



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 08:21 AM UTC

PDB ID : 2MGX / pdb_00002mgx
BMRB ID : 19607
Title : NMR structure of SRA1p C-terminal domain
Authors : Bilinovich, S.M.; Davis, C.M.; Morris, D.L.; Ray, L.A.; Prokop, J.W.; Buchan, G.J.; Leeper, T.C.
Deposited on : 2013-11-10

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

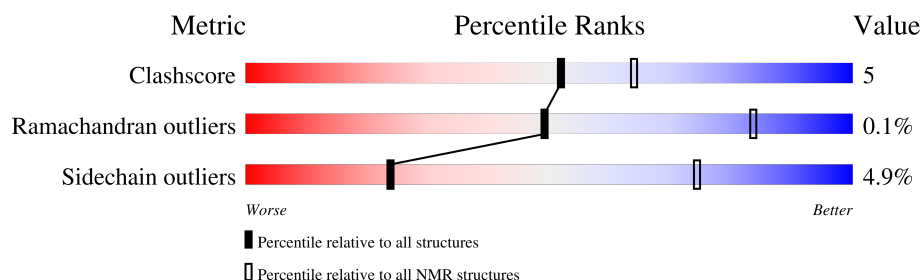
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	131	

2 Ensemble composition and analysis

This entry contains 15 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:109-A:126, A:134-A:209 (94)	0.93	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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2069 atoms, of which 1036 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Steroid receptor RNA activator 1.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			2069	636	1036	192	199	6	

There is a discrepancy between the modelled and reference sequences:

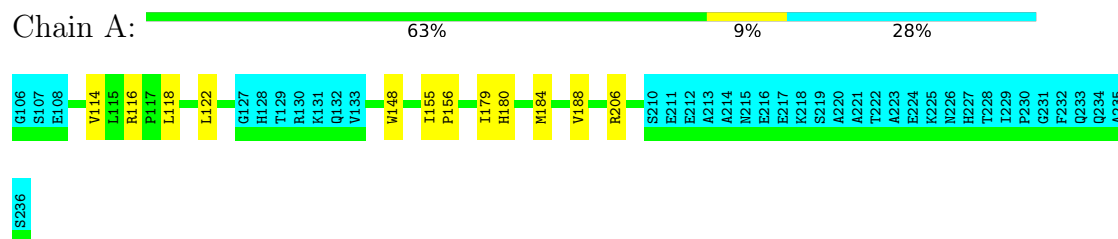
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP Q9HD15

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Steroid receptor RNA activator 1

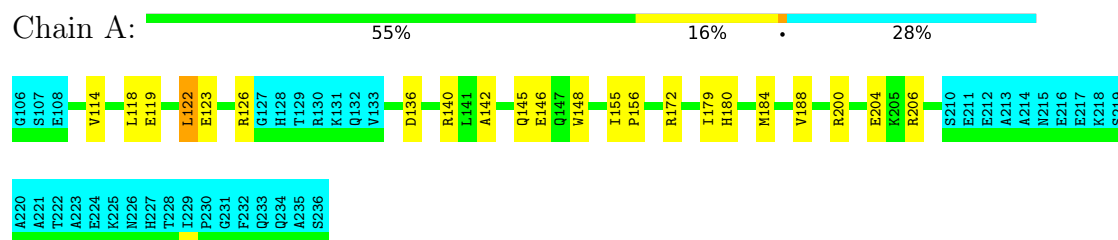


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

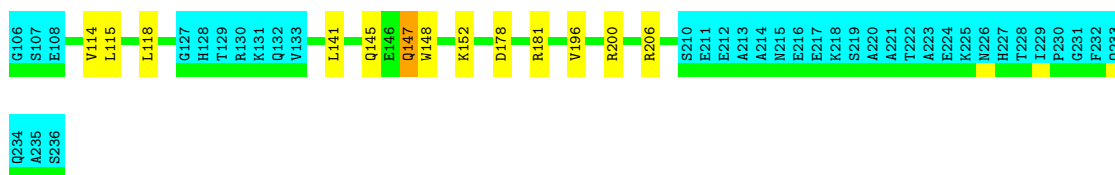
- Molecule 1: Steroid receptor RNA activator 1



4.2.2 Score per residue for model 2

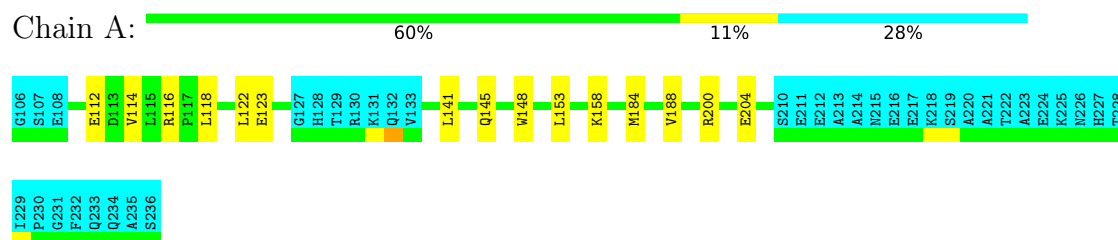
- Molecule 1: Steroid receptor RNA activator 1





