HA	4	0.29
(1,1156)	1:102:A:VAL:HG23	1:102:A:VAL:HB	8	0.29
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	1	0.29
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	7	0.29
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	5	0.29
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	2	0.29
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	5	0.29
(1,899)	1:16:A:ASN:H	1:15:A:ASP:HB3	7	0.29
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE3	6	0.29
(1,755)	1:113:A:CYS:HB3	1:112:A:ALA:HB2	6	0.29
(1,741)	1:41:A:LYS:HE2	1:38:A:ALA:HA	10	0.29
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	10	0.29
(1,631)	1:123:A:THR:H	1:122:A:PHE:HB3	8	0.29
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	9	0.29
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD12	6	0.29
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	5	0.29
(1,501)	1:94:A:ALA:HB1	1:121:A:ILE:HD12	7	0.29
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD23	3	0.29
(1,456)	1:38:A:ALA:HB3	1:35:A:GLN:HG3	2	0.29
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB2	3	0.29
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB3	6	0.29
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB3	9	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB1	1	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB3	3	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB1	5	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB3	6	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB3	7	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB2	8	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB2	9	0.29
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB3	10	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG21	1	0.29
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG22	6	0.29
(1,411)	1:21:A:ALA:HB1	1:48:A:HIS:HD2	7	0.29
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB3	3	0.29
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	8	0.29
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	10	0.29
(1,396)	1:107:A:ALA:HB3	1:77:A:SER:HB2	4	0.29
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB3	9	0.29
(1,358)	1:115:A:ALA:HB1	1:116:A:ASP:HB2	7	0.29
(1,356)	1:115:A:ALA:HB2	1:116:A:ASP:HA	8	0.29
(1,304)	1:75:A:THR:H	1:75:A:THR:HG21	5	0.29
(1,285)	1:146:A:VAL:HG21	1:90:A:SER:HA	8	0.29
(1,242)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	10	0.29
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	4	0.29
(1,228)	1:89:A:VAL:HG22	1:142:A:LYS:HA	4	0.29
(1,228)	1:89:A:VAL:HG23	1:142:A:LYS:HA	9	0.29
(1,216)	1:89:A:VAL:HG22	1:143:A:GLU:HA	6	0.29
(1,216)	1:89:A:VAL:HG21	1:143:A:GLU:HA	7	0.29
(1,216)	1:89:A:VAL:HG22	1:143:A:GLU:HA	8	0.29
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	6	0.29
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	7	0.29
(1,178)	1:67:A:LEU:H	1:67:A:LEU:HD21	8	0.29
(1,173)	1:35:A:GLN:HE21	1:31:A:VAL:HG11	4	0.29
(1,81)	1:91:A:TYR:HA	1:91:A:TYR:HD2	2	0.29
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	3	0.29
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	8	0.28
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	3	0.28
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	2	0.28
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	7	0.28
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	2	0.28
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	1	0.28
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG12	1	0.28
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	1	0.28
(1,3166)	1:131:A:CYS:HA	1:132:A:THR:HG21	10	0.28
(1,3161)	1:132:A:THR:HG23	1:100:A:ALA:HB2	4	0.28
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	3	0.28
(1,3097)	1:67:A:LEU:HD12	1:102:A:VAL:H	1	0.28
(1,3097)	1:67:A:LEU:HD13	1:102:A:VAL:H	6	0.28
(1,3055)	1:18:A:GLY:H	1:17:A:LYS:HD3	4	0.28
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	7	0.28
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	4	0.28
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	5	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2967)	1:159:A:GLU:H	1:159:A:GLU:HB3	9	0.28
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	5	0.28
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	6	0.28
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	5	0.28
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	4	0.28
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	10	0.28
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	4	0.28
(1,2864)	1:34:A:GLU:HG2	1:33:A:LEU:HD11	6	0.28
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	10	0.28
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	5	0.28
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	8	0.28
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	9	0.28
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	6	0.28
(1,2805)	1:10:A:SER:H	1:9:A:LEU:HB2	5	0.28
(1,2774)	1:56:A:LYS:HA	1:6:A:LYS:HE2	6	0.28
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	8	0.28
(1,2764)	1:74:A:LYS:H	1:53:A:ASP:HB3	9	0.28
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	2	0.28
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	6	0.28
(1,2673)	1:24:A:ILE:HD13	1:62:A:GLU:HG3	1	0.28
(1,2673)	1:24:A:ILE:HD13	1:62:A:GLU:HG3	5	0.28
(1,2673)	1:24:A:ILE:HD12	1:62:A:GLU:HG3	6	0.28
(1,2673)	1:24:A:ILE:HD12	1:62:A:GLU:HG3	7	0.28
(1,2673)	1:24:A:ILE:HD12	1:62:A:GLU:HG3	8	0.28
(1,2673)	1:24:A:ILE:HD11	1:62:A:GLU:HG3	9	0.28
(1,2639)	1:114:A:ALA:HB2	1:156:A:PHE:HE2	4	0.28
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB1	10	0.28
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	3	0.28
(1,2546)	1:150:A:THR:HG22	1:106:A:SER:HB2	8	0.28
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	7	0.28
(1,2378)	1:87:A:GLN:HE21	1:87:A:GLN:HB3	9	0.28
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB3	8	0.28
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	9	0.28
(1,1666)	1:9:A:LEU:HD23	1:33:A:LEU:HA	10	0.28
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG13	8	0.28
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG13	1	0.28
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG11	2	0.28
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG11	5	0.28
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG21	8	0.28
(1,1606)	1:33:A:LEU:HD22	1:12:A:VAL:HB	7	0.28
(1,1605)	1:33:A:LEU:HD23	1:74:A:LYS:HB3	5	0.28
(1,1541)	1:76:A:ALA:HB3	1:51:A:TYR:HE2	10	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB2	5	0.28
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB2	8	0.28
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD11	2	0.28
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	1	0.28
(1,1394)	1:95:A:PRO:HG3	1:95:A:PRO:HB2	10	0.28
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB1	3	0.28
(1,1378)	1:117:A:PRO:HB2	1:117:A:PRO:HA	2	0.28
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	3	0.28
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG21	8	0.28
(1,1156)	1:102:A:VAL:HG11	1:102:A:VAL:HB	2	0.28
(1,1156)	1:102:A:VAL:HG13	1:102:A:VAL:HB	3	0.28
(1,1156)	1:102:A:VAL:HG12	1:102:A:VAL:HB	5	0.28
(1,1156)	1:102:A:VAL:HG11	1:102:A:VAL:HB	6	0.28
(1,1156)	1:102:A:VAL:HG13	1:102:A:VAL:HB	10	0.28
(1,1075)	1:31:A:VAL:HG21	1:36:A:CYS:HB3	2	0.28
(1,964)	1:67:A:LEU:HD22	1:17:A:LYS:HB2	5	0.28
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	1	0.28
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	6	0.28
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	9	0.28
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	10	0.28
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	2	0.28
(1,742)	1:37:A:ALA:HB2	1:41:A:LYS:HE2	5	0.28
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	3	0.28
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	9	0.28
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	8	0.28
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	10	0.28
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	5	0.28
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	8	0.28
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG22	2	0.28
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG23	4	0.28
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG21	9	0.28
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG23	10	0.28
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	5	0.28
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	7	0.28
(1,523)	1:63:A:GLY:H	1:24:A:ILE:HD12	4	0.28
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	2	0.28
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	3	0.28
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	8	0.28
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	9	0.28
(1,501)	1:94:A:ALA:HB1	1:121:A:ILE:HD12	2	0.28
(1,499)	1:94:A:ALA:HB3	1:138:A:PHE:HB2	9	0.28
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB2	2	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG21	3	0.28
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG23	7	0.28
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG21	9	0.28
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB3	5	0.28
(1,439)	1:38:A:ALA:HA	1:38:A:ALA:HB1	2	0.28
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG22	3	0.28
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG21	5	0.28
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG21	8	0.28
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG21	1	0.28
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG23	6	0.28
(1,285)	1:146:A:VAL:HG22	1:90:A:SER:HA	2	0.28
(1,235)	1:103:A:THR:HG23	1:124:A:TYR:HD2	8	0.28
(1,216)	1:89:A:VAL:HG22	1:143:A:GLU:HA	1	0.28
(1,216)	1:89:A:VAL:HG23	1:143:A:GLU:HA	9	0.28
(1,216)	1:89:A:VAL:HG23	1:143:A:GLU:HA	10	0.28
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG21	1	0.28
(1,180)	1:66:A:ASP:H	1:67:A:LEU:HD23	10	0.28
(1,179)	1:68:A:TYR:H	1:67:A:LEU:HD21	2	0.28
(1,176)	1:31:A:VAL:HG12	1:58:A:CYS:HB2	10	0.28
(1,146)	1:9:A:LEU:HD22	1:37:A:ALA:HB3	7	0.28
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	3	0.27
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	9	0.27
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	2	0.27
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	2	0.27
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	5	0.27
(1,3338)	1:156:A:PHE:H	1:156:A:PHE:HA	10	0.27
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	2	0.27
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	2	0.27
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	10	0.27
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	2	0.27
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	5	0.27
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	6	0.27
(1,3266)	1:105:A:GLN:H	1:108:A:ASP:HB3	10	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG13	3	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG11	4	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG12	5	0.27
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG11	10	0.27
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	4	0.27
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	5	0.27
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	9	0.27
(1,3232)	1:60:A:VAL:H	1:61:A:LYS:H	10	0.27
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	8	0.27
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	10	0.27
(1,3202)	1:100:A:ALA:H	1:96:A:ASP:HB3	5	0.27
(1,3125)	1:123:A:THR:HG21	1:91:A:TYR:HD1	2	0.27
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD12	2	0.27
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG22	9	0.27
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD12	2	0.27
(1,3000)	1:64:A:LYS:HD2	1:116:A:ASP:HA	1	0.27
(1,2992)	1:49:A:PHE:H	1:48:A:HIS:HB3	4	0.27
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	10	0.27
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	4	0.27
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	7	0.27
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	8	0.27
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	4	0.27
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	8	0.27
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	2	0.27
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	10	0.27
(1,2834)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	3	0.27
(1,2830)	1:58:A:CYS:HB2	1:57:A:MET:HA	6	0.27
(1,2829)	1:58:A:CYS:HB2	1:51:A:TYR:HD1	4	0.27
(1,2783)	1:131:A:CYS:H	1:131:A:CYS:HB3	8	0.27
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	6	0.27
(1,2752)	1:18:A:GLY:HA3	1:70:A:LEU:HD12	4	0.27
(1,2719)	1:25:A:GLY:HA3	1:26:A:GLU:HB2	3	0.27
(1,2716)	1:160:A:GLY:HA2	1:156:A:PHE:HD2	7	0.27
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	1	0.27
(1,2692)	1:153:A:PRO:HD3	1:152:A:GLY:HA3	8	0.27
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	1	0.27
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	6	0.27
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	1	0.27
(1,2639)	1:115:A:ALA:H	1:114:A:ALA:HB3	6	0.27
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB3	2	0.27
(1,2582)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	6	0.27
(1,2582)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	7	0.27
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	6	0.27
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	7	0.27
(1,2572)	1:35:A:GLN:HA	1:35:A:GLN:HG3	3	0.27
(1,2567)	1:43:A:VAL:HG12	1:43:A:VAL:HB	7	0.27
(1,2566)	1:103:A:THR:HG22	1:102:A:VAL:HA	3	0.27
(1,2546)	1:150:A:THR:HG21	1:106:A:SER:HB2	10	0.27
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	5	0.27
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	8	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	2	0.27
(1,2531)	1:13:A:HIS:HD2	1:17:A:LYS:HB2	4	0.27
(1,2531)	1:75:A:THR:HG23	1:13:A:HIS:HD2	6	0.27
(1,2502)	1:85:A:PHE:HE2	1:107:A:ALA:HA	5	0.27
(1,2326)	1:110:A:GLN:HE22	1:85:A:PHE:HE1	3	0.27
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	7	0.27
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	3	0.27
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD23	8	0.27
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	5	0.27
(1,1666)	1:9:A:LEU:HD23	1:33:A:LEU:HA	3	0.27
(1,1666)	1:9:A:LEU:HD21	1:33:A:LEU:HA	6	0.27
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG11	3	0.27
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG13	7	0.27
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG13	3	0.27
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG12	10	0.27
(1,1640)	1:47:A:THR:HG21	1:156:A:PHE:HE2	9	0.27
(1,1606)	1:33:A:LEU:HD21	1:12:A:VAL:HB	10	0.27
(1,1605)	1:33:A:LEU:HD21	1:74:A:LYS:HB3	2	0.27
(1,1605)	1:33:A:LEU:HD21	1:74:A:LYS:HB3	10	0.27
(1,1541)	1:76:A:ALA:HB2	1:51:A:TYR:HE2	2	0.27
(1,1541)	1:76:A:ALA:HB3	1:51:A:TYR:HE2	7	0.27
(1,1541)	1:76:A:ALA:HB2	1:51:A:TYR:HE2	8	0.27
(1,1541)	1:76:A:ALA:HB3	1:51:A:TYR:HE2	9	0.27
(1,1500)	1:70:A:LEU:HG	1:70:A:LEU:HD13	4	0.27
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	4	0.27
(1,1253)	1:67:A:LEU:HD23	1:65:A:PRO:HB2	6	0.27
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	2	0.27
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	4	0.27
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	8	0.27
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	2	0.27
(1,1156)	1:102:A:VAL:HG13	1:102:A:VAL:HB	4	0.27
(1,1156)	1:102:A:VAL:HG13	1:102:A:VAL:HB	7	0.27
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	1	0.27
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	4	0.27
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	8	0.27
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	5	0.27
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	6	0.27
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	1	0.27
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	2	0.27
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	3	0.27
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG11	4	0.27
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	1	0.27
(1,698)	1:67:A:LEU:HB2	1:68:A:TYR:HA	7	0.27
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	5	0.27
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG21	2	0.27
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG23	7	0.27
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG21	8	0.27
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	1	0.27
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	4	0.27
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	6	0.27
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	10	0.27
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB2	6	0.27
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG21	1	0.27
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG21	6	0.27
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG23	8	0.27
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB1	4	0.27
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB2	6	0.27
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB1	2	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG23	2	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG21	6	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG22	7	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG23	8	0.27
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG22	9	0.27
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG21	2	0.27
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG22	6	0.27
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG23	6	0.27
(1,415)	1:21:A:ALA:HB2	1:66:A:ASP:HB2	3	0.27
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB3	2	0.27
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB2	2	0.27
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB1	7	0.27
(1,356)	1:115:A:ALA:HB3	1:116:A:ASP:HA	4	0.27
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG23	8	0.27
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG23	7	0.27
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG22	1	0.27
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG21	2	0.27
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG22	4	0.27
(1,285)	1:146:A:VAL:HG21	1:90:A:SER:HA	10	0.27
(1,240)	1:28:A:VAL:HG11	1:29:A:PRO:HD2	3	0.27
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	5	0.27
(1,240)	1:28:A:VAL:HG11	1:29:A:PRO:HD2	7	0.27
(1,228)	1:89:A:VAL:HG22	1:142:A:LYS:HA	8	0.27
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	3	0.27
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	2	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	1	0.27
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	4	0.27
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	7	0.27
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	7	0.27
(1,3523)	1:31:A:VAL:H	1:30:A:ASP:HB3	2	0.26
(1,3523)	1:31:A:VAL:H	1:30:A:ASP:HB3	5	0.26
(1,3523)	1:31:A:VAL:H	1:30:A:ASP:HB3	8	0.26
(1,3502)	1:87:A:GLN:HE21	1:150:A:THR:HA	10	0.26
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	2	0.26
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	6	0.26
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	10	0.26
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	9	0.26
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG2	3	0.26
(1,3355)	1:64:A:LYS:H	1:112:A:ALA:HA	5	0.26
(1,3354)	1:147:A:LEU:H	1:146:A:VAL:H	3	0.26
(1,3345)	1:150:A:THR:H	1:87:A:GLN:HG2	2	0.26
(1,3338)	1:156:A:PHE:H	1:156:A:PHE:HA	8	0.26
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	3	0.26
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	3	0.26
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	10	0.26
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	5	0.26
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	8	0.26
(1,3240)	1:107:A:ALA:H	1:106:A:SER:HB2	8	0.26
(1,3240)	1:107:A:ALA:H	1:106:A:SER:HB2	10	0.26
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG13	6	0.26
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG13	9	0.26
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	5	0.26
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	7	0.26
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	9	0.26
(1,3164)	1:75:A:THR:HG23	1:19:A:SER:HA	7	0.26
(1,3161)	1:132:A:THR:HG23	1:100:A:ALA:HB1	7	0.26
(1,3161)	1:100:A:ALA:HB1	1:130:A:LYS:HG2	9	0.26
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	4	0.26
(1,3137)	1:12:A:VAL:HG11	1:11:A:CYS:H	4	0.26
(1,3137)	1:12:A:VAL:HG11	1:11:A:CYS:H	5	0.26
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD11	4	0.26
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD12	7	0.26
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD11	8	0.26
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD13	10	0.26
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	2	0.26
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	1	0.26
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	2	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2916)	1:134:A:LYS:HB3	1:138:A:PHE:H	10	0.26
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	6	0.26
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	7	0.26
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	1	0.26
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	5	0.26
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	5	0.26
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	1	0.26
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	3	0.26
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	4	0.26
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	9	0.26
(1,2778)	1:113:A:CYS:HB2	1:133:A:PHE:HA	6	0.26
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	1	0.26
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	1	0.26
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	2	0.26
(1,2692)	1:153:A:PRO:HD3	1:152:A:GLY:HA3	3	0.26
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	10	0.26
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	1	0.26
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	8	0.26
(1,2595)	1:75:A:THR:HG22	1:13:A:HIS:HB2	4	0.26
(1,2567)	1:43:A:VAL:HG13	1:43:A:VAL:HB	3	0.26
(1,2567)	1:12:A:VAL:HG21	1:12:A:VAL:HB	5	0.26
(1,2567)	1:43:A:VAL:HG11	1:43:A:VAL:HB	10	0.26