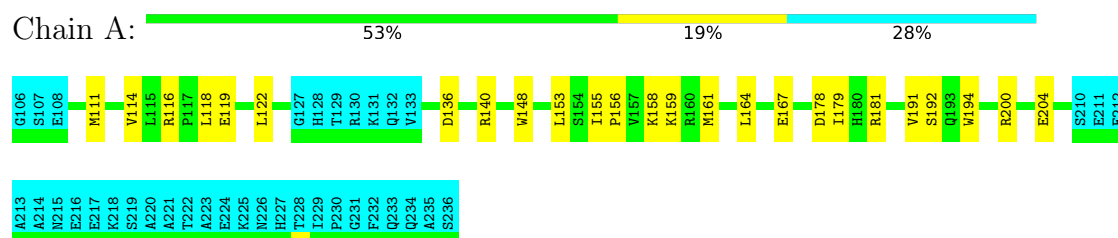
4.2.3 Score per residue for model 3

- Molecule 1: Steroid receptor RNA activator 1



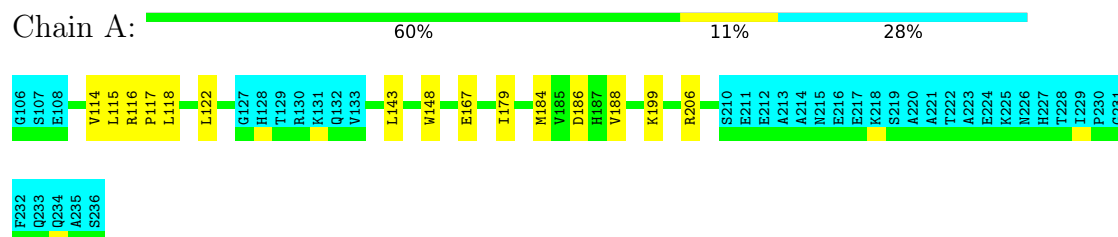
4.2.4 Score per residue for model 4

- Molecule 1: Steroid receptor RNA activator 1



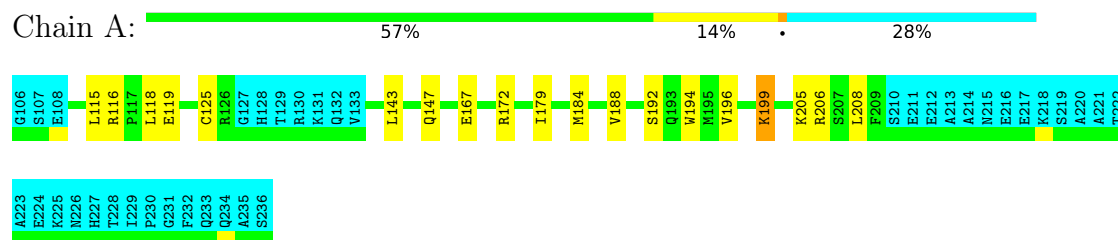
4.2.5 Score per residue for model 5

- Molecule 1: Steroid receptor RNA activator 1



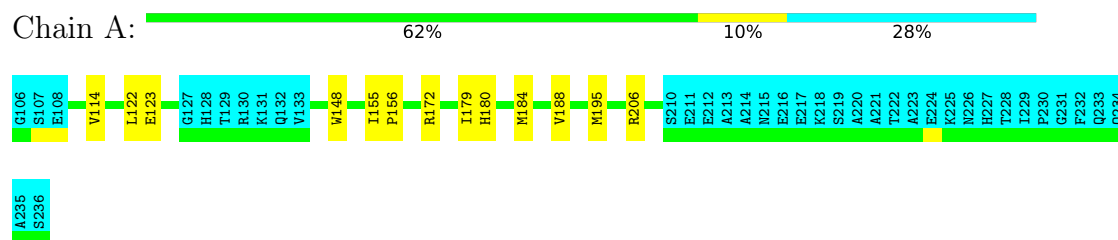
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Steroid receptor RNA activator 1



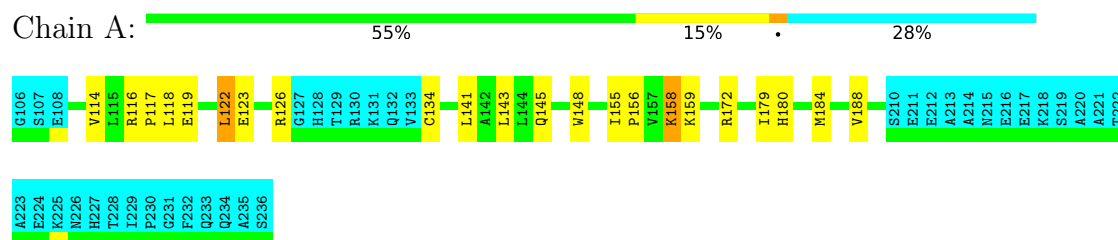
4.2.7 Score per residue for model 7

- Molecule 1: Steroid receptor RNA activator 1



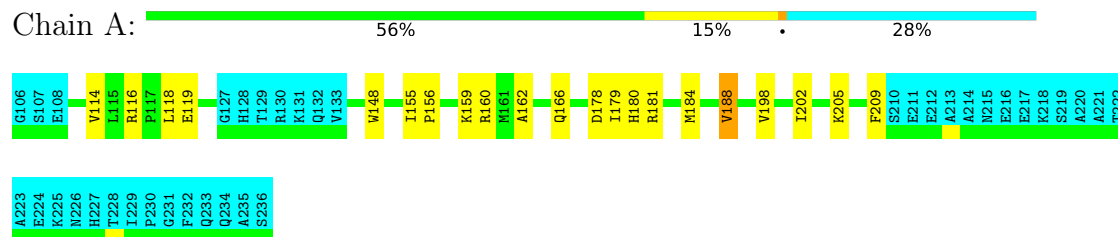
4.2.8 Score per residue for model 8

- Molecule 1: Steroid receptor RNA activator 1



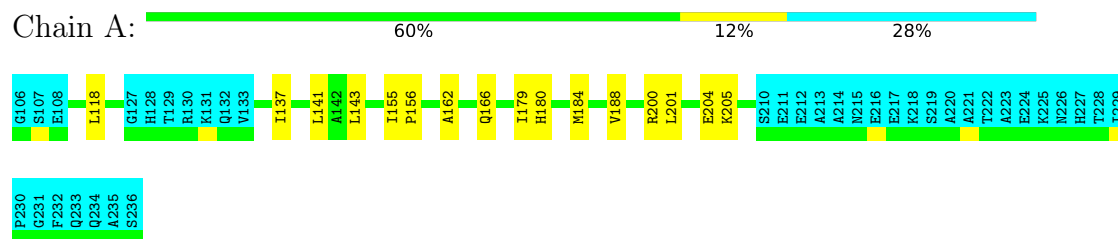
4.2.9 Score per residue for model 9

- Molecule 1: Steroid receptor RNA activator 1



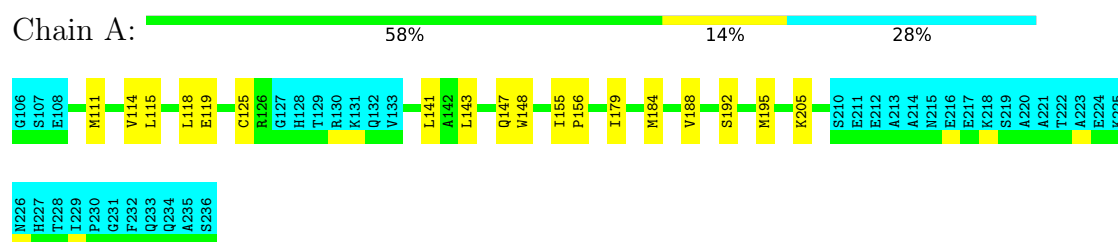
4.2.10 Score per residue for model 10

- Molecule 1: Steroid receptor RNA activator 1



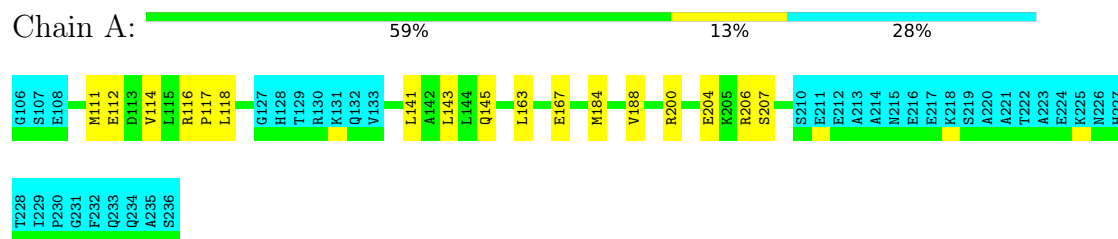
4.2.11 Score per residue for model 11

- Molecule 1: Steroid receptor RNA activator 1



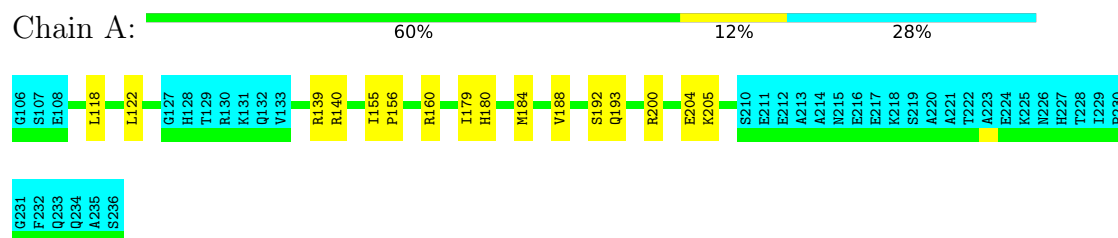
4.2.12 Score per residue for model 12

- Molecule 1: Steroid receptor RNA activator 1



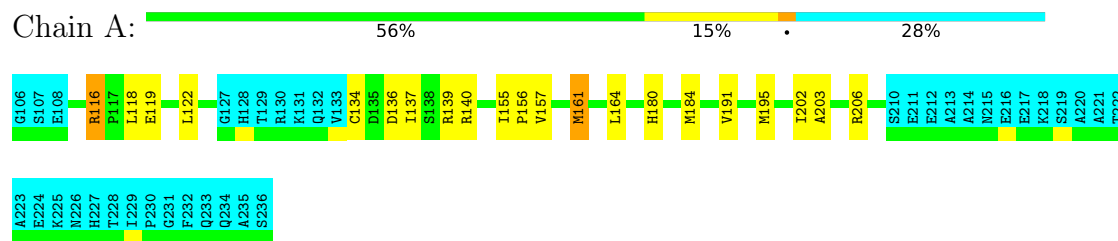
4.2.13 Score per residue for model 13

- Molecule 1: Steroid receptor RNA activator 1



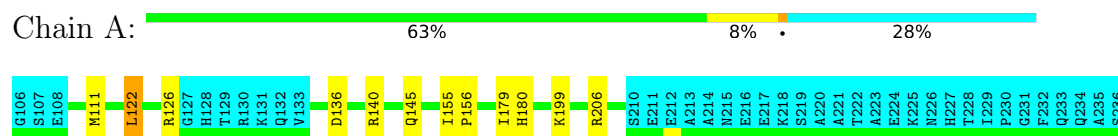
4.2.14 Score per residue for model 14

- Molecule 1: Steroid receptor RNA activator 1



4.2.15 Score per residue for model 15

- Molecule 1: Steroid receptor RNA activator 1



5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	2.3
ARIA	structure solution	2.3

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	1449
Number of shifts mapped to atoms	1449
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	757	778	775	8±3
All	All	11355	11670	11625	123