(1,2566)	1:103:A:THR:HG21	1:102:A:VAL:HA	2	0.26
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	1	0.26
(1,2536)	1:70:A:LEU:HB3	1:68:A:TYR:HE2	6	0.26
(1,2510)	1:114:A:ALA:HB3	1:156:A:PHE:HE2	10	0.26
(1,2503)	1:85:A:PHE:HE1	1:110:A:GLN:HG2	6	0.26
(1,2378)	1:87:A:GLN:HE21	1:87:A:GLN:HB3	8	0.26
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	4	0.26
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	6	0.26
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	8	0.26
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB2	2	0.26
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB2	7	0.26
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	4	0.26
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	3	0.26
(1,1666)	1:9:A:LEU:HD23	1:33:A:LEU:HA	2	0.26
(1,1666)	1:9:A:LEU:HD21	1:33:A:LEU:HA	9	0.26
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG12	4	0.26
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG12	6	0.26
(1,1640)	1:47:A:THR:HG23	1:156:A:PHE:HE2	6	0.26
(1,1577)	1:64:A:LYS:HE2	1:64:A:LYS:HG2	5	0.26
(1,1577)	1:64:A:LYS:HE2	1:64:A:LYS:HG2	8	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB1	7	0.26
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	3	0.26
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	5	0.26
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	4	0.26
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	10	0.26
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	8	0.26
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	5	0.26
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	7	0.26
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	9	0.26
(1,1156)	1:102:A:VAL:HG11	1:102:A:VAL:HB	1	0.26
(1,1156)	1:102:A:VAL:HG11	1:102:A:VAL:HB	9	0.26
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG12	3	0.26
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	8	0.26
(1,1075)	1:31:A:VAL:HG23	1:36:A:CYS:HB3	7	0.26
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	9	0.26
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	10	0.26
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	3	0.26
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	6	0.26
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	7	0.26
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	10	0.26
(1,940)	1:16:A:ASN:HB2	1:71:A:THR:HA	5	0.26
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	6	0.26
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	7	0.26
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG13	10	0.26
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	10	0.26
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	3	0.26
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	10	0.26
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	5	0.26
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	7	0.26
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	10	0.26
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	7	0.26
(1,742)	1:37:A:ALA:HB2	1:41:A:LYS:HE2	9	0.26
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	7	0.26
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	2	0.26
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG2	6	0.26
(1,709)	1:144:A:ARG:HD3	1:144:A:ARG:HG3	7	0.26
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	2	0.26
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	6	0.26
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	7	0.26
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG23	4	0.26
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG21	5	0.26
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	6	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:117:A:PRO:HD2	1:117:A:PRO:HA	7	0.26
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB2	8	0.26
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB3	9	0.26
(1,456)	1:38:A:ALA:HB1	1:35:A:GLN:HG3	8	0.26
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB1	8	0.26
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB1	9	0.26
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB2	10	0.26
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB3	1	0.26
(1,419)	1:111:A:ALA:HB1	1:156:A:PHE:HZ	1	0.26
(1,415)	1:21:A:ALA:HB2	1:66:A:ASP:HB2	2	0.26
(1,406)	1:140:A:ALA:H	1:140:A:ALA:HB1	7	0.26
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB2	3	0.26
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB2	5	0.26
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB3	8	0.26
(1,356)	1:115:A:ALA:HB1	1:116:A:ASP:HA	1	0.26
(1,356)	1:115:A:ALA:HB3	1:116:A:ASP:HA	6	0.26
(1,342)	1:149:A:VAL:HG23	1:123:A:THR:HG22	6	0.26
(1,342)	1:149:A:VAL:HG21	1:123:A:THR:HG23	10	0.26
(1,334)	1:125:A:ASN:HD22	1:149:A:VAL:HG21	9	0.26
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG21	7	0.26
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	2	0.26
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	6	0.26
(1,240)	1:28:A:VAL:HG11	1:29:A:PRO:HD2	9	0.26
(1,231)	1:104:A:SER:H	1:103:A:THR:HG21	3	0.26
(1,204)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	9	0.26
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	1	0.26
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG23	5	0.25
(1,3512)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	8	0.25
(1,3479)	1:149:A:VAL:H	1:146:A:VAL:H	10	0.25
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	2	0.25
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	4	0.25
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	5	0.25
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	7	0.25
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	10	0.25
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	4	0.25
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	6	0.25
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	8	0.25
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	3	0.25
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB3	1	0.25
(1,3280)	1:103:A:THR:H	1:129:A:GLN:HB2	1	0.25
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG12	7	0.25
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	9	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG13	9	0.25
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	8	0.25
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	10	0.25
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	7	0.25
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG12	9	0.25
(1,3164)	1:75:A:THR:HG21	1:19:A:SER:HA	6	0.25
(1,3161)	1:100:A:ALA:HB2	1:130:A:LYS:HG2	2	0.25
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	5	0.25
(1,3127)	1:132:A:THR:HG22	1:92:A:GLU:HG2	9	0.25
(1,3125)	1:123:A:THR:HG21	1:91:A:TYR:HD1	10	0.25
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD12	1	0.25
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD13	6	0.25
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	6	0.25
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD13	4	0.25
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	5	0.25
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	1	0.25
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	8	0.25
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	3	0.25
(1,3039)	1:19:A:SER:HB2	1:65:A:PRO:HB2	3	0.25
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	4	0.25
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	5	0.25
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	3	0.25
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	5	0.25
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	2	0.25
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	4	0.25
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	9	0.25
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	7	0.25
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	10	0.25
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	2	0.25
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	10	0.25
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	9	0.25
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	9	0.25
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	5	0.25
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	10	0.25
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	9	0.25
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	3	0.25
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	10	0.25
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	2	0.25
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	8	0.25
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	6	0.25
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	2	0.25
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	5	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	10	0.25
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	6	0.25
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	2	0.25
(1,2664)	1:94:A:ALA:HB3	1:95:A:PRO:HD2	7	0.25
(1,2627)	1:111:A:ALA:HB3	1:156:A:PHE:HD1	1	0.25
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB3	3	0.25
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	2	0.25
(1,2582)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	8	0.25
(1,2567)	1:43:A:VAL:HG11	1:43:A:VAL:HB	6	0.25
(1,2567)	1:43:A:VAL:HG11	1:43:A:VAL:HB	8	0.25
(1,2567)	1:43:A:VAL:HG12	1:43:A:VAL:HB	9	0.25
(1,2561)	1:89:A:VAL:HG21	1:91:A:TYR:HD1	2	0.25
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	7	0.25
(1,2531)	1:13:A:HIS:HD2	1:17:A:LYS:HB2	1	0.25
(1,2506)	1:31:A:VAL:HG12	1:29:A:PRO:HA	1	0.25
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB3	8	0.25
(1,2298)	1:130:A:LYS:H	1:124:A:TYR:HB2	9	0.25
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD23	2	0.25
(1,1888)	1:140:A:ALA:H	1:94:A:ALA:HB1	3	0.25
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	5	0.25
(1,1706)	1:93:A:GLY:H	1:92:A:GLU:HG3	9	0.25
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD21	3	0.25
(1,1666)	1:9:A:LEU:HD22	1:33:A:LEU:HA	5	0.25
(1,1666)	1:9:A:LEU:HD23	1:33:A:LEU:HA	8	0.25
(1,1655)	1:43:A:VAL:H	1:60:A:VAL:HG12	10	0.25
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG11	7	0.25
(1,1606)	1:33:A:LEU:HD23	1:12:A:VAL:HB	5	0.25
(1,1573)	1:65:A:PRO:HD2	1:64:A:LYS:HG3	2	0.25
(1,1541)	1:76:A:ALA:HB1	1:51:A:TYR:HE2	5	0.25
(1,1541)	1:76:A:ALA:HB3	1:51:A:TYR:HE2	6	0.25
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB2	4	0.25
(1,1517)	1:83:A:SER:HB2	1:157:A:CYS:HB3	7	0.25
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	3	0.25
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	4	0.25
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	6	0.25
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	8	0.25
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	9	0.25
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	10	0.25
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	4	0.25
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	10	0.25
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	1	0.25
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	10	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	3	0.25
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	5	0.25
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	7	0.25
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	5	0.25
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	6	0.25
(1,899)	1:16:A:ASN:H	1:15:A:ASP:HB3	2	0.25
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	1	0.25
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	2	0.25
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	7	0.25
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	9	0.25
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	6	0.25
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	8	0.25
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	6	0.25
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	8	0.25
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	1	0.25
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	4	0.25
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	8	0.25
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	9	0.25
(1,761)	1:64:A:LYS:HE2	1:115:A:ALA:HB2	8	0.25
(1,742)	1:37:A:ALA:HB3	1:41:A:LYS:HE2	10	0.25
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	4	0.25
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	8	0.25
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG2	9	0.25
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	9	0.25
(1,692)	1:97:A:VAL:HG23	1:133:A:PHE:HB2	3	0.25
(1,692)	1:97:A:VAL:HG22	1:133:A:PHE:HB2	7	0.25
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	2	0.25
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	7	0.25
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	10	0.25
(1,536)	1:27:A:PRO:HD3	1:23:A:THR:HG21	2	0.25
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB1	10	0.25
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG23	2	0.25
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG22	4	0.25
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG23	1	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	1	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	2	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	3	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	4	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	5	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	6	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	7	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	8	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	9	0.25
(1,459)	1:7:A:LEU:HA	1:7:A:LEU:HB2	10	0.25
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB3	1	0.25
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB3	2	0.25
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB2	3	0.25
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB3	5	0.25
(1,455)	1:38:A:ALA:H	1:38:A:ALA:HB2	7	0.25
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB1	8	0.25
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB1	10	0.25
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG23	1	0.25
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG22	4	0.25
(1,427)	1:36:A:CYS:HA	1:31:A:VAL:HG23	10	0.25
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG21	3	0.25
(1,415)	1:21:A:ALA:HB2	1:66:A:ASP:HB2	1	0.25
(1,388)	1:112:A:ALA:HB3	1:65:A:PRO:HD3	9	0.25
(1,371)	1:6:A:LYS:H	1:5:A:ALA:HB2	1	0.25
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB3	4	0.25
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB3	10	0.25
(1,356)	1:115:A:ALA:HB3	1:116:A:ASP:HA	10	0.25
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	2	0.25
(1,290)	1:102:A:VAL:HG23	1:131:A:CYS:H	6	0.25
(1,285)	1:146:A:VAL:HG21	1:90:A:SER:HA	3	0.25
(1,285)	1:146:A:VAL:HG22	1:90:A:SER:HA	5	0.25
(1,285)	1:146:A:VAL:HG21	1:90:A:SER:HA	7	0.25
(1,242)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	2	0.25
(1,242)	1:43:A:VAL:HG22	1:46:A:CYS:HB2	3	0.25
(1,242)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	6	0.25
(1,240)	1:28:A:VAL:HG11	1:29:A:PRO:HD2	10	0.25
(1,235)	1:103:A:THR:HG21	1:124:A:TYR:HD2	10	0.25
(1,169)	1:12:A:VAL:HG23	1:75:A:THR:H	6	0.25
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG23	1	0.24
(1,3512)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	7	0.24
(1,3509)	1:35:A:GLN:HE22	1:32:A:SER:HB2	4	0.24
(1,3471)	1:57:A:MET:H	1:56:A:LYS:HG2	7	0.24
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	2	0.24
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	5	0.24
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	3	0.24
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	6	0.24
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	3	0.24
(1,3338)	1:156:A:PHE:H	1:156:A:PHE:HA	1	0.24
(1,3338)	1:156:A:PHE:H	1:156:A:PHE:HA	6	0.24
(1,3321)	1:119:A:CYS:H	1:116:A:ASP:H	5	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	6	0.24
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	7	0.24
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	3	0.24
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	9	0.24
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	2	0.24
(1,3273)	1:47:A:THR:H	1:78:A:ARG:HG2	10	0.24
(1,3209)	1:70:A:LEU:H	1:69:A:ASP:HB3	4	0.24
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG11	5	0.24
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	5	0.24
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD21	3	0.24
(1,3161)	1:132:A:THR:HG21	1:100:A:ALA:HB2	6	0.24
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	6	0.24
(1,3130)	1:60:A:VAL:H	1:23:A:THR:HG22	2	0.24
(1,3125)	1:123:A:THR:HG23	1:91:A:TYR:HD1	7	0.24
(1,3119)	1:6:A:LYS:HG3	1:53:A:ASP:H	6	0.24
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD11	3	0.24
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD13	5	0.24
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	4	0.24
(1,3097)	1:67:A:LEU:HD11	1:102:A:VAL:H	7	0.24
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	5	0.24
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	9	0.24
(1,3036)	1:55:A:SER:HB3	1:57:A:MET:HG2	10	0.24
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	8	0.24
(1,3014)	1:34:A:GLU:HB3	1:9:A:LEU:HD12	7	0.24
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	4	0.24
(1,2957)	1:86:A:GLU:HB2	1:151:A:SER:HB2	2	0.24
(1,2942)	1:12:A:VAL:HG22	1:12:A:VAL:HB	8	0.24
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	7	0.24
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	4	0.24
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	7	0.24
(1,2908)	1:110:A:GLN:HG2	1:79:A:SER:HB2	5	0.24
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	2	0.24
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	6	0.24
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	3	0.24
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	4	0.24
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	5	0.24
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	10	0.24
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	5	0.24
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	7	0.24
(1,2710)	1:161:A:GLY:HA2	1:155:A:GLN:HG2	10	0.24
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	5	0.24
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	4	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	10	0.24
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	10	0.24
(1,2673)	1:24:A:ILE:HD12	1:62:A:GLU:HG3	2	0.24
(1,2673)	1:24:A:ILE:HD11	1:62:A:GLU:HG3	10	0.24
(1,2672)	1:24:A:ILE:HD12	1:46:A:CYS:HB3	3	0.24
(1,2664)	1:94:A:ALA:HB1	1:95:A:PRO:HD2	1	0.24
(1,2659)	1:40:A:CYS:H	1:37:A:ALA:HA	4	0.24
(1,2633)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	7	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	1	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	2	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	4	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	5	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	6	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	8	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	9	0.24
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	10	0.24
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG21	8	0.24
(1,2587)	1:55:A:SER:HA	1:56:A:LYS:HB2	7	0.24
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	10	0.24
(1,2567)	1:43:A:VAL:HG12	1:43:A:VAL:HB	1	0.24
(1,2567)	1:43:A:VAL:HG11	1:43:A:VAL:HB	2	0.24
(1,2567)	1:43:A:VAL:HG11	1:43:A:VAL:HB	4	0.24
(1,2503)	1:85:A:PHE:HE1	1:110:A:GLN:HG2	9	0.24
(1,2402)	1:19:A:SER:H	1:19:A:SER:HB3	9	0.24
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	3	0.24
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB1	5	0.24
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	7	0.24
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG22	10	0.24
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB3	1	0.24
(1,2048)	1:136:A:ARG:H	1:97:A:VAL:HG23	4	0.24
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	2	0.24
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG22	1	0.24
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG22	3	0.24
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD22	10	0.24
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD21	5	0.24
(1,1666)	1:9:A:LEU:HD22	1:33:A:LEU:HA	7	0.24
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG12	4	0.24
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG12	7	0.24
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG13	9	0.24
(1,1644)	1:12:A:VAL:H	1:12:A:VAL:HG13	9	0.24
(1,1577)	1:64:A:LYS:HE2	1:64:A:LYS:HG2	2	0.24
(1,1577)	1:64:A:LYS:HE2	1:64:A:LYS:HG2	9	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	2	0.24
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	7	0.24
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	8	0.24
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	1	0.24
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	2	0.24
(1,1326)	1:34:A:GLU:HB2	1:34:A:GLU:HA	7	0.24
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	5	0.24
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	6	0.24
(1,1253)	1:67:A:LEU:HD21	1:65:A:PRO:HB2	3	0.24
(1,1239)	1:78:A:ARG:H	1:78:A:ARG:HB2	6	0.24
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG22	2	0.24
(1,1223)	1:86:A:GLU:HB3	1:89:A:VAL:HG22	9	0.24
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	4	0.24
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG12	7	0.24
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG12	9	0.24
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	5	0.24
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	7	0.24
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	8	0.24
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	10	0.24
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	6	0.24
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	1	0.24
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	4	0.24
(1,899)	1:16:A:ASN:H	1:15:A:ASP:HB3	6	0.24
(1,825)	1:125:A:ASN:HD22	1:125:A:ASN:HB2	4	0.24
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	1	0.24
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	7	0.24
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	2	0.24
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	3	0.24