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:LEU:HD12	1:A:123:GLU:N	0.68	2.04	7	1
1:A:126:ARG:HG3	1:A:134:CYS:SG	0.65	2.30	8	1
1:A:136:ASP:O	1:A:139:ARG:HG2	0.64	1.93	14	1
1:A:184:MET:O	1:A:188:VAL:HB	0.63	1.92	9	10
1:A:180:HIS:O	1:A:184:MET:HG2	0.63	1.93	13	1
1:A:202:ILE:O	1:A:206:ARG:HG3	0.62	1.94	14	1
1:A:136:ASP:O	1:A:140:ARG:HG2	0.62	1.93	4	3
1:A:200:ARG:O	1:A:204:GLU:HG2	0.58	1.98	13	6
1:A:141:LEU:O	1:A:145:GLN:HG2	0.57	2.00	2	3
1:A:201:LEU:O	1:A:205:LYS:HG2	0.57	1.99	10	1
1:A:116:ARG:O	1:A:119:GLU:HG2	0.56	2.01	14	4
1:A:140:ARG:HD2	1:A:193:GLN:O	0.54	2.01	13	1
1:A:155:ILE:N	1:A:156:PRO:HD2	0.54	2.18	10	10
1:A:184:MET:SD	1:A:195:MET:HE2	0.54	2.42	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:LEU:O	1:A:208:LEU:HD13	0.54	2.03	6	1
1:A:114:VAL:HG21	1:A:148:TRP:CH2	0.53	2.39	3	8
1:A:153:LEU:HD11	1:A:194:TRP:CH2	0.53	2.38	4	1
1:A:111:MET:SD	1:A:145:GLN:HA	0.52	2.44	15	1
1:A:178:ASP:O	1:A:181:ARG:HG2	0.52	2.05	9	3
1:A:148:TRP:CH2	1:A:158:LYS:HG3	0.51	2.41	8	1
1:A:148:TRP:CZ2	1:A:158:LYS:HG3	0.51	2.41	8	1
1:A:157:VAL:HG11	1:A:191:VAL:HG11	0.51	1.81	14	1
1:A:198:VAL:O	1:A:202:ILE:HG12	0.50	2.06	9	1
1:A:122:LEU:O	1:A:126:ARG:HB3	0.49	2.07	8	2
1:A:147:GLN:OE1	1:A:152:LYS:HD2	0.48	2.08	2	1
1:A:142:ALA:O	1:A:145:GLN:HG2	0.48	2.09	1	1
1:A:122:LEU:O	1:A:122:LEU:HD22	0.48	2.08	1	1
1:A:180:HIS:HB3	1:A:184:MET:SD	0.48	2.48	14	1
1:A:125:CYS:SG	1:A:205:LYS:HE2	0.48	2.48	6	2
1:A:123:GLU:O	1:A:126:ARG:HG2	0.48	2.08	1	1
1:A:111:MET:HB3	1:A:148:TRP:CD1	0.48	2.44	11	2
1:A:122:LEU:HD13	1:A:122:LEU:C	0.48	2.34	1	1
1:A:162:ALA:O	1:A:166:GLN:HG2	0.48	2.09	10	2
1:A:136:ASP:O	1:A:140:ARG:HG3	0.47	2.09	1	1
1:A:188:VAL:O	1:A:192:SER:HB2	0.47	2.09	6	1
1:A:179:ILE:HD12	1:A:180:HIS:N	0.47	2.24	1	6
1:A:112:GLU:O	1:A:116:ARG:HG3	0.46	2.10	12	1
1:A:116:ARG:HB2	1:A:117:PRO:HD3	0.46	1.87	5	2
1:A:167:GLU:OE1	1:A:172:ARG:HD3	0.46	2.11	6	1
1:A:205:LYS:HA	1:A:208:LEU:HB3	0.46	1.88	6	1
1:A:139:ARG:C	1:A:139:ARG:HD3	0.46	2.36	13	1
1:A:119:GLU:O	1:A:123:GLU:HG3	0.45	2.11	1	2
1:A:111:MET:O	1:A:114:VAL:HG12	0.45	2.11	12	1
1:A:147:GLN:HG3	1:A:194:TRP:CZ3	0.45	2.46	6	1
1:A:172:ARG:HA	1:A:172:ARG:NE	0.45	2.26	1	1
1:A:112:GLU:O	1:A:116:ARG:HG2	0.45	2.11	3	1
1:A:188:VAL:HA	1:A:192:SER:OG	0.45	2.11	11	1
1:A:161:MET:O	1:A:164:LEU:HB3	0.44	2.13	4	2
1:A:199:LYS:NZ	1:A:199:LYS:HB2	0.44	2.28	6	1
1:A:192:SER:HA	1:A:195:MET:CG	0.44	2.42	11	1
1:A:163:LEU:O	1:A:167:GLU:HG2	0.44	2.11	12	1
1:A:202:ILE:HD12	1:A:203:ALA:N	0.44	2.27	14	1
1:A:196:VAL:O	1:A:199:LYS:HG3	0.43	2.13	6	1
1:A:115:LEU:O	1:A:119:GLU:HG3	0.43	2.13	11	1
1:A:122:LEU:HD12	1:A:122:LEU:C	0.43	2.38	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ILE:O	1:A:141:LEU:HB2	0.43	2.14	10	1
1:A:188:VAL:O	1:A:192:SER:HB3	0.43	2.14	13	1
1:A:122:LEU:HD13	1:A:123:GLU:N	0.43	2.29	1	1
1:A:196:VAL:O	1:A:200:ARG:HG3	0.43	2.14	2	1
1:A:156:PRO:O	1:A:160:ARG:HG2	0.43	2.13	9	1
1:A:153:LEU:O	1:A:158:LYS:HE3	0.42	2.13	3	1
1:A:114:VAL:O	1:A:117:PRO:HD2	0.41	2.14	8	1
1:A:205:LYS:O	1:A:209:PHE:HB2	0.41	2.15	9	1
1:A:184:MET:SD	1:A:195:MET:HE3	0.41	2.56	14	1
1:A:148:TRP:CE2	1:A:158:LYS:HD3	0.41	2.51	4	1
1:A:116:ARG:HB3	1:A:117:PRO:HD3	0.41	1.91	8	1
1:A:179:ILE:HD12	1:A:179:ILE:C	0.41	2.41	11	2
1:A:115:LEU:HD11	1:A:145:GLN:NE2	0.41	2.31	2	1
1:A:191:VAL:HA	1:A:194:TRP:CH2	0.41	2.51	4	1
1:A:122:LEU:HD12	1:A:122:LEU:HA	0.40	1.75	13	1
1:A:141:LEU:O	1:A:145:GLN:HG3	0.40	2.16	3	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	94/131 (72%)	89±2 (94±2%)	5±2 (6±2%)	0±0 (0±0%)	49	83
All	All	1410/1965 (72%)	1329 (94%)	80 (6%)	1 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	188	VAL	1

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	83/111 (75%)	79±2 (95±2%)	4±2 (5±2%)	24	74
All	All	1245/1665 (75%)	1184 (95%)	61 (5%)	24	74

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	118	LEU	13
1	A	122	LEU	7
1	A	206	ARG	7
1	A	143	LEU	6
1	A	159	LYS	3
1	A	179	ILE	3
1	A	199	LYS	3
1	A	147	GLN	2
1	A	167	GLU	2
1	A	115	LEU	2
1	A	172	ARG	2
1	A	146	GLU	1
1	A	123	GLU	1
1	A	192	SER	1
1	A	186	ASP	1
1	A	158	LYS	1
1	A	180	HIS	1
1	A	141	LEU	1
1	A	160	ARG	1
1	A	205	LYS	1
1	A	116	ARG	1
1	A	161	MET	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1449
Number of shifts mapped to atoms	1449
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	129	-1.90 ± 0.14	Should be checked
$^{13}\text{C}_\beta$	123	-1.13 ± 0.04	Should be checked
$^{13}\text{C}'$	129	-0.50 ± 0.13	None needed (< 0.5 ppm)
^{15}N	123	-0.01 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1121 atoms were assigned a chemical shift out of a possible 1352. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	469/469 (100%)	189/189 (100%)	188/188 (100%)	92/92 (100%)
Sidechain	600/813 (74%)	399/529 (75%)	197/247 (80%)	4/37 (11%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	52/70 (74%)	27/35 (77%)	22/26 (85%)	3/9 (33%)
Overall	1121/1352 (83%)	615/753 (82%)	407/461 (88%)	99/138 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1446 atoms were assigned a chemical shift out of a possible 1802. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	637/655 (97%)	256/265 (97%)	258/262 (98%)	123/128 (96%)
Sidechain	748/1051 (71%)	492/680 (72%)	252/323 (78%)	4/48 (8%)
Aromatic	61/96 (64%)	32/48 (67%)	26/35 (74%)	3/13 (23%)
Overall	1446/1802 (80%)	780/993 (79%)	536/620 (86%)	130/189 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

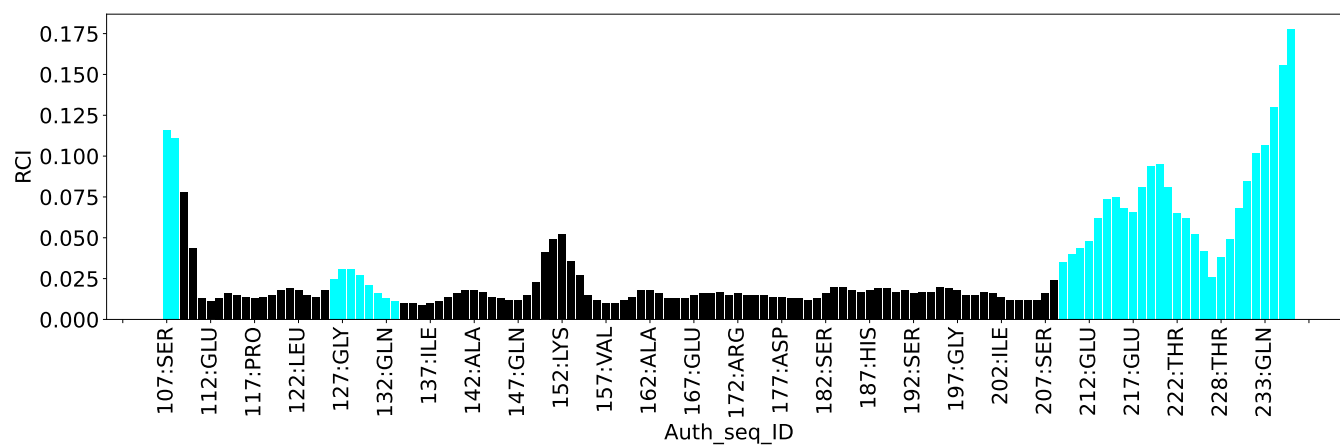
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	158	LYS	HG2	-0.98	0.13 – 2.61	-9.5
1	A	171	HIS	HA	2.08	2.49 – 6.71	-6.0

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	1898
Intra-residue ($ i-j =0$)	737
Sequential ($ i-j =1$)	365
Medium range ($ i-j >1$ and $ i-j <5$)	439
Long range ($ i-j \geq 5$)	301
Inter-chain	0
Hydrogen bond restraints	56
Disulfide bond restraints	0
Total dihedral-angle restraints	177
Number of unmapped restraints	0
Number of restraints per residue	15.8
Number of long range restraints per residue ¹	2.3

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)	43.6	0.2
0.2-0.5 (Medium)	80.5	0.5
>0.5 (Large)	126.3	47.36

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)	8.7	9.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

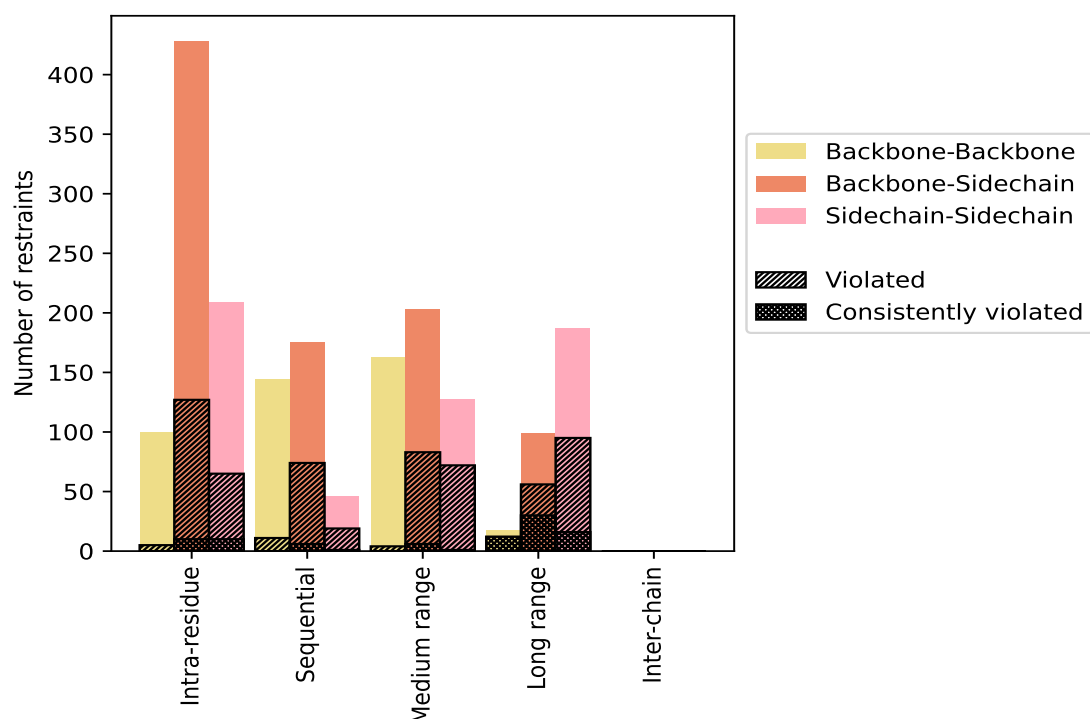
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	737	38.8	197	26.7	10.4	20	2.7	1.1
Backbone-Backbone	100	5.3	5	5.0	0.3	0	0.0	0.0
Backbone-Sidechain	428	22.6	127	29.7	6.7	10	2.3	0.5
Sidechain-Sidechain	209	11.0	65	31.1	3.4	10	4.8	0.5
Sequential ($i-j =1$)	365	19.2	104	28.5	5.5	7	1.9	0.4
Backbone-Backbone	144	7.6	11	7.6	0.6	0	0.0	0.0
Backbone-Sidechain	175	9.2	74	42.3	3.9	6	3.4	0.3
Sidechain-Sidechain	46	2.4	19	41.3	1.0	1	2.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	439	23.1	156	35.5	8.2	7	1.6	0.4
Backbone-Backbone	163	8.6	4	2.5	0.2	0	0.0	0.0
Backbone-Sidechain	149	7.9	80	53.7	4.2	6	4.0	0.3
Sidechain-Sidechain	127	6.7	72	56.7	3.8	1	0.8	0.1
Long range ($i-j \geq 5$)	301	15.9	161	53.5	8.5	56	18.6	3.0
Backbone-Backbone	17	0.9	12	70.6	0.6	12	70.6	0.6
Backbone-Sidechain	97	5.1	54	55.7	2.8	28	28.9	1.5
Sidechain-Sidechain	187	9.9	95	50.8	5.0	16	8.6	0.8
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	56	3.0	5	8.9	0.3	2	3.6	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1898	100.0	623	32.8	32.8	92	4.8	4.8
Backbone-Backbone	424	22.3	32	7.5	1.7	12	2.8	0.6
Backbone-Sidechain	905	47.7	340	37.6	17.9	52	5.7	2.7
Sidechain-Sidechain	569	30.0	251	44.1	13.2	28	4.9	1.5