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	8	0.24
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG12	5	0.24
(1,722)	1:7:A:LEU:HB3	1:34:A:GLU:HG2	10	0.24
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	3	0.24
(1,692)	1:97:A:VAL:HG23	1:133:A:PHE:HB2	6	0.24
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	3	0.24
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	6	0.24
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	4	0.24
(1,494)	1:94:A:ALA:HB2	1:141:A:PHE:HD2	8	0.24
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG23	5	0.24
(1,484)	1:25:A:GLY:H	1:24:A:ILE:HG22	10	0.24
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG23	7	0.24
(1,440)	1:38:A:ALA:HA	1:37:A:ALA:HB2	7	0.24
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG23	7	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG22	8	0.24
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB1	5	0.24
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB2	6	0.24
(1,358)	1:115:A:ALA:HB3	1:116:A:ASP:HB2	10	0.24
(1,305)	1:75:A:THR:HG23	1:19:A:SER:HB2	8	0.24
(1,285)	1:146:A:VAL:HG23	1:90:A:SER:HA	6	0.24
(1,242)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	8	0.24
(1,242)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	9	0.24
(1,235)	1:103:A:THR:HG21	1:124:A:TYR:HD2	5	0.24
(1,231)	1:104:A:SER:H	1:103:A:THR:HG23	2	0.24
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG21	7	0.24
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG21	8	0.24
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD23	10	0.24
(1,169)	1:12:A:VAL:HG23	1:75:A:THR:H	2	0.24
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	9	0.24
(1,24)	1:140:A:ALA:HB1	1:141:A:PHE:HD2	7	0.24
(1,3523)	1:31:A:VAL:H	1:56:A:LYS:HE3	4	0.23
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG22	6	0.23
(1,3493)	1:129:A:GLN:HE21	1:128:A:ASP:HB3	1	0.23
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	7	0.23
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	7	0.23
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	1	0.23
(1,3338)	1:156:A:PHE:H	1:155:A:GLN:HA	3	0.23
(1,3338)	1:156:A:PHE:H	1:156:A:PHE:HA	7	0.23
(1,3299)	1:37:A:ALA:H	1:35:A:GLN:HB3	3	0.23
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	2	0.23
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	10	0.23
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	2	0.23
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG13	10	0.23
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	8	0.23
(1,3156)	1:37:A:ALA:HA	1:9:A:LEU:HD22	4	0.23
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	9	0.23
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	2	0.23
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	3	0.23
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	2	0.23
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	10	0.23
(1,3097)	1:67:A:LEU:HD13	1:102:A:VAL:H	9	0.23
(1,3080)	1:10:A:SER:H	1:10:A:SER:HB3	5	0.23
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	5	0.23
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	8	0.23
(1,3023)	1:79:A:SER:HB3	1:156:A:PHE:HB2	9	0.23
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	8	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	5	0.23
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	6	0.23
(1,2942)	1:12:A:VAL:HG22	1:12:A:VAL:HB	4	0.23
(1,2903)	1:28:A:VAL:HB	1:57:A:MET:HA	4	0.23
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	5	0.23
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	9	0.23
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	6	0.23
(1,2881)	1:62:A:GLU:HG2	1:61:A:LYS:HA	4	0.23
(1,2878)	1:149:A:VAL:HB	1:126:A:GLU:H	8	0.23
(1,2835)	1:142:A:LYS:H	1:141:A:PHE:HB3	6	0.23
(1,2787)	1:6:A:LYS:HE3	1:6:A:LYS:HD2	6	0.23
(1,2757)	1:97:A:VAL:H	1:133:A:PHE:HB3	10	0.23
(1,2754)	1:136:A:ARG:HD3	1:120:A:GLU:HG3	2	0.23
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	7	0.23
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	6	0.23
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	5	0.23
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	9	0.23
(1,2672)	1:24:A:ILE:HD13	1:46:A:CYS:HB3	10	0.23
(1,2639)	1:114:A:ALA:HB2	1:156:A:PHE:HE2	5	0.23
(1,2627)	1:111:A:ALA:HB3	1:156:A:PHE:HD1	7	0.23
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	3	0.23
(1,2620)	1:36:A:CYS:HA	1:36:A:CYS:HB3	7	0.23
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB1	1	0.23
(1,2561)	1:89:A:VAL:HG22	1:91:A:TYR:HD1	7	0.23
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	3	0.23
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	7	0.23
(1,2532)	1:59:A:HIS:HD2	1:27:A:PRO:HG2	5	0.23
(1,2503)	1:85:A:PHE:HE2	1:107:A:ALA:HB1	10	0.23
(1,2402)	1:19:A:SER:H	1:19:A:SER:HB3	7	0.23
(1,2211)	1:17:A:LYS:H	1:73:A:GLY:HA2	4	0.23
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	5	0.23
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD21	9	0.23
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG11	2	0.23
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	8	0.23
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG11	1	0.23
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG23	5	0.23
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG23	6	0.23
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG21	7	0.23
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG23	9	0.23
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD23	4	0.23
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD21	5	0.23
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG12	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG12	5	0.23
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG11	6	0.23
(1,1627)	1:132:A:THR:HG22	1:100:A:ALA:HB2	10	0.23
(1,1577)	1:64:A:LYS:HE2	1:64:A:LYS:HG2	3	0.23
(1,1573)	1:65:A:PRO:HD2	1:64:A:LYS:HG3	3	0.23
(1,1573)	1:65:A:PRO:HD2	1:64:A:LYS:HG3	7	0.23
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	5	0.23
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	1	0.23
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	2	0.23
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	5	0.23
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	8	0.23
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	10	0.23
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	9	0.23
(1,1258)	1:86:A:GLU:HB2	1:151:A:SER:HB2	2	0.23
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	4	0.23
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	9	0.23
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG13	2	0.23
(1,1109)	1:28:A:VAL:HB	1:28:A:VAL:HG12	10	0.23
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	8	0.23
(1,982)	1:143:A:GLU:HG2	1:90:A:SER:HB3	1	0.23
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	1	0.23
(1,964)	1:67:A:LEU:HD21	1:17:A:LYS:HB2	10	0.23
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	1	0.23
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	6	0.23
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	10	0.23
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	8	0.23
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	8	0.23
(1,913)	1:131:A:CYS:H	1:130:A:LYS:HB2	7	0.23
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	2	0.23
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB3	5	0.23
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	9	0.23
(1,702)	1:61:A:LYS:HE2	1:19:A:SER:H	5	0.23
(1,680)	1:20:A:ARG:H	1:20:A:ARG:HD3	3	0.23
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG22	8	0.23
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	3	0.23
(1,494)	1:94:A:ALA:HB1	1:141:A:PHE:HD2	10	0.23
(1,456)	1:38:A:ALA:HB3	1:35:A:GLN:HG3	5	0.23
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG22	5	0.23
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG21	10	0.23
(1,412)	1:21:A:ALA:HB2	1:61:A:LYS:HA	4	0.23
(1,388)	1:112:A:ALA:HB1	1:65:A:PRO:HD3	8	0.23
(1,358)	1:115:A:ALA:HB2	1:116:A:ASP:HB2	3	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:75:A:THR:HG23	1:19:A:SER:HB2	10	0.23
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	4	0.23
(1,285)	1:146:A:VAL:HG23	1:90:A:SER:HA	4	0.23
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	8	0.23
(1,231)	1:104:A:SER:H	1:103:A:THR:HG23	9	0.23
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	5	0.23
(1,169)	1:12:A:VAL:HG21	1:75:A:THR:H	7	0.23
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	4	0.23
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	2	0.23
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	6	0.23
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	3	0.23
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	1	0.22
(1,3338)	1:156:A:PHE:H	1:155:A:GLN:HA	2	0.22
(1,3338)	1:156:A:PHE:H	1:155:A:GLN:HA	9	0.22
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	8	0.22
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	6	0.22
(1,3272)	1:43:A:VAL:H	1:41:A:LYS:HA	10	0.22
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	5	0.22
(1,3218)	1:28:A:VAL:H	1:29:A:PRO:HD2	4	0.22
(1,3202)	1:100:A:ALA:H	1:96:A:ASP:HB3	4	0.22
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	8	0.22
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	10	0.22
(1,3158)	1:9:A:LEU:HD22	1:9:A:LEU:HG	3	0.22
(1,3158)	1:9:A:LEU:HD22	1:9:A:LEU:HG	4	0.22
(1,3158)	1:9:A:LEU:HD23	1:9:A:LEU:HG	6	0.22
(1,3158)	1:9:A:LEU:HD21	1:9:A:LEU:HG	8	0.22
(1,3158)	1:9:A:LEU:HD22	1:9:A:LEU:HG	10	0.22
(1,3152)	1:71:A:THR:HB	1:70:A:LEU:HD11	6	0.22
(1,3145)	1:52:A:ASN:HB2	1:50:A:THR:HG23	6	0.22
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	10	0.22
(1,3118)	1:67:A:LEU:HG	1:67:A:LEU:HD13	9	0.22
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	8	0.22
(1,3095)	1:13:A:HIS:HB2	1:76:A:ALA:HB3	4	0.22
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	10	0.22
(1,3044)	1:88:A:HIS:HB2	1:87:A:GLN:HB2	10	0.22
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	2	0.22
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	5	0.22
(1,3027)	1:110:A:GLN:HB3	1:109:A:CYS:H	4	0.22
(1,3027)	1:110:A:GLN:HB3	1:109:A:CYS:H	6	0.22
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	2	0.22
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	9	0.22
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	4	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	6	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG13	1	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG12	2	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG12	5	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG13	6	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG12	7	0.22
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG13	10	0.22
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	8	0.22
(1,2904)	1:28:A:VAL:HB	1:31:A:VAL:HB	1	0.22
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	1	0.22
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	5	0.22
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	7	0.22
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	8	0.22
(1,2834)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	4	0.22
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	9	0.22
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	10	0.22
(1,2731)	1:45:A:GLY:HA2	1:44:A:ASP:HB3	3	0.22
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	4	0.22
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	7	0.22
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	6	0.22
(1,2672)	1:24:A:ILE:HD13	1:46:A:CYS:HB3	9	0.22
(1,2639)	1:114:A:ALA:HB3	1:156:A:PHE:HE2	2	0.22
(1,2627)	1:111:A:ALA:HB2	1:156:A:PHE:HD1	2	0.22
(1,2625)	1:112:A:ALA:HB1	1:109:A:CYS:HB3	7	0.22
(1,2600)	1:133:A:PHE:H	1:100:A:ALA:HB2	4	0.22
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB2	6	0.22
(1,2582)	1:97:A:VAL:HG11	1:135:A:GLY:HA2	2	0.22
(1,2582)	1:97:A:VAL:HG11	1:135:A:GLY:HA2	10	0.22
(1,2566)	1:103:A:THR:HG21	1:102:A:VAL:HA	6	0.22
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	6	0.22
(1,2506)	1:31:A:VAL:HG12	1:29:A:PRO:HA	9	0.22
(1,2402)	1:19:A:SER:H	1:19:A:SER:HB3	1	0.22
(1,2402)	1:19:A:SER:H	1:19:A:SER:HB3	2	0.22
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB3	3	0.22
(1,2061)	1:101:A:MET:H	1:101:A:MET:HG3	7	0.22
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	1	0.22
(1,1870)	1:7:A:LEU:H	1:7:A:LEU:HD21	5	0.22
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	6	0.22
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG21	8	0.22
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD23	1	0.22
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD23	8	0.22
(1,1627)	1:132:A:THR:HG23	1:100:A:ALA:HB2	4	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:132:A:THR:HG23	1:100:A:ALA:HB2	5	0.22
(1,1541)	1:76:A:ALA:HB1	1:51:A:TYR:HE2	1	0.22
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	1	0.22
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	6	0.22
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	9	0.22
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	3	0.22
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	4	0.22
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	6	0.22
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	7	0.22
(1,1387)	1:55:A:SER:HA	1:55:A:SER:HB2	9	0.22
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	5	0.22
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	1	0.22
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	9	0.22
(1,1227)	1:86:A:GLU:HB2	1:89:A:VAL:HG21	8	0.22
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	4	0.22
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	8	0.22
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	2	0.22
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	1	0.22
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	6	0.22
(1,982)	1:143:A:GLU:HG2	1:90:A:SER:HB3	2	0.22
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	2	0.22
(1,964)	1:67:A:LEU:HD23	1:17:A:LYS:HB2	3	0.22
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	6	0.22
(1,934)	1:72:A:GLY:H	1:16:A:ASN:HB2	3	0.22
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	8	0.22
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	2	0.22
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	5	0.22
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	9	0.22
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG11	8	0.22
(1,803)	1:68:A:TYR:HB2	1:68:A:TYR:HE2	4	0.22
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	3	0.22
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	7	0.22
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	10	0.22
(1,767)	1:40:A:CYS:HB3	1:60:A:VAL:HG13	1	0.22
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	5	0.22
(1,692)	1:97:A:VAL:HG23	1:133:A:PHE:HB2	8	0.22
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	5	0.22
(1,501)	1:94:A:ALA:HB3	1:121:A:ILE:HD12	3	0.22
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB3	1	0.22
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB1	3	0.22
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG23	9	0.22
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG22	10	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB2	3	0.22
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB2	8	0.22
(1,368)	1:42:A:ALA:H	1:42:A:ALA:HB3	1	0.22
(1,358)	1:115:A:ALA:HB3	1:116:A:ASP:HB2	6	0.22
(1,356)	1:115:A:ALA:HB3	1:116:A:ASP:HA	9	0.22
(1,242)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	5	0.22
(1,231)	1:104:A:SER:H	1:103:A:THR:HG22	7	0.22
(1,231)	1:104:A:SER:H	1:103:A:THR:HG21	10	0.22
(1,211)	1:146:A:VAL:HG11	1:149:A:VAL:H	1	0.22
(1,188)	1:67:A:LEU:HD21	1:75:A:THR:HG23	8	0.22
(1,169)	1:12:A:VAL:HG21	1:75:A:THR:H	3	0.22
(1,169)	1:12:A:VAL:HG23	1:75:A:THR:H	8	0.22
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	3	0.22
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	5	0.22
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	8	0.22
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	6	0.21
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	9	0.21
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	3	0.21
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	1	0.21
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	8	0.21
(1,3385)	1:16:A:ASN:HD22	1:16:A:ASN:H	4	0.21
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	9	0.21
(1,3350)	1:127:A:HIS:H	1:128:A:ASP:HB2	9	0.21
(1,3338)	1:156:A:PHE:H	1:155:A:GLN:HA	5	0.21
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	1	0.21
(1,3292)	1:36:A:CYS:H	1:37:A:ALA:HA	7	0.21
(1,3250)	1:91:A:TYR:H	1:92:A:GLU:HB2	2	0.21
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	2	0.21
(1,3161)	1:132:A:THR:HG22	1:100:A:ALA:HB2	1	0.21
(1,3158)	1:9:A:LEU:HD23	1:9:A:LEU:HG	1	0.21
(1,3158)	1:9:A:LEU:HD22	1:9:A:LEU:HG	2	0.21
(1,3158)	1:9:A:LEU:HD21	1:9:A:LEU:HG	7	0.21
(1,3158)	1:9:A:LEU:HD23	1:9:A:LEU:HG	9	0.21
(1,3127)	1:132:A:THR:HG21	1:92:A:GLU:HG2	3	0.21
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	9	0.21
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	5	0.21
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	8	0.21
(1,3101)	1:139:A:SER:H	1:139:A:SER:HB3	5	0.21
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	10	0.21
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG23	4	0.21
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	8	0.21
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	8	0.21
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	1	0.21
(1,2957)	1:86:A:GLU:HB2	1:151:A:SER:HB2	10	0.21
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG12	3	0.21
(1,2942)	1:12:A:VAL:HB	1:12:A:VAL:HG11	9	0.21
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	5	0.21
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	3	0.21
(1,2901)	1:129:A:GLN:HG3	1:126:A:GLU:HA	9	0.21
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	9	0.21
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	7	0.21
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	7	0.21
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	4	0.21
(1,2754)	1:136:A:ARG:HD3	1:120:A:GLU:HG3	5	0.21
(1,2716)	1:160:A:GLY:HA2	1:156:A:PHE:HD2	6	0.21
(1,2711)	1:161:A:GLY:HA2	1:155:A:GLN:HB2	9	0.21
(1,2710)	1:161:A:GLY:HA2	1:155:A:GLN:HG2	5	0.21
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	4	0.21
(1,2672)	1:24:A:ILE:HD11	1:46:A:CYS:HB3	6	0.21
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	6	0.21
(1,2643)	1:31:A:VAL:HG23	1:57:A:MET:HA	6	0.21
(1,2633)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	2	0.21
(1,2627)	1:111:A:ALA:HB1	1:156:A:PHE:HD1	10	0.21
(1,2580)	1:13:A:HIS:HA	1:12:A:VAL:HG22	3	0.21
(1,2549)	1:67:A:LEU:HD22	1:17:A:LYS:HE3	6	0.21
(1,2402)	1:19:A:SER:H	1:19:A:SER:HB3	6	0.21
(1,2383)	1:129:A:GLN:HE22	1:104:A:SER:HB3	4	0.21
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	4	0.21
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	9	0.21
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG22	7	0.21
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	6	0.21
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG23	6	0.21
(1,1963)	1:119:A:CYS:H	1:97:A:VAL:HG23	10	0.21
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD23	6	0.21
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	10	0.21
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD21	2	0.21
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD23	6	0.21
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD21	7	0.21
(1,1669)	1:147:A:LEU:H	1:147:A:LEU:HD21	9	0.21
(1,1654)	1:40:A:CYS:H	1:60:A:VAL:HG12	8	0.21
(1,1627)	1:132:A:THR:HG21	1:100:A:ALA:HB3	9	0.21
(1,1625)	1:132:A:THR:H	1:132:A:THR:HG22	5	0.21
(1,1544)	1:12:A:VAL:HB	1:76:A:ALA:HB2	3	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB3	10	0.21
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	2	0.21
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	10	0.21
(1,1496)	1:70:A:LEU:HG	1:17:A:LYS:HA	10	0.21
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	2	0.21
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	2	0.21
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	2	0.21
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	2	0.21
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	10	0.21
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	4	0.21
(1,937)	1:17:A:LYS:H	1:16:A:ASN:HB2	3	0.21
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	7	0.21
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	7	0.21
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	9	0.21
(1,826)	1:128:A:ASP:HB2	1:125:A:ASN:HB2	9	0.21
(1,761)	1:64:A:LYS:HE3	1:115:A:ALA:HB1	7	0.21
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	1	0.21
(1,709)	1:144:A:ARG:HD2	1:144:A:ARG:HG3	1	0.21
(1,709)	1:144:A:ARG:HD3	1:144:A:ARG:HG3	10	0.21
(1,692)	1:97:A:VAL:HG23	1:133:A:PHE:HB2	9	0.21
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	10	0.21
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG22	3	0.21
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG21	5	0.21
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	2	0.21
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB1	4	0.21
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB2	7	0.21
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG23	4	0.21
(1,420)	1:111:A:ALA:HB1	1:65:A:PRO:HG2	2	0.21
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB1	1	0.21
(1,358)	1:115:A:ALA:HB1	1:116:A:ASP:HB2	1	0.21
(1,356)	1:115:A:ALA:HB1	1:116:A:ASP:HA	7	0.21
(1,332)	1:125:A:ASN:HD21	1:149:A:VAL:HG21	8	0.21
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG23	3	0.21
(1,305)	1:75:A:THR:HG22	1:19:A:SER:HB2	3	0.21
(1,305)	1:75:A:THR:HG23	1:19:A:SER:HB2	4	0.21
(1,304)	1:75:A:THR:H	1:75:A:THR:HG22	4	0.21
(1,290)	1:102:A:VAL:HG22	1:131:A:CYS:H	7	0.21
(1,242)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	7	0.21
(1,240)	1:28:A:VAL:HG12	1:29:A:PRO:HD2	1	0.21
(1,235)	1:103:A:THR:HG23	1:124:A:TYR:HD2	4	0.21
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	9	0.21
(1,176)	1:31:A:VAL:HG11	1:58:A:CYS:HB2	7	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,169)	1:12:A:VAL:HG23	1:75:A:THR:H	4	0.21
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	7	0.2
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	3	0.2
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	7	0.2
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	4	0.2
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	4	0.2
(1,3335)	1:136:A:ARG:H	1:136:A:ARG:HD3	8	0.2
(1,3302)	1:142:A:LYS:H	1:140:A:ALA:H	9	0.2
(1,3290)	1:36:A:CYS:H	1:51:A:TYR:HD1	4	0.2
(1,3280)	1:103:A:THR:H	1:129:A:GLN:HB2	2	0.2
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	2	0.2
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	2	0.2
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	2	0.2
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG11	8	0.2
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	6	0.2
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	9	0.2
(1,3164)	1:75:A:THR:HG22	1:19:A:SER:HA	1	0.2
(1,3158)	1:9:A:LEU:HD21	1:9:A:LEU:HG	5	0.2
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	7	0.2
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	6	0.2
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	7	0.2
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	5	0.2
(1,3030)	1:111:A:ALA:H	1:110:A:GLN:HB2	10	0.2
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	8	0.2
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	8	0.2
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	5	0.2
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	8	0.2
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	9	0.2
(1,2928)	1:39:A:GLN:HG2	1:36:A:CYS:HA	9	0.2
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	4	0.2
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	5	0.2
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	9	0.2
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	9	0.2
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	7	0.2
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	8	0.2
(1,2882)	1:98:A:MET:HB2	1:99:A:THR:HA	10	0.2
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	1	0.2
(1,2862)	1:34:A:GLU:HG3	1:7:A:LEU:HD13	10	0.2
(1,2844)	1:156:A:PHE:HB3	1:159:A:GLU:HB3	5	0.2
(1,2803)	1:66:A:ASP:HB2	1:20:A:ARG:HB2	1	0.2
(1,2793)	1:64:A:LYS:HE2	1:117:A:PRO:HD3	4	0.2
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	1	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	6	0.2
(1,2735)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	10	0.2
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	6	0.2
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	8	0.2
(1,2672)	1:24:A:ILE:HD12	1:46:A:CYS:HB3	1	0.2
(1,2672)	1:24:A:ILE:HD11	1:46:A:CYS:HB3	2	0.2
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	4	0.2
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	10	0.2
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	9	0.2
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	4	0.2
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	6	0.2
(1,2633)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	6	0.2
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	2	0.2
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	3	0.2
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB2	8	0.2
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB2	10	0.2
(1,2625)	1:112:A:ALA:HB1	1:109:A:CYS:HB3	1	0.2
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	1	0.2
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	1	0.2
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	9	0.2
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB2	9	0.2
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG22	6	0.2
(1,2546)	1:150:A:THR:HG21	1:106:A:SER:HB2	7	0.2
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	4	0.2
(1,2542)	1:92:A:GLU:HA	1:134:A:LYS:HG3	8	0.2
(1,2485)	1:91:A:TYR:HD1	1:91:A:TYR:HE1	1	0.2
(1,2485)	1:91:A:TYR:HD2	1:91:A:TYR:HE2	2	0.2
(1,2485)	1:91:A:TYR:HD1	1:91:A:TYR:HE1	3	0.2
(1,2485)	1:91:A:TYR:HD1	1:91:A:TYR:HE1	4	0.2
(1,2485)	1:91:A:TYR:HD2	1:91:A:TYR:HE2	5	0.2
(1,2485)	1:68:A:TYR:HD2	1:68:A:TYR:HE2	6	0.2
(1,2485)	1:91:A:TYR:HD1	1:91:A:TYR:HE1	7	0.2
(1,2485)	1:91:A:TYR:HD2	1:91:A:TYR:HE2	8	0.2
(1,2485)	1:68:A:TYR:HD1	1:68:A:TYR:HE1	9	0.2
(1,2485)	1:91:A:TYR:HD1	1:91:A:TYR:HE1	10	0.2
(1,2211)	1:17:A:LYS:H	1:73:A:GLY:HA2	8	0.2
(1,2146)	1:154:A:LYS:H	1:121:A:ILE:HG22	1	0.2
(1,2146)	1:154:A:LYS:H	1:121:A:ILE:HG23	3	0.2
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	8	0.2
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG21	9	0.2
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD23	10	0.2
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	6	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1956)	1:103:A:THR:H	1:102:A:VAL:HG13	1	0.2
(1,1627)	1:132:A:THR:HG22	1:100:A:ALA:HB1	2	0.2
(1,1627)	1:132:A:THR:HG23	1:100:A:ALA:HB1	7	0.2
(1,1626)	1:130:A:LYS:HE2	1:132:A:THR:HG22	4	0.2
(1,1606)	1:33:A:LEU:HD21	1:12:A:VAL:HB	3	0.2
(1,1605)	1:33:A:LEU:HD22	1:74:A:LYS:HB3	6	0.2
(1,1429)	1:136:A:ARG:HA	1:136:A:ARG:HG3	10	0.2
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	7	0.2
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	7	0.2
(1,1258)	1:86:A:GLU:HB2	1:151:A:SER:HB2	10	0.2
(1,1253)	1:67:A:LEU:HD23	1:65:A:PRO:HB2	4	0.2
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	10	0.2
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	5	0.2
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	7	0.2
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	5	0.2
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	1	0.2
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	5	0.2
(1,794)	1:124:A:TYR:HB2	1:125:A:ASN:H	6	0.2
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	10	0.2
(1,651)	1:97:A:VAL:HG22	1:135:A:GLY:HA2	6	0.2
(1,483)	1:37:A:ALA:HA	1:9:A:LEU:HD23	8	0.2
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG21	3	0.2
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG21	6	0.2
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG23	3	0.2
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG23	7	0.2
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG21	8	0.2
(1,424)	1:32:A:SER:H	1:31:A:VAL:HG23	4	0.2
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG21	7	0.2
(1,420)	1:111:A:ALA:HB1	1:65:A:PRO:HG2	8	0.2
(1,419)	1:111:A:ALA:HB1	1:156:A:PHE:HZ	5	0.2
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB3	9	0.2
(1,358)	1:115:A:ALA:HB3	1:116:A:ASP:HB2	4	0.2
(1,357)	1:115:A:ALA:HB2	1:115:A:ALA:HA	4	0.2
(1,356)	1:115:A:ALA:HB1	1:116:A:ASP:HA	2	0.2
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG23	8	0.2
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG23	3	0.2
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG22	8	0.2
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG22	9	0.2
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	7	0.2
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG23	1	0.2
(1,174)	1:31:A:VAL:HG12	1:31:A:VAL:HA	6	0.2
(1,169)	1:12:A:VAL:HG21	1:75:A:THR:H	1	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB3	3	0.2
(1,119)	1:52:A:ASN:HA	1:50:A:THR:HG23	6	0.2
(1,81)	1:91:A:TYR:HA	1:91:A:TYR:HD2	8	0.2
(1,3533)	1:161:A:GLY:H	1:155:A:GLN:HG3	2	0.19
(1,3523)	1:31:A:VAL:H	1:30:A:ASP:HB3	6	0.19
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG23	3	0.19
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	1	0.19
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	2	0.19
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	4	0.19
(1,3424)	1:54:A:ASP:H	1:57:A:MET:HG2	8	0.19
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG2	6	0.19
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	1	0.19
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	5	0.19
(1,3370)	1:46:A:CYS:H	1:44:A:ASP:HB3	5	0.19
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	6	0.19
(1,3345)	1:150:A:THR:H	1:87:A:GLN:HG2	3	0.19
(1,3345)	1:150:A:THR:H	1:87:A:GLN:HG2	9	0.19
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	1	0.19
(1,3338)	1:156:A:PHE:H	1:155:A:GLN:HA	4	0.19
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	6	0.19
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	5	0.19
(1,3235)	1:61:A:LYS:H	1:60:A:VAL:HG13	1	0.19
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	4	0.19
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	1	0.19
(1,3204)	1:100:A:ALA:H	1:132:A:THR:HG22	8	0.19
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	1	0.19
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	6	0.19
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	3	0.19
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	6	0.19
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG13	4	0.19
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG11	7	0.19
(1,3161)	1:100:A:ALA:HB3	1:130:A:LYS:HG2	5	0.19
(1,3152)	1:71:A:THR:HB	1:70:A:LEU:HD12	1	0.19
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	6	0.19
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	4	0.19
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	4	0.19
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	9	0.19
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	3	0.19
(1,3080)	1:10:A:SER:H	1:10:A:SER:HB3	2	0.19
(1,3080)	1:10:A:SER:H	1:10:A:SER:HB3	4	0.19
(1,3080)	1:10:A:SER:H	1:10:A:SER:HB3	10	0.19
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	2	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	4	0.19
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	6	0.19
(1,3015)	1:33:A:LEU:H	1:34:A:GLU:HB2	6	0.19
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	9	0.19
(1,2977)	1:26:A:GLU:HB3	1:26:A:GLU:H	1	0.19
(1,2910)	1:88:A:HIS:H	1:87:A:GLN:HG2	1	0.19
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	4	0.19
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	2	0.19
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	8	0.19
(1,2879)	1:150:A:THR:HB	1:85:A:PHE:HD2	10	0.19
(1,2877)	1:61:A:LYS:HB3	1:21:A:ALA:HA	10	0.19
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	10	0.19
(1,2803)	1:66:A:ASP:HB2	1:20:A:ARG:HB2	3	0.19
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HG3	5	0.19
(1,2794)	1:64:A:LYS:HE3	1:64:A:LYS:HG3	7	0.19
(1,2784)	1:101:A:MET:H	1:131:A:CYS:HB3	8	0.19
(1,2766)	1:133:A:PHE:HB2	1:134:A:LYS:HA	6	0.19
(1,2765)	1:133:A:PHE:HB2	1:97:A:VAL:H	1	0.19
(1,2765)	1:54:A:ASP:H	1:53:A:ASP:HB3	2	0.19
(1,2765)	1:54:A:ASP:H	1:53:A:ASP:HB3	3	0.19
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	5	0.19
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	10	0.19
(1,2760)	1:18:A:GLY:HA2	1:75:A:THR:HA	3	0.19
(1,2731)	1:45:A:GLY:HA2	1:44:A:ASP:HB3	9	0.19
(1,2725)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	6	0.19
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	4	0.19
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	8	0.19
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	9	0.19
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	4	0.19
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	1	0.19
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	2	0.19
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	8	0.19
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	7	0.19
(1,2625)	1:112:A:ALA:HB1	1:109:A:CYS:HB3	5	0.19
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	2	0.19
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	10	0.19
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	6	0.19
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB2	4	0.19
(1,2506)	1:31:A:VAL:HG11	1:29:A:PRO:HA	5	0.19
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	1	0.19
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG23	5	0.19
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG23	7	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:119:A:CYS:H	1:97:A:VAL:HG12	1	0.19
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	9	0.19
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	9	0.19
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	9	0.19
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG12	4	0.19
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG23	4	0.19
(1,1674)	1:28:A:VAL:HG13	1:28:A:VAL:HA	10	0.19
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD23	1	0.19
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD21	2	0.19
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD23	6	0.19
(1,1627)	1:132:A:THR:HG23	1:100:A:ALA:HB2	3	0.19
(1,1627)	1:132:A:THR:HG21	1:100:A:ALA:HB2	6	0.19
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	2	0.19
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	3	0.19
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	4	0.19
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	5	0.19
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	8	0.19
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB1	1	0.19
(1,1536)	1:61:A:LYS:HG3	1:21:A:ALA:HB1	9	0.19
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD12	9	0.19
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	2	0.19
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	8	0.19
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	10	0.19
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	1	0.19
(1,1292)	1:32:A:SER:HB2	1:35:A:GLN:HB3	2	0.19
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	8	0.19
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	1	0.19
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	3	0.19
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	5	0.19
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	7	0.19
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	8	0.19
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	10	0.19
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	6	0.19
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	10	0.19
(1,1062)	1:35:A:GLN:HG2	1:31:A:VAL:HA	7	0.19
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	1	0.19
(1,994)	1:61:A:LYS:HE3	1:50:A:THR:HB	3	0.19
(1,974)	1:86:A:GLU:H	1:85:A:PHE:HB2	9	0.19
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG13	4	0.19
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB2	2	0.19
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB2	7	0.19
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	8	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,747)	1:142:A:LYS:HE2	1:89:A:VAL:HG22	10	0.19
(1,742)	1:37:A:ALA:HB3	1:41:A:LYS:HE2	1	0.19
(1,742)	1:37:A:ALA:HB3	1:41:A:LYS:HE3	8	0.19
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	7	0.19
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	2	0.19
(1,492)	1:141:A:PHE:H	1:94:A:ALA:HB3	5	0.19
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG23	5	0.19
(1,401)	1:37:A:ALA:HB3	1:51:A:TYR:HE1	4	0.19
(1,401)	1:37:A:ALA:HB1	1:51:A:TYR:HE1	6	0.19
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB2	1	0.19
(1,388)	1:112:A:ALA:HB2	1:65:A:PRO:HD3	1	0.19
(1,388)	1:112:A:ALA:HB3	1:65:A:PRO:HD3	4	0.19
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB1	2	0.19
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB3	6	0.19
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB1	7	0.19
(1,357)	1:115:A:ALA:HB3	1:115:A:ALA:HA	2	0.19
(1,357)	1:115:A:ALA:HB3	1:115:A:ALA:HA	7	0.19
(1,357)	1:115:A:ALA:HB2	1:115:A:ALA:HA	10	0.19
(1,342)	1:149:A:VAL:HG22	1:123:A:THR:HG23	3	0.19
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG22	8	0.19
(1,327)	1:101:A:MET:H	1:100:A:ALA:HB1	8	0.19
(1,277)	1:143:A:GLU:H	1:146:A:VAL:HG23	4	0.19
(1,211)	1:146:A:VAL:HG12	1:149:A:VAL:H	4	0.19
(1,211)	1:146:A:VAL:HG12	1:149:A:VAL:H	10	0.19
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG22	1	0.19
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG21	2	0.19
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG21	7	0.19
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	10	0.19
(1,24)	1:140:A:ALA:HB1	1:141:A:PHE:HD2	8	0.19
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	6	0.19
(1,10)	1:133:A:PHE:HD2	1:112:A:ALA:HB1	10	0.19
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	10	0.18
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	2	0.18
(1,3422)	1:54:A:ASP:H	1:72:A:GLY:HA2	1	0.18
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	5	0.18
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	8	0.18
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	9	0.18
(1,3296)	1:151:A:SER:H	1:86:A:GLU:HB3	2	0.18
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	4	0.18
(1,3284)	1:119:A:CYS:H	1:117:A:PRO:HG2	9	0.18
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB3	7	0.18
(1,3240)	1:107:A:ALA:H	1:11:A:CYS:HB2	5	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	3	0.18
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	3	0.18
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	9	0.18
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	10	0.18
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG12	3	0.18
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG12	6	0.18
(1,3152)	1:71:A:THR:HB	1:70:A:LEU:HD11	5	0.18
(1,3141)	1:106:A:SER:HA	1:105:A:GLN:HB2	5	0.18
(1,3134)	1:27:A:PRO:HD3	1:23:A:THR:HG21	2	0.18
(1,3130)	1:60:A:VAL:H	1:23:A:THR:HG22	5	0.18
(1,3110)	1:56:A:LYS:HG2	1:56:A:LYS:H	2	0.18
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	2	0.18
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	2	0.18
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD11	3	0.18
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD12	9	0.18
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	4	0.18
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	1	0.18
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	7	0.18
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	9	0.18
(1,3046)	1:65:A:PRO:HG3	1:108:A:ASP:HA	3	0.18
(1,3041)	1:118:A:SER:HB3	1:117:A:PRO:HG2	9	0.18
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	10	0.18
(1,3027)	1:110:A:GLN:HB3	1:156:A:PHE:HD1	2	0.18
(1,3023)	1:79:A:SER:HB3	1:156:A:PHE:HB2	3	0.18
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	6	0.18
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	7	0.18
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	2	0.18
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	4	0.18
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	4	0.18
(1,2963)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	8	0.18
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	5	0.18
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	5	0.18
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	4	0.18
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	8	0.18
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	1	0.18
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	6	0.18
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	7	0.18
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	1	0.18
(1,2847)	1:91:A:TYR:HB2	1:138:A:PHE:HB3	3	0.18
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HG3	8	0.18
(1,2765)	1:54:A:ASP:H	1:53:A:ASP:HB3	8	0.18
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	9	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2754)	1:136:A:ARG:HD3	1:120:A:GLU:HG3	7	0.18
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	5	0.18
(1,2730)	1:45:A:GLY:HA3	1:44:A:ASP:HB3	3	0.18
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	3	0.18
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	6	0.18
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	9	0.18
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	7	0.18
(1,2625)	1:112:A:ALA:HB2	1:109:A:CYS:HB3	4	0.18
(1,2625)	1:112:A:ALA:HB2	1:109:A:CYS:HB3	9	0.18
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	1	0.18
(1,2558)	1:149:A:VAL:HG11	1:126:A:GLU:H	8	0.18
(1,2524)	1:48:A:HIS:HA	1:49:A:PHE:HD1	4	0.18
(1,2510)	1:47:A:THR:HG21	1:156:A:PHE:HE2	8	0.18
(1,2311)	1:112:A:ALA:H	1:65:A:PRO:HD2	6	0.18
(1,2269)	1:141:A:PHE:H	1:142:A:LYS:HB3	4	0.18
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG21	4	0.18
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	7	0.18
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG22	2	0.18
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG23	3	0.18
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB1	4	0.18
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG21	8	0.18
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	3	0.18
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	4	0.18
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	7	0.18
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	2	0.18
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	2	0.18
(1,1767)	1:82:A:ARG:H	1:82:A:ARG:HB3	9	0.18
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG21	1	0.18
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG22	4	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD23	4	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD21	5	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD21	7	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD23	8	0.18
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD21	9	0.18
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD21	9	0.18
(1,1606)	1:33:A:LEU:HD22	1:12:A:VAL:HB	6	0.18
(1,1605)	1:33:A:LEU:HD21	1:74:A:LYS:HB3	3	0.18
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	6	0.18
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	10	0.18
(1,1555)	1:67:A:LEU:HD23	1:67:A:LEU:HD12	7	0.18
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	6	0.18
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	10	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	1	0.18
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	8	0.18
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	1	0.18
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	10	0.18
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	8	0.18
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	9	0.18
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	6	0.18
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	7	0.18
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	8	0.18
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	9	0.18
(1,1268)	1:20:A:ARG:HB3	1:68:A:TYR:HE1	9	0.18
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	3	0.18