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	70	32	55	91	0	248	8.66	46.95	15.55	0.5
2	67	41	51	88	0	247	4.84	36.9	9.52	0.53
3	68	39	66	86	0	259	6.79	47.36	12.78	0.53
4	70	42	62	89	0	263	5.33	33.79	9.72	0.49
5	70	36	53	98	0	257	6.86	43.62	12.63	0.46
6	68	34	56	104	0	262	4.85	36.58	9.15	0.49
7	66	38	55	88	0	247	7.07	41.55	12.72	0.49
8	72	39	46	89	0	246	6.23	39.38	11.32	0.48
9	75	45	54	91	0	265	6.89	39.66	12.74	0.52
10	71	36	61	90	0	258	6.83	38.54	12.35	0.6

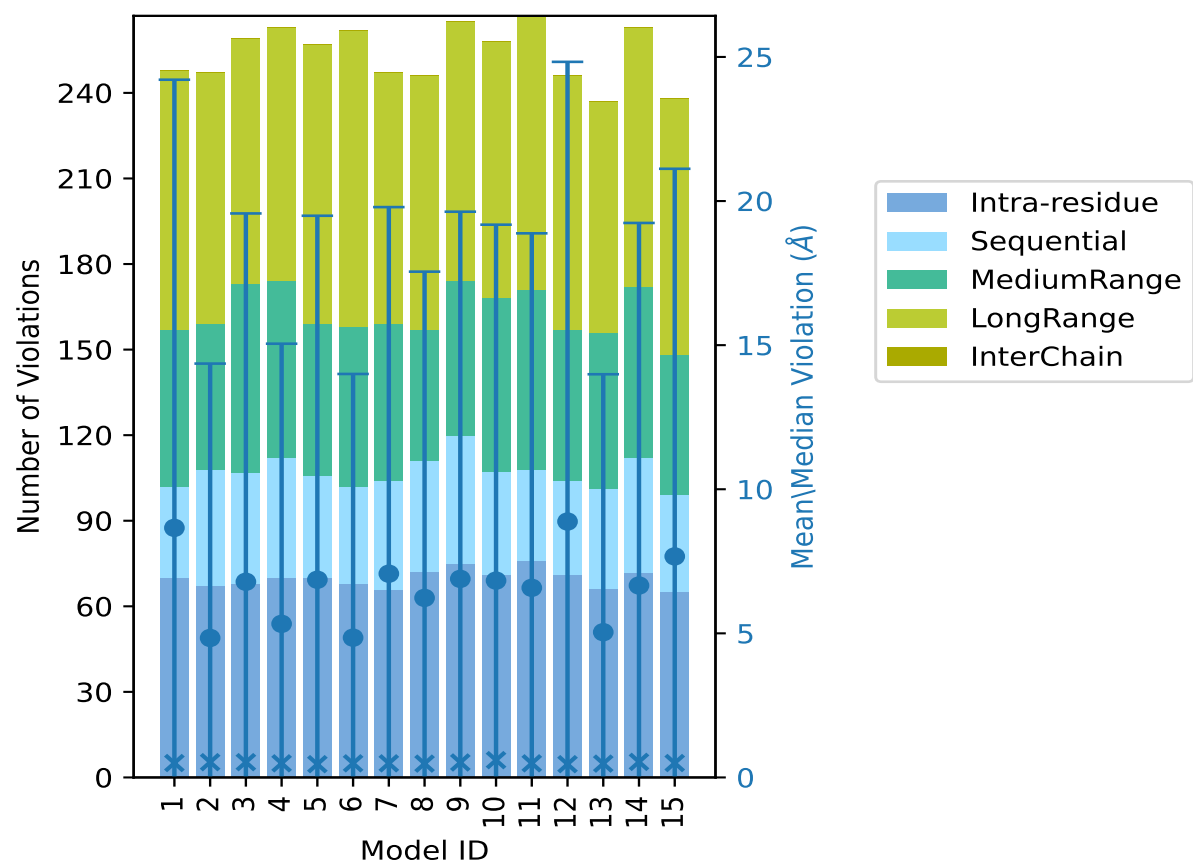
Continued on next page...

Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	76	32	63	96	0	267	6.58	41.77	12.3	0.49
12	71	33	53	89	0	246	8.88	45.18	15.95	0.46
13	66	35	55	81	0	237	5.04	33.41	8.95	0.48
14	72	40	60	91	0	263	6.66	46.83	12.58	0.54
15	65	34	49	90	0	238	7.67	44.13	13.45	0.5

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

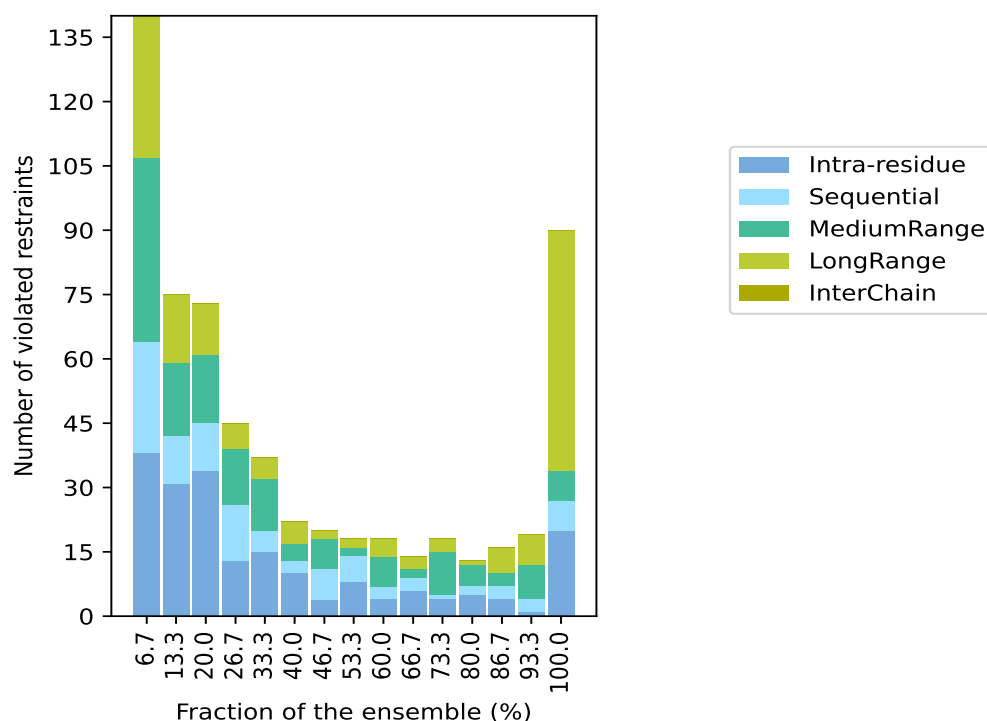
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1224(IR:540, SQ:261, MR:283, LR:140, IC:0) restraints are 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	%
38	26	43	33	0	140	1	6.7
31	11	17	16	0	75	2	13.3
34	11	16	12	0	73	3	20.0
13	13	13	6	0	45	4	26.7
15	5	12	5	0	37	5	33.3
10	3	4	5	0	22	6	40.0
4	7	7	2	0	20	7	46.7
8	6	2	2	0	18	8	53.3
4	3	7	4	0	18	9	60.0
6	3	2	3	0	14	10	66.7
4	1	10	3	0	18	11	73.3
5	2	5	1	0	13	12	80.0
4	3	3	6	0	16	13	86.7
1	3	8	7	0	19	14	93.3
20	7	7	56	0	90	15	100.0