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	6	0.18
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	5	0.18
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	2	0.18
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	4	0.18
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	6	0.18
(1,1212)	1:27:A:PRO:HB2	1:27:A:PRO:HA	9	0.18
(1,1062)	1:35:A:GLN:HG2	1:31:A:VAL:HA	1	0.18
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	5	0.18
(1,982)	1:143:A:GLU:HG2	1:90:A:SER:HB3	6	0.18
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	3	0.18
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	5	0.18
(1,860)	1:30:A:ASP:HB3	1:31:A:VAL:HG12	3	0.18
(1,821)	1:52:A:ASN:HB3	1:51:A:TYR:HA	4	0.18
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	9	0.18
(1,741)	1:41:A:LYS:HE3	1:38:A:ALA:HA	8	0.18
(1,739)	1:131:A:CYS:HB2	1:100:A:ALA:HB2	7	0.18
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	2	0.18
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	7	0.18
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	1	0.18
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	8	0.18
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	8	0.18
(1,489)	1:24:A:ILE:HG21	1:24:A:ILE:HB	1	0.18
(1,489)	1:24:A:ILE:HG22	1:24:A:ILE:HB	9	0.18
(1,420)	1:111:A:ALA:HB1	1:65:A:PRO:HG2	3	0.18
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB3	10	0.18
(1,363)	1:108:A:ASP:HA	1:77:A:SER:HB3	1	0.18
(1,357)	1:115:A:ALA:HB3	1:115:A:ALA:HA	1	0.18
(1,357)	1:115:A:ALA:HB1	1:115:A:ALA:HA	3	0.18
(1,357)	1:115:A:ALA:HB2	1:115:A:ALA:HA	6	0.18
(1,357)	1:115:A:ALA:HB2	1:115:A:ALA:HA	9	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:101:A:MET:H	1:100:A:ALA:HB3	10	0.18
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG22	7	0.18
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG21	1	0.18
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG21	7	0.18
(1,235)	1:103:A:THR:HG22	1:124:A:TYR:HD2	7	0.18
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	6	0.18
(1,221)	1:89:A:VAL:HG23	1:144:A:ARG:HG3	9	0.18
(1,211)	1:146:A:VAL:HG11	1:149:A:VAL:H	2	0.18
(1,211)	1:146:A:VAL:HG12	1:149:A:VAL:H	5	0.18
(1,211)	1:146:A:VAL:HG13	1:149:A:VAL:H	6	0.18
(1,211)	1:146:A:VAL:HG11	1:149:A:VAL:H	9	0.18
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG23	8	0.18
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	2	0.18
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	3	0.18
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	7	0.18
(1,169)	1:12:A:VAL:HG21	1:75:A:THR:H	5	0.18
(1,169)	1:12:A:VAL:HG21	1:75:A:THR:H	10	0.18
(1,41)	1:50:A:THR:HG22	1:75:A:THR:HA	6	0.18
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	1	0.17
(1,3470)	1:125:A:ASN:HD22	1:130:A:LYS:HE3	1	0.17
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	9	0.17
(1,3464)	1:110:A:GLN:HE22	1:79:A:SER:H	2	0.17
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	5	0.17
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	2	0.17
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG2	7	0.17
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	6	0.17
(1,3335)	1:136:A:ARG:H	1:136:A:ARG:HD3	6	0.17
(1,3307)	1:111:A:ALA:H	1:109:A:CYS:H	1	0.17
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB3	10	0.17
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	9	0.17
(1,3202)	1:100:A:ALA:H	1:96:A:ASP:HB3	1	0.17
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	7	0.17
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD21	2	0.17
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD23	5	0.17
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD22	6	0.17
(1,3145)	1:52:A:ASN:HB2	1:50:A:THR:HG23	3	0.17
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	6	0.17
(1,3097)	1:67:A:LEU:HD11	1:102:A:VAL:H	2	0.17
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD11	2	0.17
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD11	6	0.17
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	6	0.17
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	7	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:10:A:SER:H	1:10:A:SER:HB3	8	0.17
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	3	0.17
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	6	0.17
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	3	0.17
(1,3046)	1:65:A:PRO:HG3	1:108:A:ASP:HA	2	0.17
(1,3041)	1:118:A:SER:HB2	1:117:A:PRO:HG2	7	0.17
(1,3027)	1:110:A:GLN:HB3	1:109:A:CYS:H	9	0.17
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	6	0.17
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	2	0.17
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	4	0.17
(1,2944)	1:101:A:MET:HG3	1:65:A:PRO:HB2	7	0.17
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	10	0.17
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	1	0.17
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	2	0.17
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	3	0.17
(1,2901)	1:22:A:PRO:HD3	1:62:A:GLU:HG3	8	0.17
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	7	0.17
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	1	0.17
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	2	0.17
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	3	0.17
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	5	0.17
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	10	0.17
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	2	0.17
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HG3	3	0.17
(1,2725)	1:160:A:GLY:HA3	1:159:A:GLU:HB2	4	0.17
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	7	0.17
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	5	0.17
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	3	0.17
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	5	0.17
(1,2664)	1:94:A:ALA:HB3	1:95:A:PRO:HD2	8	0.17
(1,2633)	1:107:A:ALA:HB2	1:108:A:ASP:HB2	5	0.17
(1,2633)	1:107:A:ALA:HB1	1:108:A:ASP:HB2	8	0.17
(1,2633)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	9	0.17
(1,2633)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	10	0.17
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	1	0.17
(1,2625)	1:112:A:ALA:HB2	1:109:A:CYS:HB3	6	0.17
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	7	0.17
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	8	0.17
(1,2599)	1:113:A:CYS:HA	1:112:A:ALA:HB1	5	0.17
(1,2588)	1:75:A:THR:HG21	1:76:A:ALA:HA	1	0.17
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	7	0.17
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	4	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2546)	1:150:A:THR:HG21	1:106:A:SER:HB2	5	0.17
(1,2531)	1:75:A:THR:HG23	1:13:A:HIS:HD2	2	0.17
(1,2527)	1:17:A:LYS:HD2	1:17:A:LYS:HA	6	0.17
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	10	0.17
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	8	0.17
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	10	0.17
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG21	9	0.17
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG22	6	0.17
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG22	9	0.17
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG22	3	0.17
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	5	0.17
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	8	0.17
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG22	8	0.17
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	2	0.17
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	4	0.17
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD21	3	0.17
(1,1671)	1:147:A:LEU:HG	1:147:A:LEU:HD22	10	0.17
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD23	4	0.17
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD21	7	0.17
(1,1577)	1:64:A:LYS:HE3	1:64:A:LYS:HG2	4	0.17
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	7	0.17
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	7	0.17
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	5	0.17
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	5	0.17
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	10	0.17
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD12	2	0.17
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD12	3	0.17
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD11	4	0.17
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	1	0.17
(1,1392)	1:19:A:SER:HB2	1:21:A:ALA:HB3	4	0.17
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	1	0.17
(1,1252)	1:65:A:PRO:HB2	1:67:A:LEU:HD13	1	0.17
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	9	0.17
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	3	0.17
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	9	0.17
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	3	0.17
(1,1000)	1:112:A:ALA:HB2	1:109:A:CYS:HB2	4	0.17
(1,982)	1:143:A:GLU:HG2	1:90:A:SER:HB3	10	0.17
(1,930)	1:16:A:ASN:HB3	1:16:A:ASN:HD21	3	0.17
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	8	0.17
(1,899)	1:16:A:ASN:H	1:15:A:ASP:HB3	8	0.17
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB3	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	1	0.17
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	2	0.17
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	10	0.17
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	8	0.17
(1,733)	1:132:A:THR:H	1:131:A:CYS:HB2	2	0.17
(1,733)	1:132:A:THR:H	1:131:A:CYS:HB2	10	0.17
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	3	0.17
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	6	0.17
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	8	0.17
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	10	0.17
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	2	0.17
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	6	0.17
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	5	0.17
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	9	0.17
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG23	10	0.17
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	6	0.17
(1,489)	1:24:A:ILE:HG21	1:24:A:ILE:HB	2	0.17
(1,489)	1:24:A:ILE:HG21	1:24:A:ILE:HB	5	0.17
(1,489)	1:24:A:ILE:HG22	1:24:A:ILE:HB	6	0.17
(1,489)	1:24:A:ILE:HG21	1:24:A:ILE:HB	7	0.17
(1,489)	1:24:A:ILE:HG23	1:24:A:ILE:HB	10	0.17
(1,401)	1:37:A:ALA:HB2	1:51:A:TYR:HE1	1	0.17
(1,401)	1:37:A:ALA:HB2	1:51:A:TYR:HE1	2	0.17
(1,401)	1:37:A:ALA:HB1	1:51:A:TYR:HE1	5	0.17
(1,401)	1:37:A:ALA:HB2	1:51:A:TYR:HE1	8	0.17
(1,401)	1:37:A:ALA:HB2	1:51:A:TYR:HE1	10	0.17
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB3	4	0.17
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB1	5	0.17
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB1	6	0.17
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB1	9	0.17
(1,358)	1:115:A:ALA:HB3	1:116:A:ASP:HB2	9	0.17
(1,357)	1:115:A:ALA:HB3	1:115:A:ALA:HA	5	0.17
(1,357)	1:115:A:ALA:HB1	1:115:A:ALA:HA	8	0.17
(1,356)	1:115:A:ALA:HB1	1:116:A:ASP:HA	5	0.17
(1,330)	1:150:A:THR:H	1:149:A:VAL:HG22	10	0.17
(1,261)	1:105:A:GLN:HE22	1:13:A:HIS:HA	4	0.17
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG23	10	0.17
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	2	0.17
(1,211)	1:146:A:VAL:HG11	1:149:A:VAL:H	7	0.17
(1,211)	1:146:A:VAL:HG12	1:149:A:VAL:H	8	0.17
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG23	4	0.17
(1,188)	1:67:A:LEU:HD22	1:75:A:THR:HG23	10	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:19:A:SER:H	1:67:A:LEU:HD22	3	0.17
(1,174)	1:31:A:VAL:HG11	1:31:A:VAL:HA	4	0.17
(1,174)	1:31:A:VAL:HG12	1:31:A:VAL:HA	5	0.17
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	8	0.17
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	9	0.17
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	1	0.17
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	10	0.17
(1,41)	1:50:A:THR:HG21	1:75:A:THR:HA	2	0.17
(1,3543)	1:79:A:SER:H	1:77:A:SER:HB3	5	0.16
(1,3476)	1:149:A:VAL:H	1:88:A:HIS:HB3	8	0.16
(1,3471)	1:57:A:MET:H	1:56:A:LYS:HG2	3	0.16
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	4	0.16
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	9	0.16
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	7	0.16
(1,3423)	1:54:A:ASP:H	1:52:A:ASN:HB2	7	0.16
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	5	0.16
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	6	0.16
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG2	1	0.16
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	1	0.16
(1,3296)	1:151:A:SER:H	1:86:A:GLU:HB3	6	0.16
(1,3280)	1:103:A:THR:H	1:129:A:GLN:HB2	9	0.16
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	1	0.16
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	8	0.16
(1,3208)	1:70:A:LEU:H	1:16:A:ASN:HB3	9	0.16
(1,3205)	1:131:A:CYS:H	1:103:A:THR:H	10	0.16
(1,3187)	1:76:A:ALA:H	1:48:A:HIS:HB3	2	0.16
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	1	0.16
(1,3161)	1:100:A:ALA:HB3	1:130:A:LYS:HG2	3	0.16
(1,3147)	1:155:A:GLN:HB3	1:156:A:PHE:HA	10	0.16
(1,3110)	1:56:A:LYS:HG2	1:56:A:LYS:H	7	0.16
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	7	0.16
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD11	7	0.16
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD13	8	0.16
(1,3080)	1:11:A:CYS:H	1:10:A:SER:HB3	6	0.16
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	4	0.16
(1,3021)	1:105:A:GLN:HB3	1:108:A:ASP:H	6	0.16
(1,3000)	1:87:A:GLN:HB3	1:88:A:HIS:HA	5	0.16
(1,2998)	1:32:A:SER:H	1:35:A:GLN:HB2	1	0.16
(1,2986)	1:131:A:CYS:H	1:130:A:LYS:HD2	7	0.16
(1,2977)	1:26:A:GLU:HB3	1:26:A:GLU:H	4	0.16
(1,2916)	1:134:A:LYS:HB3	1:121:A:ILE:H	6	0.16
(1,2916)	1:134:A:LYS:HB3	1:138:A:PHE:H	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	6	0.16
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	7	0.16
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	4	0.16
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	5	0.16
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	7	0.16
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	3	0.16
(1,2866)	1:159:A:GLU:H	1:159:A:GLU:HG3	9	0.16
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	3	0.16
(1,2804)	1:66:A:ASP:HB2	1:20:A:ARG:HG3	3	0.16
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HG3	2	0.16
(1,2765)	1:133:A:PHE:HB2	1:97:A:VAL:H	10	0.16
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	2	0.16
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	6	0.16
(1,2751)	1:18:A:GLY:HA3	1:50:A:THR:HG21	6	0.16
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	1	0.16
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	10	0.16
(1,2735)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	2	0.16
(1,2735)	1:43:A:VAL:HG22	1:46:A:CYS:HB2	3	0.16
(1,2735)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	6	0.16
(1,2725)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	7	0.16
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	1	0.16
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	2	0.16
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	3	0.16
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	7	0.16
(1,2672)	1:24:A:ILE:HD11	1:46:A:CYS:HB3	7	0.16
(1,2668)	1:42:A:ALA:H	1:42:A:ALA:HA	9	0.16
(1,2664)	1:94:A:ALA:HB2	1:95:A:PRO:HD2	4	0.16
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB2	3	0.16
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB1	8	0.16
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	4	0.16
(1,2625)	1:112:A:ALA:HB3	1:109:A:CYS:HB3	8	0.16
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	3	0.16
(1,2572)	1:35:A:GLN:HA	1:35:A:GLN:HG3	6	0.16
(1,2510)	1:114:A:ALA:HB1	1:156:A:PHE:HE2	7	0.16
(1,2506)	1:31:A:VAL:HG13	1:29:A:PRO:HA	4	0.16
(1,2506)	1:150:A:THR:HA	1:89:A:VAL:HG13	10	0.16
(1,2502)	1:85:A:PHE:HE2	1:107:A:ALA:HA	9	0.16
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	3	0.16
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	6	0.16
(1,2317)	1:125:A:ASN:HD22	1:128:A:ASP:HB2	1	0.16
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	8	0.16
(1,2146)	1:154:A:LYS:H	1:121:A:ILE:HG22	10	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2117)	1:68:A:TYR:H	1:68:A:TYR:HD1	9	0.16
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG23	10	0.16
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	2	0.16
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	8	0.16
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	7	0.16
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	10	0.16
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	4	0.16
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	5	0.16
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG23	7	0.16
(1,1737)	1:124:A:TYR:H	1:149:A:VAL:HG11	9	0.16
(1,1713)	1:24:A:ILE:H	1:23:A:THR:HG21	10	0.16
(1,1640)	1:47:A:THR:HG21	1:156:A:PHE:HE2	10	0.16
(1,1606)	1:33:A:LEU:HD21	1:12:A:VAL:HB	2	0.16
(1,1569)	1:74:A:LYS:HG2	1:12:A:VAL:HB	1	0.16
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	4	0.16
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	3	0.16
(1,1515)	1:34:A:GLU:HG3	1:9:A:LEU:HD11	5	0.16
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	4	0.16
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	7	0.16
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	9	0.16
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	1	0.16
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	7	0.16
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD12	6	0.16
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD12	7	0.16
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD13	9	0.16
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	3	0.16
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	7	0.16
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	10	0.16
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	4	0.16
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	5	0.16
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	10	0.16
(1,964)	1:67:A:LEU:HD23	1:17:A:LYS:HB2	9	0.16
(1,892)	1:101:A:MET:HB3	1:101:A:MET:HG3	7	0.16
(1,888)	1:101:A:MET:HB3	1:102:A:VAL:H	7	0.16
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	3	0.16
(1,830)	1:57:A:MET:H	1:52:A:ASN:HB2	8	0.16
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	6	0.16
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	4	0.16
(1,713)	1:53:A:ASP:HB3	1:74:A:LYS:HG3	5	0.16
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	3	0.16
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	9	0.16
(1,658)	1:50:A:THR:H	1:49:A:PHE:HB3	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:24:A:ILE:HG22	1:25:A:GLY:HA3	10	0.16
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	7	0.16
(1,501)	1:94:A:ALA:HB1	1:121:A:ILE:HD11	8	0.16
(1,489)	1:24:A:ILE:HG22	1:24:A:ILE:HB	3	0.16
(1,489)	1:24:A:ILE:HG23	1:24:A:ILE:HB	4	0.16
(1,489)	1:24:A:ILE:HG21	1:24:A:ILE:HB	8	0.16
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG21	2	0.16
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG23	9	0.16
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG21	10	0.16
(1,401)	1:37:A:ALA:HB3	1:51:A:TYR:HE1	7	0.16
(1,379)	1:115:A:ALA:H	1:115:A:ALA:HB3	4	0.16
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	3	0.16
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	5	0.16
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	9	0.16
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG21	4	0.16
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	8	0.16
(1,191)	1:127:A:HIS:HA	1:126:A:GLU:HB2	5	0.16
(1,174)	1:31:A:VAL:HG11	1:31:A:VAL:HA	10	0.16
(1,119)	1:52:A:ASN:HA	1:50:A:THR:HG23	3	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	2	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	3	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	4	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	5	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	6	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	7	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	8	0.16
(1,92)	1:88:A:HIS:HB2	1:88:A:HIS:HA	9	0.16
(1,41)	1:50:A:THR:HG22	1:75:A:THR:HA	1	0.16
(1,41)	1:50:A:THR:HG21	1:75:A:THR:HA	7	0.16
(1,21)	1:156:A:PHE:HD2	1:114:A:ALA:HB2	9	0.16
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	2	0.16
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	5	0.16
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG2	3	0.15
(1,3510)	1:35:A:GLN:HE22	1:35:A:GLN:HG2	6	0.15
(1,3491)	1:18:A:GLY:H	1:68:A:TYR:HB3	3	0.15
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	8	0.15
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	6	0.15
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	1	0.15
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	4	0.15
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	10	0.15
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	10	0.15
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	6	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	1	0.15
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	9	0.15
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	4	0.15
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	8	0.15
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	10	0.15
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	3	0.15
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	9	0.15
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	2	0.15
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	6	0.15
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	7	0.15
(1,3164)	1:75:A:THR:HG23	1:19:A:SER:HA	4	0.15
(1,3152)	1:71:A:THR:HB	1:70:A:LEU:HD12	3	0.15
(1,3140)	1:106:A:SER:HA	1:150:A:THR:HB	9	0.15
(1,3125)	1:123:A:THR:HG23	1:91:A:TYR:HD1	5	0.15
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD11	5	0.15
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG22	3	0.15
(1,3064)	1:24:A:ILE:HG12	1:25:A:GLY:H	8	0.15
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	5	0.15
(1,2990)	1:13:A:HIS:HB2	1:12:A:VAL:HA	1	0.15
(1,2977)	1:26:A:GLU:HB3	1:26:A:GLU:H	8	0.15
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	10	0.15
(1,2933)	1:57:A:MET:HG3	1:27:A:PRO:HB3	2	0.15
(1,2933)	1:57:A:MET:HG3	1:27:A:PRO:HB3	4	0.15
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	9	0.15
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	8	0.15
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	8	0.15
(1,2859)	1:71:A:THR:HG23	1:16:A:ASN:HB2	9	0.15
(1,2840)	1:30:A:ASP:HB2	1:29:A:PRO:HB2	9	0.15
(1,2833)	1:125:A:ASN:HB2	1:130:A:LYS:HG2	9	0.15
(1,2797)	1:130:A:LYS:HE2	1:130:A:LYS:HD3	2	0.15
(1,2797)	1:130:A:LYS:HE2	1:130:A:LYS:HD3	5	0.15
(1,2797)	1:130:A:LYS:HE2	1:130:A:LYS:HD3	6	0.15
(1,2797)	1:130:A:LYS:HE3	1:130:A:LYS:HD2	7	0.15
(1,2797)	1:130:A:LYS:HE2	1:130:A:LYS:HD3	9	0.15
(1,2794)	1:64:A:LYS:HE2	1:64:A:LYS:HG3	9	0.15
(1,2785)	1:130:A:LYS:HE2	1:125:A:ASN:HD21	3	0.15
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	3	0.15
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	10	0.15
(1,2735)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	8	0.15
(1,2735)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	9	0.15
(1,2725)	1:160:A:GLY:HA3	1:159:A:GLU:HB2	1	0.15
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	10	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	8	0.15
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	3	0.15
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	2	0.15
(1,2681)	1:95:A:PRO:HD3	1:94:A:ALA:H	1	0.15
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB3	2	0.15
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB1	7	0.15
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB3	10	0.15
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	5	0.15
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	6	0.15
(1,2625)	1:112:A:ALA:HB3	1:109:A:CYS:HB3	2	0.15
(1,2625)	1:112:A:ALA:HB1	1:109:A:CYS:HB3	3	0.15
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	4	0.15
(1,2607)	1:149:A:VAL:HG13	1:149:A:VAL:HG21	4	0.15
(1,2607)	1:149:A:VAL:HG23	1:146:A:VAL:HG12	8	0.15
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	10	0.15
(1,2582)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	5	0.15
(1,2582)	1:97:A:VAL:HG13	1:135:A:GLY:HA2	9	0.15
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	3	0.15
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	5	0.15
(1,2326)	1:110:A:GLN:HE22	1:85:A:PHE:HE1	7	0.15
(1,2211)	1:17:A:LYS:H	1:73:A:GLY:HA2	6	0.15
(1,2211)	1:17:A:LYS:H	1:73:A:GLY:HA2	7	0.15
(1,2091)	1:56:A:LYS:H	1:56:A:LYS:HB3	6	0.15
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG22	2	0.15
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG22	4	0.15
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	5	0.15
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	8	0.15
(1,1879)	1:94:A:ALA:H	1:141:A:PHE:HD2	8	0.15
(1,1877)	1:7:A:LEU:H	1:32:A:SER:H	7	0.15
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	4	0.15
(1,1841)	1:107:A:ALA:H	1:11:A:CYS:HA	5	0.15
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	1	0.15
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	2	0.15
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG23	2	0.15
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG22	10	0.15
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	2	0.15
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	3	0.15
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	7	0.15
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	8	0.15
(1,1674)	1:28:A:VAL:HG13	1:28:A:VAL:HA	7	0.15
(1,1674)	1:28:A:VAL:HG13	1:28:A:VAL:HA	9	0.15
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD22	10	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1627)	1:132:A:THR:HG22	1:100:A:ALA:HB2	1	0.15
(1,1606)	1:33:A:LEU:HD22	1:12:A:VAL:HB	4	0.15
(1,1605)	1:33:A:LEU:HD22	1:74:A:LYS:HB3	4	0.15
(1,1555)	1:67:A:LEU:HD23	1:67:A:LEU:HD12	2	0.15
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	9	0.15
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	3	0.15
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	6	0.15
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	7	0.15
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	2	0.15
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	3	0.15
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	5	0.15
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	8	0.15
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	6	0.15
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD11	8	0.15
(1,1449)	1:79:A:SER:H	1:77:A:SER:HB2	6	0.15
(1,1428)	1:136:A:ARG:H	1:136:A:ARG:HG3	10	0.15
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	2	0.15
(1,1421)	1:108:A:ASP:HA	1:65:A:PRO:HG2	5	0.15
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD11	6	0.15
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	1	0.15
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	5	0.15
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	8	0.15
(1,1260)	1:156:A:PHE:HB3	1:159:A:GLU:HB3	2	0.15
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	7	0.15
(1,1179)	1:64:A:LYS:HB3	1:112:A:ALA:HA	1	0.15
(1,1175)	1:58:A:CYS:H	1:57:A:MET:HG3	4	0.15
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	2	0.15
(1,935)	1:73:A:GLY:H	1:16:A:ASN:HB2	10	0.15
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	2	0.15
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	4	0.15
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	6	0.15
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	2	0.15
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	6	0.15
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	7	0.15
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	10	0.15
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB1	3	0.15
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB3	9	0.15
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	4	0.15
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	5	0.15
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	6	0.15
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	7	0.15
(1,838)	1:125:A:ASN:H	1:125:A:ASN:HB3	9	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	3	0.15
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	7	0.15
(1,758)	1:64:A:LYS:H	1:64:A:LYS:HE3	4	0.15
(1,748)	1:96:A:ASP:H	1:96:A:ASP:HB3	10	0.15
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	4	0.15
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	1	0.15
(1,549)	1:74:A:LYS:H	1:73:A:GLY:HA3	10	0.15
(1,532)	1:24:A:ILE:HD12	1:24:A:ILE:HG12	7	0.15
(1,532)	1:24:A:ILE:HD11	1:24:A:ILE:HG12	10	0.15
(1,428)	1:31:A:VAL:HG22	1:58:A:CYS:HB3	3	0.15
(1,428)	1:31:A:VAL:HG21	1:58:A:CYS:HB3	5	0.15
(1,420)	1:111:A:ALA:HB3	1:65:A:PRO:HG2	10	0.15
(1,412)	1:21:A:ALA:HB1	1:61:A:LYS:HA	3	0.15
(1,401)	1:37:A:ALA:HB1	1:51:A:TYR:HE1	9	0.15
(1,358)	1:115:A:ALA:HB1	1:116:A:ASP:HB2	5	0.15
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG23	2	0.15
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG21	6	0.15
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG22	3	0.15
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG22	6	0.15
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	9	0.15
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG22	3	0.15
(1,243)	1:149:A:VAL:HG12	1:149:A:VAL:HG23	6	0.15
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG23	7	0.15
(1,239)	1:103:A:THR:HG23	1:108:A:ASP:HB2	3	0.15
(1,223)	1:104:A:SER:H	1:13:A:HIS:HA	10	0.15
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	4	0.15
(1,200)	1:71:A:THR:HG22	1:71:A:THR:HB	7	0.15
(1,191)	1:127:A:HIS:HA	1:126:A:GLU:HB2	7	0.15
(1,174)	1:31:A:VAL:HG13	1:31:A:VAL:HA	1	0.15
(1,127)	1:88:A:HIS:HB2	1:88:A:HIS:HD2	10	0.15
(1,41)	1:50:A:THR:HG22	1:75:A:THR:HA	3	0.15
(1,41)	1:50:A:THR:HG21	1:75:A:THR:HA	5	0.15
(1,41)	1:50:A:THR:HG23	1:75:A:THR:HA	10	0.15
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	4	0.15
(1,3512)	1:39:A:GLN:HE22	1:43:A:VAL:HG11	2	0.14
(1,3512)	1:39:A:GLN:HE22	1:60:A:VAL:HG22	10	0.14
(1,3491)	1:18:A:GLY:H	1:68:A:TYR:HB3	4	0.14
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB3	3	0.14
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	5	0.14
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	10	0.14
(1,3471)	1:57:A:MET:H	1:56:A:LYS:HG2	9	0.14
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3466)	1:52:A:ASN:H	1:57:A:MET:H	8	0.14
(1,3459)	1:118:A:SER:H	1:118:A:SER:HB2	1	0.14
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	3	0.14
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	7	0.14
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	8	0.14
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	8	0.14
(1,3335)	1:136:A:ARG:H	1:136:A:ARG:HD3	9	0.14
(1,3273)	1:47:A:THR:H	1:78:A:ARG:HG2	3	0.14
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	4	0.14
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	6	0.14
(1,3251)	1:33:A:LEU:H	1:32:A:SER:HB2	3	0.14
(1,3238)	1:107:A:ALA:H	1:77:A:SER:HB3	3	0.14
(1,3225)	1:85:A:PHE:H	1:152:A:GLY:HA2	9	0.14
(1,3214)	1:147:A:LEU:H	1:149:A:VAL:H	5	0.14
(1,3205)	1:131:A:CYS:H	1:103:A:THR:H	9	0.14
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	6	0.14
(1,3170)	1:51:A:TYR:H	1:49:A:PHE:HE1	7	0.14
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD22	7	0.14
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD21	10	0.14
(1,3155)	1:37:A:ALA:H	1:9:A:LEU:HD21	4	0.14
(1,3145)	1:52:A:ASN:HB2	1:50:A:THR:HG23	9	0.14
(1,3125)	1:123:A:THR:HG23	1:91:A:TYR:HD1	6	0.14
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	3	0.14
(1,3097)	1:67:A:LEU:HD11	1:102:A:VAL:H	3	0.14
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD13	1	0.14
(1,3086)	1:41:A:LYS:HG2	1:40:A:CYS:HB3	2	0.14
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	1	0.14
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	9	0.14
(1,3023)	1:79:A:SER:HB3	1:156:A:PHE:HB2	6	0.14
(1,3021)	1:105:A:GLN:HB3	1:108:A:ASP:H	4	0.14
(1,3021)	1:105:A:GLN:HB3	1:108:A:ASP:H	5	0.14
(1,2978)	1:26:A:GLU:HB3	1:27:A:PRO:HD3	6	0.14
(1,2978)	1:26:A:GLU:HB2	1:27:A:PRO:HD3	9	0.14
(1,2914)	1:142:A:LYS:HE3	1:142:A:LYS:HB2	8	0.14
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	5	0.14
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	1	0.14
(1,2879)	1:150:A:THR:HB	1:85:A:PHE:HD2	8	0.14
(1,2857)	1:16:A:ASN:HB3	1:71:A:THR:HA	2	0.14
(1,2833)	1:125:A:ASN:HB2	1:130:A:LYS:HG2	10	0.14
(1,2823)	1:125:A:ASN:HD21	1:125:A:ASN:HB3	2	0.14
(1,2823)	1:125:A:ASN:HD21	1:125:A:ASN:HB3	5	0.14
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	8	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2801)	1:64:A:LYS:HE2	1:116:A:ASP:H	9	0.14
(1,2797)	1:130:A:LYS:HE3	1:130:A:LYS:HD2	4	0.14
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	4	0.14
(1,2787)	1:56:A:LYS:HE2	1:56:A:LYS:HD3	5	0.14
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	7	0.14
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	8	0.14
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	9	0.14
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	3	0.14
(1,2763)	1:136:A:ARG:HD3	1:136:A:ARG:HG3	7	0.14
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	2	0.14
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	6	0.14
(1,2739)	1:122:A:PHE:HB3	1:109:A:CYS:HB2	2	0.14
(1,2725)	1:160:A:GLY:HA3	1:159:A:GLU:HB2	8	0.14
(1,2725)	1:145:A:GLY:HA3	1:144:A:ARG:HB3	9	0.14
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	5	0.14
(1,2692)	1:153:A:PRO:HD2	1:152:A:GLY:HA3	9	0.14
(1,2672)	1:24:A:ILE:HD12	1:46:A:CYS:HB3	5	0.14
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB2	4	0.14
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB2	5	0.14
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB2	6	0.14
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	9	0.14
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	8	0.14
(1,2607)	1:149:A:VAL:HG12	1:149:A:VAL:HG23	6	0.14
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG23	3	0.14
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	9	0.14
(1,2576)	1:33:A:LEU:HA	1:6:A:LYS:HB3	2	0.14
(1,2562)	1:89:A:VAL:HG22	1:89:A:VAL:HA	8	0.14
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	6	0.14
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	7	0.14
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	9	0.14
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	2	0.14
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	8	0.14
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	2	0.14
(1,2112)	1:133:A:PHE:H	1:132:A:THR:HG21	6	0.14
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB2	8	0.14
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB3	9	0.14
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG21	1	0.14
(1,2057)	1:150:A:THR:H	1:150:A:THR:HG21	3	0.14
(1,2004)	1:111:A:ALA:H	1:112:A:ALA:HB2	9	0.14
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	6	0.14
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD22	3	0.14
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD23	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD21	5	0.14
(1,1841)	1:107:A:ALA:H	1:11:A:CYS:HA	8	0.14
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	10	0.14
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	5	0.14
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	6	0.14
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD23	6	0.14
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD23	4	0.14
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	7	0.14
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	3	0.14
(1,1514)	1:30:A:ASP:HB2	1:29:A:PRO:HG2	9	0.14
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	6	0.14
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	3	0.14
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD12	5	0.14
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD11	10	0.14
(1,1421)	1:108:A:ASP:HA	1:65:A:PRO:HG2	9	0.14
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD12	1	0.14
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	2	0.14
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	4	0.14
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	8	0.14
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	4	0.14
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	8	0.14
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	2	0.14
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	1	0.14
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	3	0.14
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	6	0.14
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	6	0.14
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	7	0.14
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	4	0.14
(1,1059)	1:32:A:SER:H	1:35:A:GLN:HG2	8	0.14
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	3	0.14
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	5	0.14
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	10	0.14
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	1	0.14
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	3	0.14
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	4	0.14
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	9	0.14
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB1	4	0.14
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB2	8	0.14
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	1	0.14
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	4	0.14
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	4	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	1	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	2	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	3	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	4	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	5	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	6	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	7	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	8	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	9	0.14
(1,784)	1:147:A:LEU:HA	1:147:A:LEU:HB2	10	0.14
(1,741)	1:41:A:LYS:HE3	1:38:A:ALA:HA	4	0.14
(1,651)	1:97:A:VAL:HG21	1:135:A:GLY:HA2	7	0.14
(1,650)	1:97:A:VAL:HG12	1:135:A:GLY:HA2	4	0.14
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	5	0.14
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	6	0.14
(1,532)	1:24:A:ILE:HD13	1:24:A:ILE:HG12	2	0.14
(1,532)	1:24:A:ILE:HD11	1:24:A:ILE:HG12	3	0.14
(1,532)	1:24:A:ILE:HD13	1:24:A:ILE:HG12	4	0.14
(1,532)	1:24:A:ILE:HD13	1:24:A:ILE:HG12	6	0.14
(1,532)	1:24:A:ILE:HD13	1:24:A:ILE:HG12	8	0.14
(1,532)	1:24:A:ILE:HD12	1:24:A:ILE:HG12	9	0.14
(1,428)	1:31:A:VAL:HG21	1:58:A:CYS:HB3	6	0.14
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG23	5	0.14
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG21	9	0.14
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB3	3	0.14
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB1	5	0.14
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB2	7	0.14
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB1	10	0.14
(1,420)	1:111:A:ALA:HB2	1:65:A:PRO:HG2	7	0.14
(1,412)	1:21:A:ALA:HB1	1:61:A:LYS:HA	2	0.14
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB2	2	0.14
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB2	8	0.14
(1,358)	1:115:A:ALA:HB2	1:116:A:ASP:HB2	8	0.14
(1,337)	1:149:A:VAL:HG23	1:90:A:SER:HA	2	0.14
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG22	1	0.14
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	2	0.14
(1,251)	1:39:A:GLN:HA	1:42:A:ALA:HB2	5	0.14
(1,243)	1:149:A:VAL:HG11	1:149:A:VAL:HG23	2	0.14
(1,228)	1:89:A:VAL:HG22	1:142:A:LYS:HA	5	0.14
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	2	0.14
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	5	0.14
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	9	0.14
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG23	3	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG22	5	0.14
(1,191)	1:127:A:HIS:HA	1:126:A:GLU:HB2	1	0.14
(1,188)	1:67:A:LEU:HD23	1:75:A:THR:HG22	5	0.14
(1,173)	1:35:A:GLN:HE21	1:31:A:VAL:HG13	7	0.14
(1,164)	1:150:A:THR:HG23	1:150:A:THR:HA	1	0.14
(1,164)	1:150:A:THR:HG23	1:150:A:THR:HA	3	0.14
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	2	0.14
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	5	0.14
(1,14)	1:126:A:GLU:HG3	1:124:A:TYR:HD1	9	0.14
(1,3526)	1:31:A:VAL:H	1:29:A:PRO:HB2	1	0.13
(1,3523)	1:31:A:VAL:H	1:30:A:ASP:HB3	1	0.13
(1,3512)	1:39:A:GLN:HE22	1:43:A:VAL:HG12	9	0.13
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	5	0.13
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	8	0.13
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	2	0.13
(1,3466)	1:52:A:ASN:H	1:57:A:MET:H	3	0.13
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	5	0.13
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	10	0.13
(1,3422)	1:54:A:ASP:H	1:72:A:GLY:HA2	8	0.13
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	10	0.13
(1,3403)	1:48:A:HIS:H	1:61:A:LYS:HB3	10	0.13
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	10	0.13
(1,3350)	1:127:A:HIS:H	1:128:A:ASP:HB2	10	0.13
(1,3339)	1:156:A:PHE:H	1:110:A:GLN:HG3	7	0.13
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	3	0.13
(1,3329)	1:39:A:GLN:H	1:28:A:VAL:HG21	9	0.13
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	7	0.13
(1,3296)	1:151:A:SER:H	1:86:A:GLU:HB3	3	0.13
(1,3287)	1:114:A:ALA:H	1:110:A:GLN:HG2	6	0.13
(1,3251)	1:33:A:LEU:H	1:32:A:SER:HB2	5	0.13
(1,3250)	1:91:A:TYR:H	1:149:A:VAL:HB	5	0.13
(1,3250)	1:91:A:TYR:H	1:149:A:VAL:HB	7	0.13
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	5	0.13
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	9	0.13
(1,3216)	1:147:A:LEU:H	1:146:A:VAL:HG12	5	0.13
(1,3213)	1:87:A:GLN:H	1:150:A:THR:HA	3	0.13
(1,3208)	1:70:A:LEU:H	1:16:A:ASN:HB3	2	0.13
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	4	0.13
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	5	0.13
(1,3136)	1:52:A:ASN:H	1:50:A:THR:HG21	10	0.13
(1,3125)	1:123:A:THR:HG23	1:91:A:TYR:HD1	9	0.13
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	10	0.13
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	6	0.13
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	7	0.13
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	8	0.13
(1,3051)	1:108:A:ASP:HB2	1:65:A:PRO:HG2	10	0.13
(1,3023)	1:79:A:SER:HB3	1:156:A:PHE:HB2	4	0.13
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	1	0.13
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	1	0.13
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	3	0.13
(1,2914)	1:142:A:LYS:HE3	1:89:A:VAL:HB	1	0.13
(1,2912)	1:153:A:PRO:HB2	1:121:A:ILE:HA	1	0.13
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	2	0.13
(1,2902)	1:28:A:VAL:H	1:28:A:VAL:HB	10	0.13
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	4	0.13
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	3	0.13
(1,2883)	1:62:A:GLU:HG2	1:22:A:PRO:HD2	6	0.13
(1,2877)	1:61:A:LYS:HB3	1:23:A:THR:HA	6	0.13
(1,2877)	1:61:A:LYS:HB3	1:23:A:THR:HA	7	0.13
(1,2877)	1:61:A:LYS:HB3	1:23:A:THR:HA	8	0.13
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	4	0.13
(1,2857)	1:16:A:ASN:HB3	1:71:A:THR:HA	4	0.13
(1,2823)	1:125:A:ASN:HD21	1:125:A:ASN:HB3	6	0.13
(1,2823)	1:125:A:ASN:HB3	1:129:A:GLN:H	9	0.13
(1,2797)	1:130:A:LYS:HE2	1:130:A:LYS:HD3	3	0.13
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	1	0.13
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	2	0.13
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	10	0.13
(1,2786)	1:41:A:LYS:HE2	1:41:A:LYS:HG2	2	0.13
(1,2765)	1:54:A:ASP:H	1:53:A:ASP:HB3	4	0.13
(1,2764)	1:74:A:LYS:H	1:18:A:GLY:HA2	10	0.13
(1,2763)	1:136:A:ARG:HD3	1:136:A:ARG:HG3	8	0.13
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	7	0.13
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	8	0.13
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	9	0.13
(1,2754)	1:136:A:ARG:HD3	1:120:A:GLU:HG3	6	0.13
(1,2740)	1:145:A:GLY:H	1:145:A:GLY:HA3	4	0.13
(1,2740)	1:145:A:GLY:H	1:145:A:GLY:HA3	7	0.13
(1,2735)	1:43:A:VAL:HG21	1:46:A:CYS:HB2	5	0.13
(1,2717)	1:160:A:GLY:HA2	1:155:A:GLN:HG3	8	0.13
(1,2696)	1:65:A:PRO:HD3	1:65:A:PRO:HB3	9	0.13
(1,2691)	1:153:A:PRO:HD2	1:85:A:PHE:HD1	9	0.13
(1,2682)	1:95:A:PRO:HD3	1:141:A:PHE:HD2	5	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB3	1	0.13
(1,2631)	1:111:A:ALA:HA	1:111:A:ALA:HB3	5	0.13
(1,2627)	1:111:A:ALA:HB3	1:156:A:PHE:HD1	4	0.13
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	10	0.13