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

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

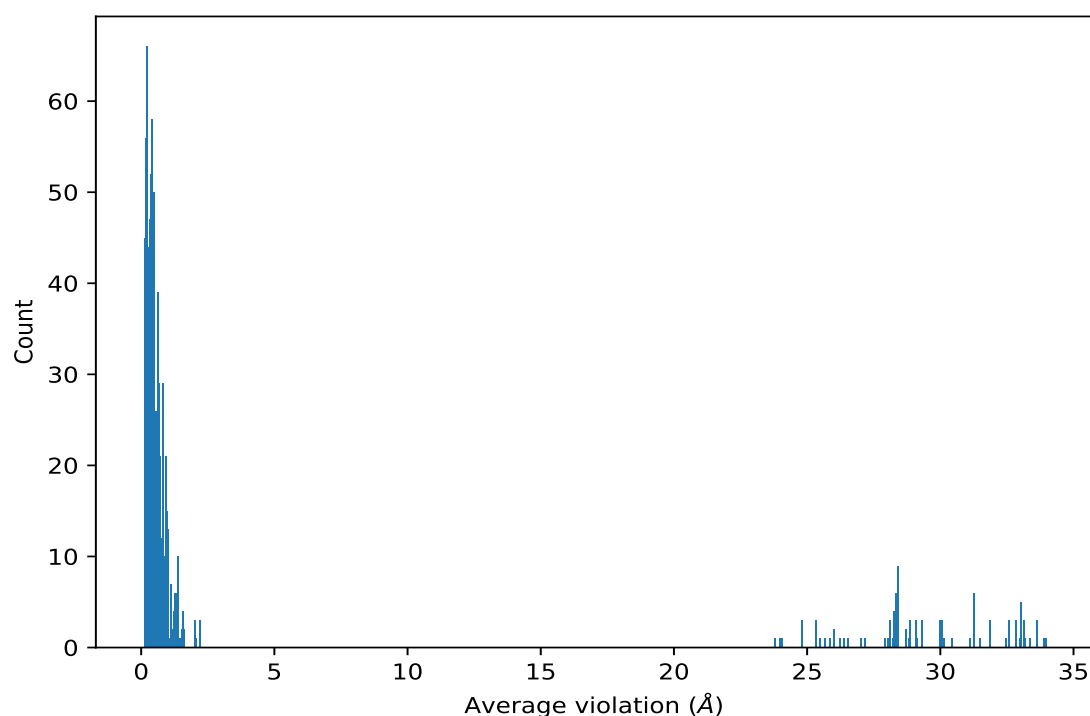
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	15	33.96	9.93	36.3
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	15	33.86	8.74	35.8
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	15	33.62	4.08	33.79
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB1	15	33.62	4.08	33.79
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB2	15	33.62	4.08	33.79
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	15	33.36	9.04	32.03
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	15	33.19	9.66	36.9
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	15	33.14	3.88	32.81
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB1	15	33.14	3.88	32.81
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB2	15	33.14	3.88	32.81
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	15	33.04	3.79	33.25
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	15	33.01	8.72	31.86
(1,739)	1:133:A:VAL:HG11	1:235:A:ALA:H	15	33.01	8.72	31.86
(1,739)	1:133:A:VAL:HG13	1:235:A:ALA:H	15	33.01	8.72	31.86
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	15	33.0	9.31	35.51
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	15	32.95	7.93	32.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	15	32.81	3.59	32.15
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB1	15	32.81	3.59	32.15
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB2	15	32.81	3.59	32.15
(1,595)	1:133:A:VAL:HG21	1:235:A:ALA:H	15	32.59	8.97	31.61
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	15	32.59	8.97	31.61
(1,595)	1:133:A:VAL:HG22	1:235:A:ALA:H	15	32.59	8.97	31.61
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	15	32.48	8.58	30.1
(1,674)	1:110:A:VAL:HG13	1:215:A:ASN:H	15	31.88	4.16	31.33
(1,674)	1:110:A:VAL:HG12	1:215:A:ASN:H	15	31.88	4.16	31.33
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	15	31.88	4.16	31.33
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	15	31.49	10.02	35.49
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	15	31.29	3.84	31.24
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB1	15	31.29	3.84	31.24
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB2	15	31.29	3.84	31.24
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	15	31.26	8.04	31.17
(1,1212)	1:110:A:VAL:HG21	1:217:A:GLU:HG3	15	31.26	8.04	31.17
(1,1212)	1:110:A:VAL:HG22	1:217:A:GLU:HG3	15	31.26	8.04	31.17
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	15	31.12	8.11	33.58
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	15	30.44	9.35	32.22
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	15	30.12	3.61	30.27
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	15	30.05	8.95	31.72
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD22	15	30.05	8.95	31.72
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD23	15	30.05	8.95	31.72
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD12	15	29.96	9.14	31.83
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD13	15	29.96	9.14	31.83
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	15	29.96	9.14	31.83
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	15	29.33	3.89	28.19
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB1	15	29.33	3.89	28.19
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB2	15	29.33	3.89	28.19
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	15	29.11	9.42	29.09
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	15	29.09	9.44	31.77
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	15	29.07	7.43	28.89
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	15	29.07	7.43	28.89
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	15	28.86	4.06	28.13
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB1	15	28.86	4.06	28.13
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB2	15	28.86	4.06	28.13
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	15	28.8	9.49	27.71
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	15	28.74	3.2	28.55
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	15	28.74	3.2	28.55
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB3	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB1	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB3	15	28.41	4.54	28.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB2	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB3	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB2	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB1	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB2	15	28.41	4.54	28.89
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB1	15	28.41	4.54	28.89
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG13	15	28.33	3.68	27.59
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG13	15	28.33	3.68	27.59
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG12	15	28.33	3.68	27.59
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG12	15	28.33	3.68	27.59
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	15	28.33	3.68	27.59
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	15	28.33	3.68	27.59
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	15	28.28	7.86	30.04
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	15	28.27	8.42	29.65
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	15	28.27	8.42	29.65
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD11	15	28.27	8.42	29.65
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	15	28.21	9.08	29.51
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	15	28.13	9.01	30.08
(1,1460)	1:122:A:LEU:HD13	1:227:A:HIS:HB2	15	28.13	9.01	30.08
(1,1460)	1:122:A:LEU:HD11	1:227:A:HIS:HB2	15	28.13	9.01	30.08
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	15	28.04	8.79	30.01
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	15	27.9	9.23	28.9
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	15	27.15	3.95	26.82