(1,2607)	1:149:A:VAL:HG11	1:149:A:VAL:HG23	2	0.13
(1,2607)	1:149:A:VAL:HG22	1:146:A:VAL:HG11	7	0.13
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG23	5	0.13
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	3	0.13
(1,2586)	1:55:A:SER:HA	1:52:A:ASN:HB3	6	0.13
(1,2556)	1:71:A:THR:HG21	1:54:A:ASP:HB2	2	0.13
(1,2527)	1:17:A:LYS:HD2	1:17:A:LYS:HA	3	0.13
(1,2510)	1:47:A:THR:HG22	1:156:A:PHE:HE2	3	0.13
(1,2506)	1:31:A:VAL:HG12	1:29:A:PRO:HA	7	0.13
(1,2502)	1:152:A:GLY:HA3	1:85:A:PHE:HE1	3	0.13
(1,2502)	1:85:A:PHE:HE2	1:107:A:ALA:HA	6	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	2	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	3	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	4	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	5	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	8	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	9	0.13
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	10	0.13
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	7	0.13
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	10	0.13
(1,2403)	1:19:A:SER:H	1:19:A:SER:HB2	3	0.13
(1,2333)	1:57:A:MET:H	1:56:A:LYS:HG3	6	0.13
(1,2311)	1:112:A:ALA:H	1:65:A:PRO:HD2	5	0.13
(1,2218)	1:115:A:ALA:H	1:111:A:ALA:HB3	2	0.13
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	6	0.13
(1,2188)	1:139:A:SER:H	1:140:A:ALA:HB1	8	0.13
(1,2180)	1:108:A:ASP:H	1:108:A:ASP:HB3	2	0.13
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	5	0.13
(1,2091)	1:56:A:LYS:H	1:56:A:LYS:HB3	7	0.13
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD21	6	0.13
(1,1963)	1:119:A:CYS:H	1:97:A:VAL:HG21	5	0.13
(1,1879)	1:94:A:ALA:H	1:141:A:PHE:HD2	10	0.13
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	3	0.13
(1,1868)	1:7:A:LEU:H	1:6:A:LYS:HB3	5	0.13
(1,1799)	1:120:A:GLU:H	1:120:A:GLU:HG3	9	0.13
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG23	9	0.13
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	8	0.13
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	9	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	3	0.13
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	10	0.13
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	4	0.13
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	9	0.13
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	8	0.13
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD23	8	0.13
(1,1643)	1:74:A:LYS:H	1:50:A:THR:HG22	3	0.13
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD11	1	0.13
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	5	0.13
(1,1507)	1:122:A:PHE:H	1:121:A:ILE:HG12	4	0.13
(1,1487)	1:9:A:LEU:HG	1:9:A:LEU:HD11	1	0.13
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	6	0.13
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	7	0.13
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	9	0.13
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	3	0.13
(1,1251)	1:65:A:PRO:HB2	1:75:A:THR:HG23	10	0.13
(1,1236)	1:78:A:ARG:HB3	1:78:A:ARG:HD3	2	0.13
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	1	0.13
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	5	0.13
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	6	0.13
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	8	0.13
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	9	0.13
(1,1062)	1:35:A:GLN:HG2	1:31:A:VAL:HA	9	0.13
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	3	0.13
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	4	0.13
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	8	0.13
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	9	0.13
(1,938)	1:16:A:ASN:HD22	1:16:A:ASN:HB2	2	0.13
(1,938)	1:16:A:ASN:HD22	1:16:A:ASN:HB2	9	0.13
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	7	0.13
(1,906)	1:24:A:ILE:HB	1:62:A:GLU:HG2	5	0.13
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	2	0.13
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	5	0.13
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	10	0.13
(1,824)	1:125:A:ASN:HD22	1:125:A:ASN:HB3	8	0.13
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	2	0.13
(1,733)	1:132:A:THR:H	1:131:A:CYS:HB2	3	0.13
(1,680)	1:20:A:ARG:H	1:20:A:ARG:HD3	4	0.13
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	2	0.13
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	4	0.13
(1,534)	1:4:A:PRO:HD3	1:32:A:SER:HB3	5	0.13
(1,532)	1:24:A:ILE:HD11	1:24:A:ILE:HG12	1	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,532)	1:24:A:ILE:HD11	1:24:A:ILE:HG12	5	0.13
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB2	9	0.13
(1,428)	1:31:A:VAL:HG23	1:58:A:CYS:HB3	2	0.13
(1,425)	1:36:A:CYS:H	1:31:A:VAL:HG22	5	0.13
(1,388)	1:112:A:ALA:HB2	1:65:A:PRO:HD3	5	0.13
(1,355)	1:115:A:ALA:HB3	1:156:A:PHE:HZ	8	0.13
(1,326)	1:100:A:ALA:H	1:100:A:ALA:HB1	10	0.13
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG23	4	0.13
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG21	5	0.13
(1,276)	1:97:A:VAL:HG11	1:97:A:VAL:HG22	10	0.13
(1,251)	1:39:A:GLN:HA	1:42:A:ALA:HB3	4	0.13
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	4	0.13
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	8	0.13
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG23	5	0.13
(1,243)	1:149:A:VAL:HG12	1:149:A:VAL:HG21	9	0.13
(1,238)	1:103:A:THR:HG23	1:101:A:MET:HG3	4	0.13
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG22	6	0.13
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG21	7	0.13
(1,211)	1:146:A:VAL:HG13	1:149:A:VAL:H	3	0.13
(1,200)	1:71:A:THR:HG23	1:71:A:THR:HB	1	0.13
(1,200)	1:71:A:THR:HG23	1:71:A:THR:HB	3	0.13
(1,200)	1:71:A:THR:HG23	1:71:A:THR:HB	6	0.13
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	10	0.13
(1,198)	1:72:A:GLY:H	1:71:A:THR:HG23	5	0.13
(1,188)	1:67:A:LEU:HD22	1:75:A:THR:HG23	4	0.13
(1,164)	1:150:A:THR:HG22	1:150:A:THR:HA	10	0.13
(1,146)	1:9:A:LEU:HD23	1:37:A:ALA:HB2	8	0.13
(1,13)	1:124:A:TYR:HD1	1:126:A:GLU:HA	5	0.13
(1,3507)	1:35:A:GLN:HE21	1:35:A:GLN:HB2	8	0.12
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB2	2	0.12
(1,3458)	1:57:A:MET:H	1:51:A:TYR:HB3	2	0.12
(1,3456)	1:125:A:ASN:HD21	1:128:A:ASP:HB2	2	0.12
(1,3410)	1:115:A:ALA:H	1:114:A:ALA:HA	6	0.12
(1,3384)	1:129:A:GLN:H	1:129:A:GLN:HG2	4	0.12
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	6	0.12
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	5	0.12
(1,3347)	1:101:A:MET:H	1:131:A:CYS:HB3	10	0.12
(1,3345)	1:150:A:THR:H	1:87:A:GLN:HG2	4	0.12
(1,3337)	1:38:A:ALA:H	1:35:A:GLN:HG3	5	0.12
(1,3251)	1:33:A:LEU:H	1:32:A:SER:HB2	2	0.12
(1,3250)	1:91:A:TYR:H	1:149:A:VAL:HB	10	0.12
(1,3234)	1:61:A:LYS:H	1:61:A:LYS:HB3	10	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3200)	1:52:A:ASN:H	1:53:A:ASP:H	1	0.12
(1,3184)	1:76:A:ALA:H	1:48:A:HIS:HA	7	0.12
(1,3180)	1:143:A:GLU:H	1:142:A:LYS:H	8	0.12
(1,3177)	1:59:A:HIS:H	1:60:A:VAL:HG11	2	0.12
(1,3127)	1:132:A:THR:HG22	1:92:A:GLU:HG2	6	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	1	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	2	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	3	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	4	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	5	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	6	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	7	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	8	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	9	0.12
(1,3114)	1:24:A:ILE:HB	1:24:A:ILE:HA	10	0.12
(1,3104)	1:74:A:LYS:HG2	1:53:A:ASP:HB2	10	0.12
(1,3089)	1:9:A:LEU:HB2	1:9:A:LEU:HD13	10	0.12
(1,3080)	1:11:A:CYS:H	1:10:A:SER:HB3	3	0.12
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	2	0.12
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	4	0.12
(1,3023)	1:79:A:SER:HB3	1:156:A:PHE:HB2	1	0.12
(1,3021)	1:105:A:GLN:HB3	1:108:A:ASP:H	9	0.12
(1,2977)	1:26:A:GLU:HB3	1:26:A:GLU:H	9	0.12
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	9	0.12
(1,2968)	1:159:A:GLU:HB3	1:159:A:GLU:HG3	7	0.12
(1,2965)	1:65:A:PRO:HD3	1:65:A:PRO:HB2	10	0.12
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	8	0.12
(1,2893)	1:36:A:CYS:HB3	1:35:A:GLN:HB3	7	0.12
(1,2880)	1:150:A:THR:HB	1:87:A:GLN:HG2	8	0.12
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	5	0.12
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	10	0.12
(1,2787)	1:6:A:LYS:HE2	1:6:A:LYS:HD2	3	0.12
(1,2766)	1:133:A:PHE:HB2	1:96:A:ASP:HA	2	0.12
(1,2766)	1:133:A:PHE:HB2	1:96:A:ASP:HA	5	0.12
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	2	0.12
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	5	0.12
(1,2735)	1:43:A:VAL:HG23	1:46:A:CYS:HB2	7	0.12
(1,2709)	1:148:A:GLY:HA2	1:147:A:LEU:HB3	10	0.12
(1,2648)	1:114:A:ALA:HA	1:114:A:ALA:HB2	9	0.12
(1,2633)	1:107:A:ALA:HB3	1:108:A:ASP:HB2	1	0.12
(1,2625)	1:112:A:ALA:HB1	1:109:A:CYS:HB3	10	0.12
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	5	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2612)	1:53:A:ASP:HA	1:53:A:ASP:HB2	6	0.12
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	2	0.12
(1,2607)	1:149:A:VAL:HG13	1:149:A:VAL:HG23	5	0.12
(1,2605)	1:77:A:SER:HA	1:76:A:ALA:HB1	3	0.12
(1,2563)	1:89:A:VAL:HG22	1:89:A:VAL:HG11	2	0.12
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB3	2	0.12
(1,2546)	1:150:A:THR:HG23	1:106:A:SER:HB2	2	0.12
(1,2546)	1:150:A:THR:HG23	1:106:A:SER:HB2	6	0.12
(1,2501)	1:29:A:PRO:HB2	1:29:A:PRO:HA	1	0.12
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	4	0.12
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	5	0.12
(1,2403)	1:19:A:SER:H	1:19:A:SER:HB2	8	0.12
(1,2403)	1:19:A:SER:H	1:19:A:SER:HB2	10	0.12
(1,2233)	1:98:A:MET:H	1:96:A:ASP:HA	10	0.12
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	2	0.12
(1,2118)	1:68:A:TYR:H	1:68:A:TYR:HE1	3	0.12
(1,2067)	1:92:A:GLU:H	1:94:A:ALA:HB1	3	0.12
(1,2004)	1:111:A:ALA:H	1:112:A:ALA:HB3	6	0.12
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG23	5	0.12
(1,1963)	1:119:A:CYS:H	1:97:A:VAL:HG23	4	0.12
(1,1938)	1:69:A:ASP:H	1:68:A:TYR:HE2	10	0.12
(1,1772)	1:125:A:ASN:H	1:124:A:TYR:HD2	4	0.12
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG21	3	0.12
(1,1754)	1:71:A:THR:H	1:71:A:THR:HG22	5	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	2	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	4	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	5	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	6	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	7	0.12
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	8	0.12
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD23	1	0.12
(1,1625)	1:132:A:THR:H	1:132:A:THR:HG22	4	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD13	3	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD21	5	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD13	6	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD13	7	0.12
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD11	10	0.12
(1,1555)	1:67:A:LEU:HD23	1:67:A:LEU:HD11	6	0.12
(1,1555)	1:67:A:LEU:HD22	1:67:A:LEU:HD11	10	0.12
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	2	0.12
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	5	0.12
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	6	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	10	0.12
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	1	0.12
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	2	0.12
(1,1492)	1:74:A:LYS:H	1:70:A:LEU:HG	2	0.12
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	1	0.12
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	2	0.12
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	3	0.12
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	8	0.12
(1,1328)	1:105:A:GLN:HE22	1:105:A:GLN:HG3	9	0.12
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	10	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	1	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	2	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	3	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	4	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	5	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	6	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	7	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	8	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	9	0.12
(1,1306)	1:87:A:GLN:HB2	1:87:A:GLN:HA	10	0.12
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	3	0.12
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	1	0.12
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	8	0.12
(1,1207)	1:57:A:MET:HG3	1:27:A:PRO:HB3	4	0.12
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	1	0.12
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	5	0.12
(1,1159)	1:29:A:PRO:HB3	1:57:A:MET:HA	8	0.12
(1,1130)	1:39:A:GLN:HE22	1:39:A:GLN:HG2	2	0.12
(1,1130)	1:39:A:GLN:HE22	1:39:A:GLN:HG2	9	0.12
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	2	0.12
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	7	0.12
(1,1114)	1:87:A:GLN:H	1:87:A:GLN:HG2	1	0.12
(1,1060)	1:36:A:CYS:H	1:35:A:GLN:HG2	8	0.12
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	1	0.12
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	2	0.12
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	5	0.12
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	7	0.12
(1,953)	1:7:A:LEU:H	1:34:A:GLU:HG2	10	0.12
(1,932)	1:16:A:ASN:HD22	1:16:A:ASN:HB3	8	0.12
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	8	0.12
(1,921)	1:138:A:PHE:HB3	1:138:A:PHE:HE1	9	0.12
(1,914)	1:125:A:ASN:H	1:130:A:LYS:HB2	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:102:A:VAL:H	1:101:A:MET:HB2	4	0.12
(1,888)	1:101:A:MET:HB3	1:102:A:VAL:H	10	0.12
(1,857)	1:141:A:PHE:HB3	1:94:A:ALA:HB1	10	0.12
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	9	0.12
(1,830)	1:57:A:MET:H	1:52:A:ASN:HB2	3	0.12
(1,830)	1:57:A:MET:H	1:52:A:ASN:HB2	9	0.12
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG13	6	0.12
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	7	0.12
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	1	0.12
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	3	0.12
(1,773)	1:66:A:ASP:HB3	1:65:A:PRO:HA	9	0.12
(1,741)	1:41:A:LYS:HE3	1:38:A:ALA:HA	2	0.12
(1,739)	1:131:A:CYS:HB2	1:100:A:ALA:HB3	3	0.12
(1,733)	1:132:A:THR:H	1:131:A:CYS:HB2	6	0.12
(1,692)	1:97:A:VAL:HG22	1:133:A:PHE:HB2	1	0.12
(1,651)	1:97:A:VAL:HG21	1:135:A:GLY:HA2	1	0.12
(1,622)	1:45:A:GLY:HA3	1:43:A:VAL:HG22	3	0.12
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	1	0.12
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	6	0.12
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	2	0.12
(1,555)	1:73:A:GLY:HA2	1:70:A:LEU:HB3	3	0.12
(1,536)	1:27:A:PRO:HD3	1:23:A:THR:HG21	5	0.12
(1,494)	1:94:A:ALA:HB3	1:141:A:PHE:HD2	5	0.12
(1,471)	1:112:A:ALA:H	1:109:A:CYS:HA	9	0.12
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG21	7	0.12
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB2	1	0.12
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB1	4	0.12
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB3	8	0.12
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB3	3	0.12
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB2	10	0.12
(1,326)	1:100:A:ALA:H	1:100:A:ALA:HB1	4	0.12
(1,279)	1:144:A:ARG:H	1:146:A:VAL:HG23	5	0.12
(1,277)	1:143:A:GLU:H	1:146:A:VAL:HG22	5	0.12
(1,276)	1:97:A:VAL:HG12	1:97:A:VAL:HG22	8	0.12
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	4	0.12
(1,251)	1:39:A:GLN:HA	1:42:A:ALA:HB3	1	0.12
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	3	0.12
(1,200)	1:71:A:THR:HG21	1:71:A:THR:HB	8	0.12
(1,196)	1:100:A:ALA:H	1:99:A:THR:HG22	2	0.12
(1,191)	1:127:A:HIS:HA	1:126:A:GLU:HB2	3	0.12
(1,182)	1:67:A:LEU:HD21	1:19:A:SER:HA	1	0.12
(1,180)	1:66:A:ASP:H	1:67:A:LEU:HD22	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:31:A:VAL:HG13	1:31:A:VAL:HB	7	0.12
(1,164)	1:150:A:THR:HG21	1:150:A:THR:HA	2	0.12
(1,164)	1:150:A:THR:HG21	1:150:A:THR:HA	4	0.12
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	5	0.12
(1,69)	1:82:A:ARG:HG2	1:85:A:PHE:HZ	9	0.12
(1,60)	1:85:A:PHE:HD2	1:82:A:ARG:HB2	4	0.12
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	7	0.12
(1,3525)	1:31:A:VAL:H	1:56:A:LYS:HB2	3	0.11
(1,3491)	1:18:A:GLY:H	1:68:A:TYR:HB3	8	0.11
(1,3491)	1:18:A:GLY:H	1:68:A:TYR:HB3	10	0.11
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	4	0.11
(1,3488)	1:155:A:GLN:HE21	1:115:A:ALA:HA	6	0.11
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB1	9	0.11
(1,3481)	1:132:A:THR:H	1:100:A:ALA:HB2	10	0.11
(1,3477)	1:149:A:VAL:H	1:146:A:VAL:HB	8	0.11
(1,3471)	1:57:A:MET:H	1:56:A:LYS:HG2	10	0.11
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	10	0.11
(1,3466)	1:56:A:LYS:H	1:57:A:MET:H	1	0.11
(1,3422)	1:54:A:ASP:H	1:72:A:GLY:HA2	9	0.11
(1,3411)	1:115:A:ALA:H	1:113:A:CYS:HB3	1	0.11
(1,3410)	1:115:A:ALA:H	1:114:A:ALA:HA	7	0.11
(1,3410)	1:115:A:ALA:H	1:114:A:ALA:HA	9	0.11
(1,3394)	1:32:A:SER:H	1:31:A:VAL:HG23	3	0.11
(1,3359)	1:64:A:LYS:H	1:64:A:LYS:HG3	4	0.11
(1,3350)	1:127:A:HIS:H	1:128:A:ASP:HB2	4	0.11
(1,3334)	1:134:A:LYS:H	1:121:A:ILE:HG12	6	0.11
(1,3322)	1:116:A:ASP:H	1:114:A:ALA:HA	6	0.11
(1,3296)	1:151:A:SER:H	1:86:A:GLU:HB3	9	0.11
(1,3283)	1:119:A:CYS:H	1:118:A:SER:HB3	6	0.11
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	7	0.11
(1,3251)	1:33:A:LEU:H	1:32:A:SER:HB2	9	0.11
(1,3240)	1:107:A:ALA:H	1:11:A:CYS:HB2	6	0.11
(1,3238)	1:107:A:ALA:H	1:77:A:SER:HB3	8	0.11
(1,3145)	1:52:A:ASN:HB2	1:50:A:THR:HG21	10	0.11
(1,3125)	1:123:A:THR:HG21	1:91:A:TYR:HD1	3	0.11
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG23	7	0.11
(1,3084)	1:65:A:PRO:HA	1:75:A:THR:HG23	10	0.11
(1,3054)	1:147:A:LEU:HA	1:147:A:LEU:HG	10	0.11
(1,2978)	1:26:A:GLU:HB3	1:27:A:PRO:HD3	3	0.11
(1,2978)	1:26:A:GLU:HB2	1:27:A:PRO:HD3	4	0.11
(1,2978)	1:26:A:GLU:HB3	1:27:A:PRO:HD3	5	0.11
(1,2971)	1:159:A:GLU:HB2	1:156:A:PHE:HA	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	6	0.11
(1,2956)	1:86:A:GLU:HB2	1:85:A:PHE:HA	7	0.11
(1,2940)	1:9:A:LEU:HB3	1:12:A:VAL:HB	5	0.11
(1,2914)	1:142:A:LYS:HE3	1:89:A:VAL:HB	4	0.11
(1,2914)	1:142:A:LYS:HE3	1:89:A:VAL:HB	6	0.11
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	3	0.11
(1,2888)	1:157:A:CYS:HB2	1:156:A:PHE:HA	3	0.11
(1,2863)	1:34:A:GLU:HG2	1:9:A:LEU:HB2	6	0.11
(1,2844)	1:156:A:PHE:HB3	1:159:A:GLU:HB3	10	0.11
(1,2829)	1:58:A:CYS:HB2	1:51:A:TYR:HD1	6	0.11
(1,2818)	1:54:A:ASP:HB2	1:72:A:GLY:HA2	4	0.11
(1,2803)	1:66:A:ASP:HB2	1:20:A:ARG:HB2	7	0.11
(1,2786)	1:41:A:LYS:HE2	1:41:A:LYS:HG2	4	0.11
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	4	0.11
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	4	0.11
(1,2740)	1:136:A:ARG:H	1:135:A:GLY:HA2	2	0.11
(1,2740)	1:136:A:ARG:H	1:135:A:GLY:HA2	6	0.11
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	8	0.11
(1,2730)	1:45:A:GLY:HA3	1:44:A:ASP:HB3	9	0.11
(1,2656)	1:107:A:ALA:HA	1:85:A:PHE:HZ	10	0.11
(1,2654)	1:97:A:VAL:HG21	1:134:A:LYS:HA	10	0.11
(1,2646)	1:38:A:ALA:HA	1:37:A:ALA:HA	3	0.11
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	10	0.11
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	7	0.11
(1,2607)	1:149:A:VAL:HG12	1:149:A:VAL:HG21	9	0.11
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG22	2	0.11
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG21	7	0.11
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG23	9	0.11
(1,2588)	1:75:A:THR:HG23	1:76:A:ALA:HA	2	0.11
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB2	1	0.11
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB3	7	0.11
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB3	8	0.11
(1,2527)	1:17:A:LYS:HD2	1:17:A:LYS:HA	10	0.11
(1,2506)	1:150:A:THR:HA	1:89:A:VAL:HG12	8	0.11
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	2	0.11
(1,2410)	1:31:A:VAL:H	1:6:A:LYS:H	8	0.11
(1,2252)	1:113:A:CYS:H	1:122:A:PHE:HB2	5	0.11
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	3	0.11
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	7	0.11
(1,2198)	1:48:A:HIS:H	1:46:A:CYS:HB2	10	0.11
(1,2149)	1:88:A:HIS:H	1:150:A:THR:HG21	2	0.11
(1,2085)	1:102:A:VAL:H	1:101:A:MET:H	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2005)	1:15:A:ASP:H	1:16:A:ASN:H	4	0.11
(1,2004)	1:111:A:ALA:H	1:112:A:ALA:HB2	5	0.11
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG23	4	0.11
(1,1977)	1:151:A:SER:H	1:151:A:SER:HB2	8	0.11
(1,1963)	1:119:A:CYS:H	1:97:A:VAL:HG21	9	0.11
(1,1934)	1:67:A:LEU:H	1:67:A:LEU:HD11	4	0.11
(1,1901)	1:12:A:VAL:H	1:80:A:CYS:HB3	3	0.11
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	3	0.11
(1,1879)	1:94:A:ALA:H	1:141:A:PHE:HD2	6	0.11
(1,1879)	1:94:A:ALA:H	1:141:A:PHE:HD2	9	0.11
(1,1867)	1:66:A:ASP:H	1:65:A:PRO:HG2	10	0.11
(1,1799)	1:120:A:GLU:H	1:120:A:GLU:HG3	7	0.11
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	3	0.11
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	6	0.11
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	1	0.11
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	2	0.11
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	3	0.11
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	6	0.11
(1,1724)	1:63:A:GLY:H	1:48:A:HIS:H	7	0.11
(1,1722)	1:74:A:LYS:H	1:74:A:LYS:HB3	1	0.11
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	10	0.11
(1,1678)	1:70:A:LEU:HG	1:70:A:LEU:HA	10	0.11
(1,1674)	1:28:A:VAL:HG11	1:28:A:VAL:HA	1	0.11
(1,1674)	1:28:A:VAL:HG13	1:28:A:VAL:HA	3	0.11
(1,1656)	1:60:A:VAL:HG13	1:49:A:PHE:HA	1	0.11
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD13	2	0.11
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD13	8	0.11
(1,1609)	1:7:A:LEU:HG	1:7:A:LEU:HD12	9	0.11
(1,1573)	1:65:A:PRO:HD2	1:64:A:LYS:HG3	8	0.11
(1,1555)	1:67:A:LEU:HD23	1:67:A:LEU:HD12	8	0.11
(1,1547)	1:61:A:LYS:H	1:61:A:LYS:HG2	1	0.11
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	6	0.11
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	7	0.11
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	8	0.11
(1,1482)	1:153:A:PRO:HG2	1:154:A:LYS:HB2	3	0.11
(1,1482)	1:153:A:PRO:HG2	1:154:A:LYS:HB2	10	0.11
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	5	0.11
(1,1422)	1:65:A:PRO:HG2	1:65:A:PRO:HA	9	0.11
(1,1380)	1:55:A:SER:H	1:55:A:SER:HB3	8	0.11
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD11	5	0.11
(1,1325)	1:35:A:GLN:HB2	1:36:A:CYS:H	3	0.11
(1,1313)	1:143:A:GLU:HB2	1:90:A:SER:HB3	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1305)	1:88:A:HIS:H	1:87:A:GLN:HB2	6	0.11
(1,1298)	1:48:A:HIS:HB3	1:65:A:PRO:HG2	10	0.11
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	5	0.11
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	7	0.11
(1,1213)	1:27:A:PRO:HB2	1:57:A:MET:HG3	9	0.11
(1,1207)	1:57:A:MET:HG3	1:27:A:PRO:HB3	2	0.11
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	3	0.11
(1,1116)	1:29:A:PRO:HB2	1:57:A:MET:HA	10	0.11
(1,1053)	1:75:A:THR:HB	1:74:A:LYS:HA	9	0.11
(1,1027)	1:75:A:THR:HB	1:18:A:GLY:HA3	4	0.11
(1,1020)	1:149:A:VAL:HB	1:90:A:SER:HB2	1	0.11
(1,926)	1:121:A:ILE:HD11	1:138:A:PHE:HB3	10	0.11
(1,894)	1:102:A:VAL:H	1:101:A:MET:HB2	2	0.11
(1,888)	1:101:A:MET:HB3	1:102:A:VAL:H	8	0.11
(1,791)	1:150:A:THR:HG23	1:124:A:TYR:HB3	5	0.11
(1,760)	1:64:A:LYS:HE2	1:116:A:ASP:HB2	2	0.11
(1,688)	1:133:A:PHE:HB2	1:98:A:MET:HG3	8	0.11
(1,644)	1:119:A:CYS:HB3	1:97:A:VAL:HG21	7	0.11
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	7	0.11
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	9	0.11
(1,607)	1:24:A:ILE:HG23	1:25:A:GLY:HA3	7	0.11
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	5	0.11
(1,595)	1:70:A:LEU:HB2	1:18:A:GLY:HA2	7	0.11
(1,537)	1:22:A:PRO:HD3	1:21:A:ALA:HB3	2	0.11
(1,537)	1:22:A:PRO:HD3	1:21:A:ALA:HB2	10	0.11
(1,519)	1:118:A:SER:H	1:117:A:PRO:HD3	5	0.11
(1,501)	1:94:A:ALA:HB2	1:121:A:ILE:HD12	5	0.11
(1,494)	1:94:A:ALA:HB1	1:141:A:PHE:HD2	4	0.11
(1,460)	1:135:A:GLY:H	1:97:A:VAL:HG21	2	0.11
(1,454)	1:155:A:GLN:HE22	1:114:A:ALA:HB2	4	0.11
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG21	9	0.11
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG22	1	0.11
(1,423)	1:58:A:CYS:H	1:31:A:VAL:HG22	2	0.11
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB1	2	0.11
(1,412)	1:21:A:ALA:HB1	1:61:A:LYS:HA	6	0.11
(1,412)	1:21:A:ALA:HB2	1:61:A:LYS:HA	8	0.11
(1,400)	1:37:A:ALA:H	1:37:A:ALA:HB3	7	0.11
(1,388)	1:112:A:ALA:HB2	1:65:A:PRO:HD3	10	0.11
(1,383)	1:36:A:CYS:HA	1:58:A:CYS:HB3	1	0.11
(1,380)	1:112:A:ALA:HB3	1:65:A:PRO:HG3	9	0.11
(1,374)	1:111:A:ALA:HA	1:156:A:PHE:HD1	9	0.11
(1,370)	1:5:A:ALA:HB1	1:5:A:ALA:HA	2	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:5:A:ALA:HB1	1:5:A:ALA:HA	4	0.11
(1,370)	1:5:A:ALA:HB1	1:5:A:ALA:HA	5	0.11
(1,370)	1:5:A:ALA:HB1	1:5:A:ALA:HA	6	0.11
(1,326)	1:100:A:ALA:H	1:100:A:ALA:HB2	8	0.11
(1,294)	1:39:A:GLN:HE22	1:28:A:VAL:HG23	3	0.11
(1,277)	1:143:A:GLU:H	1:146:A:VAL:HG21	7	0.11
(1,276)	1:97:A:VAL:HG13	1:97:A:VAL:HG21	9	0.11
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	1	0.11
(1,264)	1:136:A:ARG:HA	1:137:A:GLY:HA2	6	0.11
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	1	0.11
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	6	0.11
(1,243)	1:149:A:VAL:HG12	1:149:A:VAL:HG21	1	0.11
(1,243)	1:149:A:VAL:HG13	1:149:A:VAL:HG21	10	0.11
(1,235)	1:103:A:THR:HG21	1:124:A:TYR:HD2	3	0.11
(1,233)	1:108:A:ASP:H	1:103:A:THR:HG23	5	0.11
(1,229)	1:131:A:CYS:H	1:103:A:THR:HG23	7	0.11
(1,214)	1:146:A:VAL:HG12	1:146:A:VAL:HB	4	0.11
(1,214)	1:146:A:VAL:HG12	1:146:A:VAL:HB	5	0.11
(1,177)	1:31:A:VAL:HG12	1:31:A:VAL:HB	5	0.11
(1,177)	1:31:A:VAL:HG13	1:31:A:VAL:HB	9	0.11
(1,177)	1:31:A:VAL:HG11	1:31:A:VAL:HB	10	0.11
(1,164)	1:150:A:THR:HG23	1:150:A:THR:HA	8	0.11
(1,164)	1:150:A:THR:HG21	1:150:A:THR:HA	9	0.11
(1,145)	1:43:A:VAL:HG23	1:24:A:ILE:HB	3	0.11
(1,137)	1:59:A:HIS:HD2	1:27:A:PRO:HB2	5	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	2	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	3	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	4	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	6	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	7	0.11
(1,134)	1:59:A:HIS:HB3	1:59:A:HIS:HD2	9	0.11
(1,42)	1:75:A:THR:HG21	1:75:A:THR:HA	4	0.11
(1,41)	1:50:A:THR:HG23	1:75:A:THR:HA	4	0.11
(1,41)	1:50:A:THR:HG22	1:75:A:THR:HA	8	0.11
(1,17)	1:156:A:PHE:HD1	1:156:A:PHE:HA	2	0.11
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	1	0.11
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	9	0.11
(1,3524)	1:31:A:VAL:H	1:58:A:CYS:HB2	4	0.1
(1,3509)	1:35:A:GLN:HE22	1:35:A:GLN:HA	9	0.1
(1,3469)	1:57:A:MET:H	1:55:A:SER:HA	3	0.1
(1,3449)	1:130:A:LYS:H	1:128:A:ASP:HB2	5	0.1
(1,3375)	1:89:A:VAL:H	1:149:A:VAL:H	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3333)	1:75:A:THR:H	1:17:A:LYS:HB2	3	0.1
(1,3313)	1:111:A:ALA:H	1:110:A:GLN:HB2	1	0.1
(1,3312)	1:111:A:ALA:H	1:110:A:GLN:HG3	2	0.1
(1,3280)	1:103:A:THR:H	1:129:A:GLN:HB2	4	0.1
(1,3273)	1:47:A:THR:H	1:78:A:ARG:HG2	7	0.1
(1,3258)	1:94:A:ALA:H	1:91:A:TYR:HB2	3	0.1
(1,3238)	1:107:A:ALA:H	1:77:A:SER:HB3	7	0.1
(1,3205)	1:131:A:CYS:H	1:103:A:THR:H	2	0.1
(1,3199)	1:52:A:ASN:H	1:57:A:MET:HB2	1	0.1
(1,3199)	1:52:A:ASN:H	1:57:A:MET:HB2	3	0.1
(1,3169)	1:51:A:TYR:H	1:33:A:LEU:HD23	1	0.1
(1,3108)	1:130:A:LYS:HG2	1:131:A:CYS:HB2	5	0.1
(1,3077)	1:39:A:GLN:HB3	1:60:A:VAL:HG11	8	0.1
(1,2968)	1:159:A:GLU:HB3	1:159:A:GLU:HG3	6	0.1
(1,2912)	1:142:A:LYS:HB3	1:143:A:GLU:HA	6	0.1
(1,2879)	1:150:A:THR:HB	1:85:A:PHE:HD2	4	0.1
(1,2871)	1:123:A:THR:HB	1:151:A:SER:HA	6	0.1
(1,2762)	1:67:A:LEU:HB3	1:68:A:TYR:HA	7	0.1
(1,2759)	1:134:A:LYS:H	1:133:A:PHE:HB2	1	0.1
(1,2748)	1:82:A:ARG:HD3	1:82:A:ARG:HA	5	0.1
(1,2739)	1:152:A:GLY:HA2	1:153:A:PRO:HG3	3	0.1
(1,2703)	1:116:A:ASP:HB2	1:119:A:CYS:HB3	2	0.1
(1,2646)	1:38:A:ALA:HA	1:37:A:ALA:HA	2	0.1
(1,2646)	1:38:A:ALA:HA	1:37:A:ALA:HA	7	0.1
(1,2646)	1:38:A:ALA:HA	1:37:A:ALA:HA	9	0.1
(1,2645)	1:155:A:GLN:HA	1:155:A:GLN:HG2	9	0.1
(1,2608)	1:53:A:ASP:HA	1:51:A:TYR:HB2	5	0.1
(1,2607)	1:149:A:VAL:HG13	1:149:A:VAL:HG21	10	0.1
(1,2593)	1:49:A:PHE:H	1:75:A:THR:HG21	10	0.1
(1,2572)	1:35:A:GLN:HA	1:35:A:GLN:HG3	10	0.1
(1,2561)	1:89:A:VAL:HG23	1:91:A:TYR:HD1	8	0.1
(1,2550)	1:13:A:HIS:HA	1:13:A:HIS:HB3	6	0.1
(1,2233)	1:98:A:MET:H	1:96:A:ASP:HA	5	0.1
(1,2091)	1:56:A:LYS:H	1:56:A:LYS:HB3	3	0.1
(1,2085)	1:102:A:VAL:H	1:101:A:MET:H	3	0.1
(1,2085)	1:102:A:VAL:H	1:101:A:MET:H	10	0.1
(1,2078)	1:159:A:GLU:H	1:159:A:GLU:HB3	1	0.1
(1,2004)	1:111:A:ALA:H	1:112:A:ALA:HB3	4	0.1
(1,1992)	1:37:A:ALA:H	1:9:A:LEU:HD21	1	0.1
(1,1982)	1:151:A:SER:H	1:89:A:VAL:HG21	2	0.1
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD22	2	0.1
(1,1904)	1:12:A:VAL:H	1:9:A:LEU:HD22	8	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1892)	1:86:A:GLU:H	1:85:A:PHE:HD1	6	0.1
(1,1841)	1:107:A:ALA:H	1:11:A:CYS:HA	2	0.1
(1,1841)	1:107:A:ALA:H	1:11:A:CYS:HA	4	0.1
(1,1782)	1:52:A:ASN:H	1:57:A:MET:HB3	8	0.1
(1,1693)	1:20:A:ARG:HG2	1:19:A:SER:HA	6	0.1
(1,1678)	1:70:A:LEU:HG	1:70:A:LEU:HA	2	0.1
(1,1678)	1:70:A:LEU:HG	1:70:A:LEU:HA	4	0.1
(1,1678)	1:70:A:LEU:HG	1:70:A:LEU:HA	8	0.1
(1,1678)	1:70:A:LEU:HG	1:70:A:LEU:HA	9	0.1
(1,1668)	1:148:A:GLY:H	1:147:A:LEU:HD21	2	0.1
(1,1656)	1:60:A:VAL:HG13	1:49:A:PHE:HA	9	0.1
(1,1531)	1:61:A:LYS:HG3	1:62:A:GLU:H	9	0.1
(1,1482)	1:153:A:PRO:HG2	1:154:A:LYS:HB2	1	0.1
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD12	3	0.1
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD13	7	0.1
(1,1341)	1:71:A:THR:HA	1:70:A:LEU:HD12	8	0.1
(1,1333)	1:79:A:SER:H	1:79:A:SER:HB3	5	0.1
(1,1304)	1:6:A:LYS:HD3	1:56:A:LYS:HB2	5	0.1
(1,1296)	1:56:A:LYS:HA	1:6:A:LYS:HD2	1	0.1
(1,888)	1:101:A:MET:HB3	1:102:A:VAL:H	6	0.1
(1,832)	1:52:A:ASN:HB2	1:51:A:TYR:HA	8	0.1
(1,830)	1:57:A:MET:H	1:52:A:ASN:HB2	6	0.1
(1,828)	1:55:A:SER:H	1:52:A:ASN:HB2	2	0.1
(1,828)	1:55:A:SER:H	1:52:A:ASN:HB2	4	0.1
(1,818)	1:9:A:LEU:HB2	1:12:A:VAL:HG12	2	0.1
(1,733)	1:132:A:THR:H	1:131:A:CYS:HB2	9	0.1
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	2	0.1
(1,625)	1:44:A:ASP:HA	1:45:A:GLY:HA2	4	0.1
(1,471)	1:112:A:ALA:H	1:109:A:CYS:HA	2	0.1
(1,471)	1:112:A:ALA:H	1:109:A:CYS:HA	6	0.1
(1,471)	1:112:A:ALA:H	1:109:A:CYS:HA	8	0.1
(1,428)	1:31:A:VAL:HG23	1:58:A:CYS:HB3	10	0.1
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG23	5	0.1
(1,426)	1:31:A:VAL:H	1:31:A:VAL:HG22	8	0.1
(1,421)	1:114:A:ALA:H	1:114:A:ALA:HB1	9	0.1
(1,413)	1:21:A:ALA:HB2	1:21:A:ALA:HA	1	0.1
(1,413)	1:21:A:ALA:HB3	1:21:A:ALA:HA	4	0.1
(1,383)	1:36:A:CYS:HA	1:58:A:CYS:HB3	8	0.1
(1,370)	1:5:A:ALA:HB3	1:5:A:ALA:HA	3	0.1
(1,370)	1:5:A:ALA:HB1	1:5:A:ALA:HA	8	0.1
(1,285)	1:146:A:VAL:HG22	1:90:A:SER:HA	9	0.1
(1,276)	1:97:A:VAL:HG11	1:97:A:VAL:HG22	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,248)	1:42:A:ALA:H	1:39:A:GLN:HA	2	0.1
(1,246)	1:119:A:CYS:HA	1:116:A:ASP:HB3	2	0.1
(1,231)	1:104:A:SER:H	1:103:A:THR:HG23	8	0.1
(1,214)	1:146:A:VAL:HG11	1:146:A:VAL:HB	2	0.1
(1,177)	1:31:A:VAL:HG11	1:31:A:VAL:HB	4	0.1
(1,89)	1:51:A:TYR:HD1	1:51:A:TYR:HA	9	0.1
(1,15)	1:50:A:THR:H	1:49:A:PHE:HD1	10	0.1

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

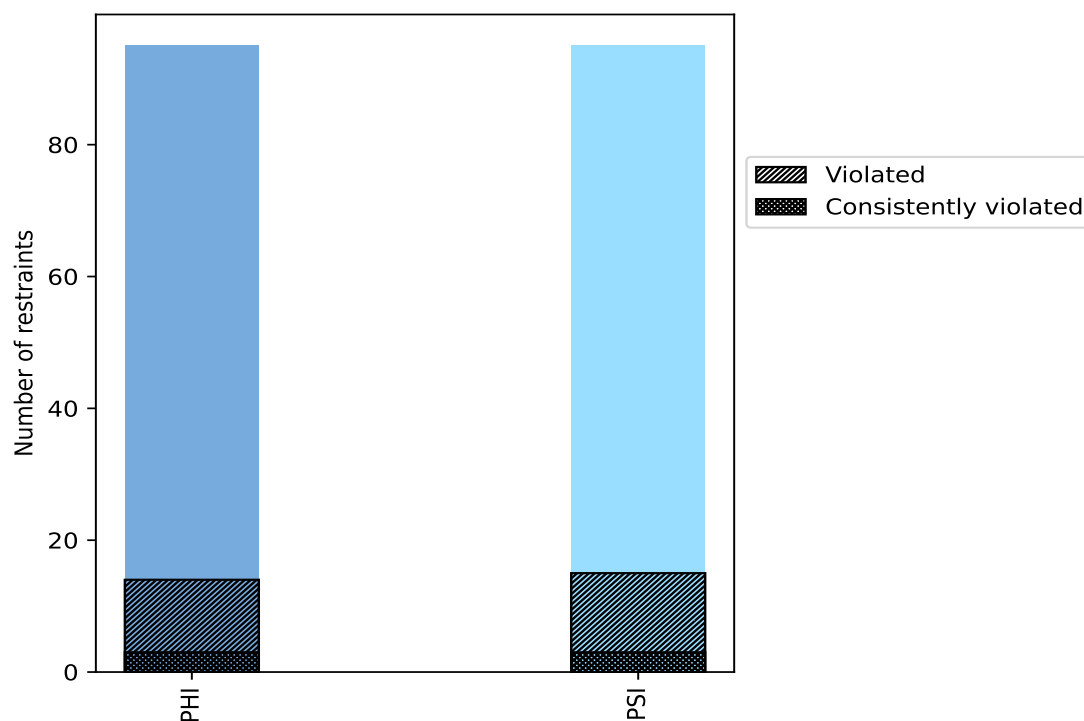
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	95	50.0	14	14.7	7.4	3	3.2	1.6
PSI	95	50.0	15	15.8	7.9	3	3.2	1.6
Total	190	100.0	29	15.3	15.3	6	3.2	3.2

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

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



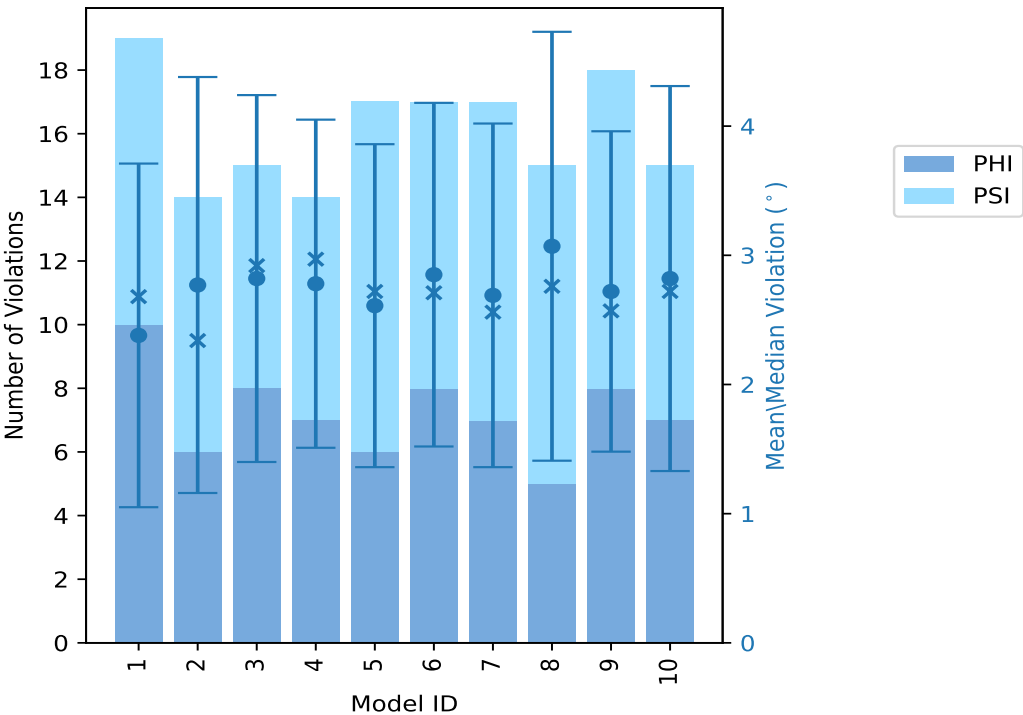
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	10	9	19	2.38	6.45	1.33	2.68
2	6	8	14	2.77	6.36	1.61	2.34
3	8	7	15	2.82	6.76	1.42	2.92
4	7	7	14	2.78	6.05	1.27	2.97
5	6	11	17	2.61	5.92	1.25	2.72
6	8	9	17	2.85	6.57	1.33	2.71
7	7	10	17	2.69	6.73	1.33	2.56
8	5	10	15	3.07	8.04	1.66	2.76
9	8	10	18	2.72	5.88	1.24	2.57
10	7	8	15	2.82	6.55	1.49	2.72

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

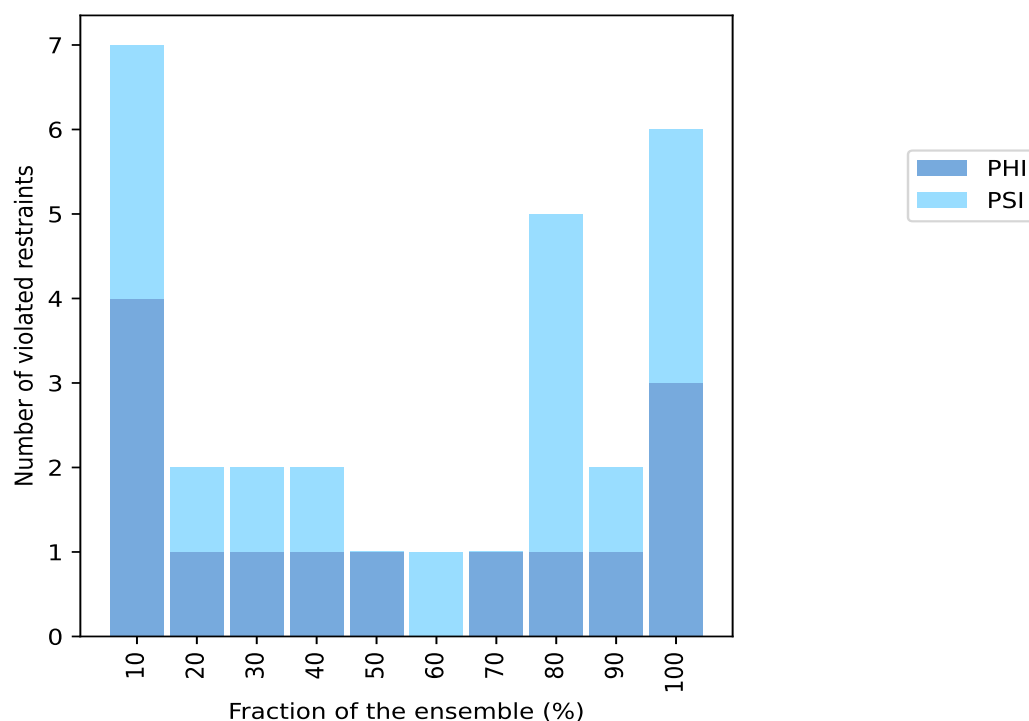
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
4	3	7	1	10.0
1	1	2	2	20.0
1	1	2	3	30.0
1	1	2	4	40.0
1	0	1	5	50.0
0	1	1	6	60.0
1	0	1	7	70.0
1	4	5	8	80.0
1	1	2	9	90.0
3	3	6	10	100.0

¹ Number of models with violations

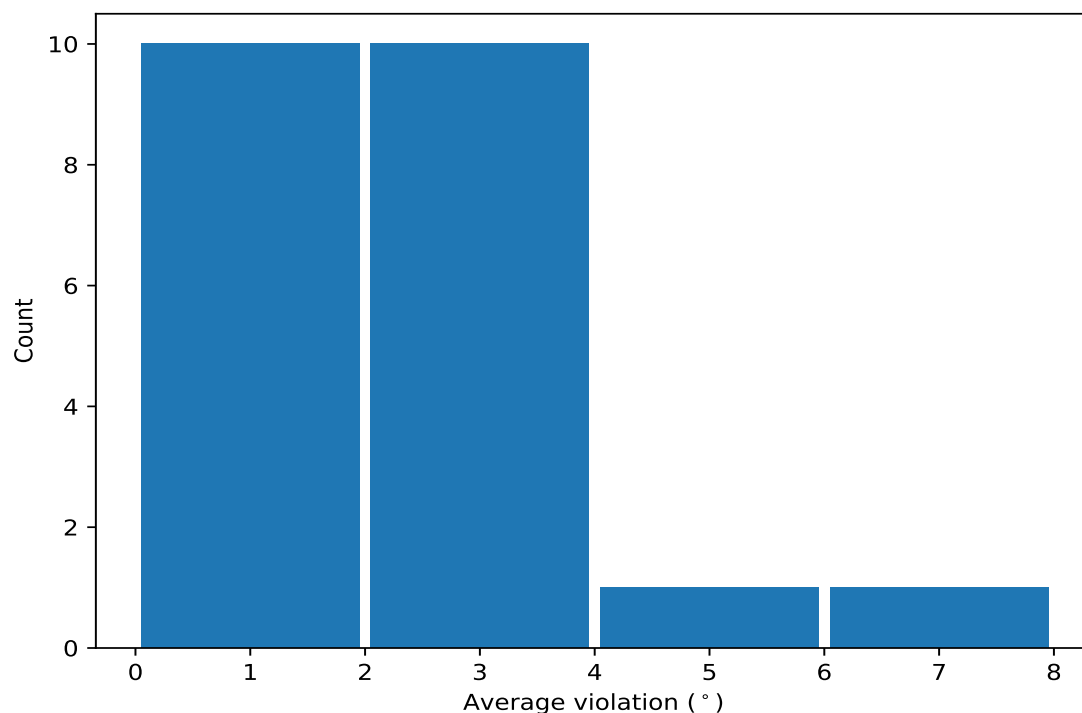
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	10	6.53	0.59	6.5
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	10	4.04	0.4	3.98
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	10	3.83	0.73	3.88
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	10	3.43	0.48	3.4
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	10	3.43	0.46	3.6
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	10	2.68	0.52	2.68
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	9	2.96	0.71	3.14
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	9	1.38	0.27	1.27
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	8	3.04	0.46	2.91
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	8	2.62	0.69	2.62
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	8	2.61	0.54	2.54
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	8	2.4	0.39	2.3
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	8	1.45	0.28	1.47

Continued on next page...

Continued from previous page...

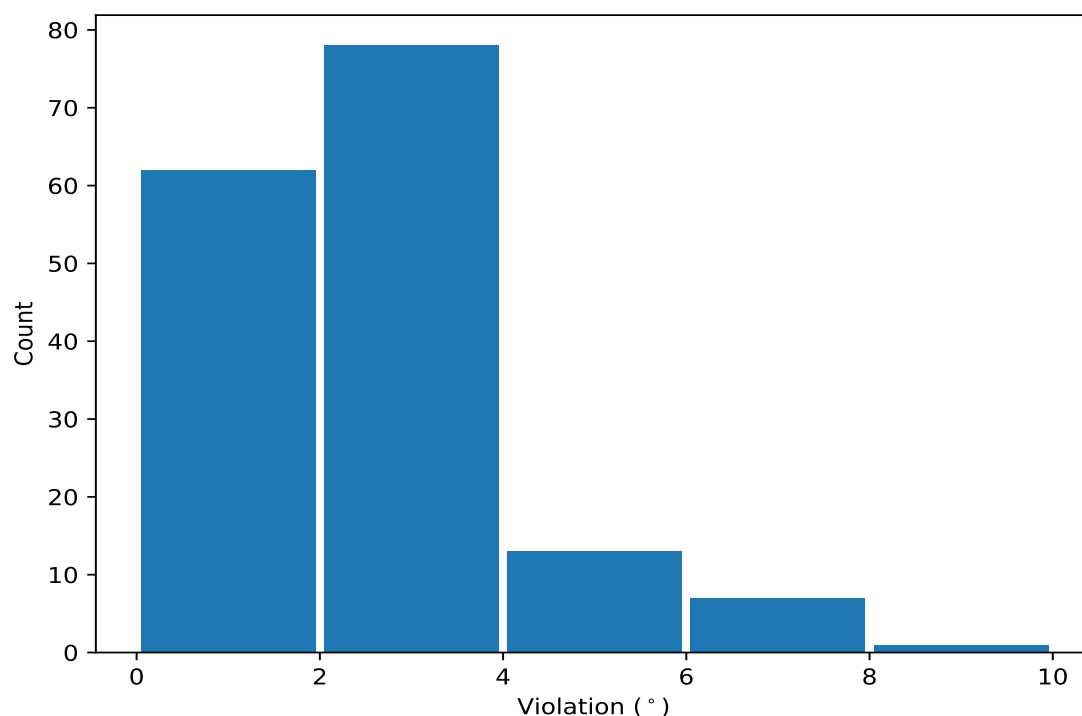
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	7	1.51	0.28	1.6
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	6	1.46	0.28	1.5
(1,54)	1:90:A:SER:C	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	5	1.55	0.2	1.59
(1,99)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:VAL:N	4	2.01	0.58	2.1
(1,28)	1:50:A:THR:C	1:51:A:TYR:N	1:51:A:TYR:CA	1:51:A:TYR:C	4	1.41	0.18	1.43
(1,76)	1:126:A:GLU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	3	1.81	0.67	1.61
(1,118)	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	1:43:A:VAL:N	3	1.3	0.16	1.3
(1,162)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:ALA:N	2	1.78	0.36	1.78
(1,62)	1:104:A:SER:C	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	2	1.21	0.12	1.21

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	8	8.04
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	3	6.76
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	7	6.73
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	6	6.57
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	10	6.55
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	1	6.45
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	2	6.36
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	4	6.05
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	5	5.92
(1,133)	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1:63:A:GLY:N	9	5.88
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	2	5.44
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	5	4.7
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	10	4.53
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	6	4.39
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	8	4.38
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	9	4.36
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	9	4.16
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	10	4.03
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	4	4.01
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	8	4.0
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	2	4.0
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1	3.98
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	7	3.98
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	8	3.97
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	6	3.94
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	10	3.89
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	2	3.82
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	3	3.81
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	3	3.81
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	6	3.78
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	3	3.74
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	7	3.73
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	2	3.68
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	6	3.67
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	4	3.66
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	9	3.61
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	5	3.59
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	3	3.59
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	9	3.53
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	9	3.53
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	8	3.49
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	4	3.47
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	10	3.43
(1,38)	1:61:A:LYS:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	3	3.42
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	6	3.4
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	8	3.4
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	7	3.38
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	1	3.32
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	10	3.29
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	8	3.27
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	9	3.24
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	5	3.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	4	3.2
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	7	3.16
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	7	3.14
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	6	3.13
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	7	3.11
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	10	3.11
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	3	3.11
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	1	3.1
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	4	3.06
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	4	2.99
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	1	2.98
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	4	2.95
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	3	2.92
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	1	2.92
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	5	2.87
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	1	2.86
(1,149)	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1:92:A:GLU:N	5	2.82
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	1	2.82
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	5	2.78
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	5	2.77
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	8	2.76
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	5	2.72
(1,99)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:VAL:N	10	2.72
(1,76)	1:126:A:GLU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	6	2.71
(1,39)	1:62:A:GLU:C	1:63:A:GLY:N	1:63:A:GLY:CA	1:63:A:GLY:C	6	2.71
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	1	2.7
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	7	2.69
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	8	2.68
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	1	2.68
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	9	2.68
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	9	2.57
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	9	2.57
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	7	2.56
(1,26)	1:45:A:GLY:C	1:46:A:CYS:N	1:46:A:CYS:CA	1:46:A:CYS:C	5	2.54
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	6	2.5
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	2	2.44
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	8	2.39
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	2	2.37
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	2	2.31
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	10	2.3
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	6	2.28
(1,99)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:VAL:N	7	2.24
(1,176)	1:133:A:PHE:N	1:133:A:PHE:CA	1:133:A:PHE:C	1:134:A:LYS:N	7	2.22
(1,162)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:ALA:N	5	2.13
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	9	2.05
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	10	2.04
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	7	2.02
(1,103)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:ALA:N	8	1.95
(1,99)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:VAL:N	8	1.95
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	1	1.94
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	2	1.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	3	1.84
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	5	1.8
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	9	1.8
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	4	1.79
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	6	1.77
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	2	1.77
(1,54)	1:90:A:SER:C	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	10	1.77
(1,96)	1:5:A:ALA:N	1:5:A:ALA:CA	1:5:A:ALA:C	1:6:A:LYS:N	3	1.76
(1,54)	1:90:A:SER:C	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	4	1.75
(1,94)	1:151:A:SER:C	1:152:A:GLY:N	1:152:A:GLY:CA	1:152:A:GLY:C	9	1.74
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	3	1.73
(1,46)	1:75:A:THR:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	9	1.67
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	7	1.64
(1,28)	1:50:A:THR:C	1:51:A:TYR:N	1:51:A:TYR:CA	1:51:A:TYR:C	3	1.64
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	6	1.63
(1,76)	1:126:A:GLU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	5	1.61
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	4	1.6
(1,54)	1:90:A:SER:C	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	3	1.59
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	1	1.57
(1,139)	1:74:A:LYS:N	1:74:A:LYS:CA	1:74:A:LYS:C	1:75:A:THR:N	4	1.56
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	6	1.52
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	8	1.52
(1,118)	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	1:43:A:VAL:N	5	1.5
(1,28)	1:50:A:THR:C	1:51:A:TYR:N	1:51:A:TYR:CA	1:51:A:TYR:C	6	1.5
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	9	1.48
(1,33)	1:56:A:LYS:C	1:57:A:MET:N	1:57:A:MET:CA	1:57:A:MET:C	6	1.45
(1,5)	1:11:A:CYS:C	1:12:A:VAL:N	1:12:A:VAL:CA	1:12:A:VAL:C	6	1.43
(1,162)	1:111:A:ALA:N	1:111:A:ALA:CA	1:111:A:ALA:C	1:112:A:ALA:N	4	1.42
(1,156)	1:103:A:THR:N	1:103:A:THR:CA	1:103:A:THR:C	1:104:A:SER:N	4	1.38
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	7	1.38
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	9	1.37
(1,54)	1:90:A:SER:C	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	7	1.36
(1,28)	1:50:A:THR:C	1:51:A:TYR:N	1:51:A:TYR:CA	1:51:A:TYR:C	10	1.36
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	9	1.35
(1,62)	1:104:A:SER:C	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	3	1.33
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	7	1.32
(1,118)	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	1:43:A:VAL:N	9	1.3
(1,54)	1:90:A:SER:C	1:91:A:TYR:N	1:91:A:TYR:CA	1:91:A:TYR:C	1	1.28
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	3	1.27
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	2	1.26
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	1	1.22
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	5	1.19
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	8	1.19
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	2	1.16
(1,28)	1:50:A:THR:C	1:51:A:TYR:N	1:51:A:TYR:CA	1:51:A:TYR:C	5	1.15
(1,188)	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	1:152:A:GLY:N	10	1.14
(1,99)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:VAL:N	2	1.12
(1,118)	1:42:A:ALA:N	1:42:A:ALA:CA	1:42:A:ALA:C	1:43:A:VAL:N	8	1.11
(1,76)	1:126:A:GLU:C	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	1	1.11
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	1	1.1
(1,93)	1:150:A:THR:C	1:151:A:SER:N	1:151:A:SER:CA	1:151:A:SER:C	2	1.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,62)	1:104:A:SER:C	1:105:A:GLN:N	1:105:A:GLN:CA	1:105:A:GLN:C	1	1.09
(1,52)	1:88:A:HIS:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1	1.08
(1,154)	1:101:A:MET:N	1:101:A:MET:CA	1:101:A:MET:C	1:102:A:VAL:N	7	1.07
(1,171)	1:127:A:HIS:N	1:127:A:HIS:CA	1:127:A:HIS:C	1:128:A:ASP:N	1	1.05
(1,70)	1:118:A:SER:C	1:119:A:CYS:N	1:119:A:CYS:CA	1:119:A:CYS:C	10	1.04
(1,130)	1:59:A:HIS:N	1:59:A:HIS:CA	1:59:A:HIS:C	1:60:A:VAL:N	10	1.03
(1,105)	1:23:A:THR:N	1:23:A:THR:CA	1:23:A:THR:C	1:24:A:ILE:N	5	1.0