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	15	27.03	7.02	26.83
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	15	26.5	9.89	27.56
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	15	26.35	8.75	26.33
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	15	26.24	9.17	26.59
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	15	26.04	7.37	26.54
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	15	26.02	6.57	27.46
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	15	25.85	9.76	26.0
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	15	25.67	9.49	26.42
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	15	25.47	6.49	25.19
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	15	25.34	6.83	25.11
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	15	25.32	8.03	28.05
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	15	25.32	6.6	25.31
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	15	24.81	4.16	23.55
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB1	15	24.81	4.16	23.55
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB2	15	24.81	4.16	23.55
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	15	24.07	9.07	26.64
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	15	23.99	9.92	25.28
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	15	23.76	9.71	25.55
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG11	15	2.2	0.49	2.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	15	2.2	0.49	2.38
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG13	15	2.2	0.49	2.38
(1,250)	1:191:A:VAL:HG23	1:185:A:VAL:H	15	1.02	0.13	1.05
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	15	1.02	0.13	1.05
(1,250)	1:191:A:VAL:HG21	1:185:A:VAL:H	15	1.02	0.13	1.05
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	15	1.01	0.14	1.1
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	15	0.98	0.29	1.02
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	15	0.98	0.29	1.02
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD22	15	0.98	0.29	1.02
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	15	0.9	0.42	0.8
(1,1500)	1:185:A:VAL:HG11	1:187:A:HIS:HA	15	0.9	0.42	0.8
(1,1500)	1:185:A:VAL:HG12	1:187:A:HIS:HA	15	0.9	0.42	0.8
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	15	0.87	0.05	0.87
(1,370)	1:198:A:VAL:HG13	1:198:A:VAL:H	15	0.85	0.03	0.85
(1,370)	1:198:A:VAL:HG12	1:198:A:VAL:H	15	0.85	0.03	0.85
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	15	0.85	0.03	0.85
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG22	15	0.84	0.23	0.9
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	15	0.84	0.23	0.9
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG23	15	0.84	0.23	0.9
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	15	0.8	0.07	0.78
(1,1769)	1:144:A:LEU:HD22	1:194:A:TRP:HZ2	15	0.8	0.07	0.78
(1,1769)	1:144:A:LEU:HD23	1:194:A:TRP:HZ2	15	0.8	0.07	0.78
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD11	15	0.72	0.15	0.77
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD12	15	0.72	0.15	0.77
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	15	0.72	0.15	0.77
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	15	0.69	0.29	0.84
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	15	0.65	0.14	0.61
(1,273)	1:142:A:ALA:HB1	1:145:A:GLN:H	15	0.65	0.14	0.61
(1,273)	1:142:A:ALA:HB3	1:145:A:GLN:H	15	0.65	0.14	0.61
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	15	0.64	0.03	0.64
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	15	0.64	0.26	0.59
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD13	15	0.64	0.26	0.59
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD11	15	0.64	0.26	0.59
(1,796)	1:168:A:LEU:HD21	1:168:A:LEU:H	15	0.62	0.03	0.62
(1,796)	1:168:A:LEU:HD23	1:168:A:LEU:H	15	0.62	0.03	0.62
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	15	0.62	0.03	0.62
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	15	0.57	0.07	0.56
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	15	0.53	0.23	0.47
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	15	0.5	0.21	0.51
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	15	0.49	0.09	0.5
(1,566)	1:144:A:LEU:HD22	1:194:A:TRP:HE1	15	0.49	0.09	0.5
(1,566)	1:144:A:LEU:HD23	1:194:A:TRP:HE1	15	0.49	0.09	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,503)	1:153:A:LEU:HD11	1:149:A:ALA:H	15	0.48	0.14	0.48
(1,503)	1:153:A:LEU:HD13	1:149:A:ALA:H	15	0.48	0.14	0.48
(1,503)	1:153:A:LEU:HD12	1:149:A:ALA:H	15	0.48	0.14	0.48
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	15	0.48	0.57	0.31
(1,520)	1:164:A:LEU:HD22	1:166:A:GLN:H	15	0.48	0.57	0.31
(1,520)	1:164:A:LEU:HD23	1:166:A:GLN:H	15	0.48	0.57	0.31
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	15	0.47	0.09	0.48
(1,403)	1:137:A:ILE:HG23	1:137:A:ILE:H	15	0.45	0.03	0.44
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	15	0.45	0.03	0.44
(1,403)	1:137:A:ILE:HG22	1:137:A:ILE:H	15	0.45	0.03	0.44
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	15	0.45	0.12	0.5
(1,378)	1:149:A:ALA:HB3	1:146:A:GLU:H	15	0.44	0.11	0.47
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	15	0.44	0.11	0.47
(1,378)	1:149:A:ALA:HB1	1:146:A:GLU:H	15	0.44	0.11	0.47
(1,80)	1:202:A:ILE:HD11	1:201:A:LEU:H	15	0.39	0.15	0.41
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	15	0.39	0.15	0.41
(1,80)	1:202:A:ILE:HD12	1:201:A:LEU:H	15	0.39	0.15	0.41
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	15	0.39	0.02	0.39
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	15	0.39	0.04	0.39
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	15	0.38	0.07	0.38
(1,119)	1:183:A:LEU:HD23	1:183:A:LEU:H	15	0.37	0.21	0.32
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	15	0.37	0.21	0.32
(1,119)	1:183:A:LEU:HD21	1:183:A:LEU:H	15	0.37	0.21	0.32
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	15	0.37	0.07	0.35
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD21	15	0.37	0.07	0.35
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD22	15	0.37	0.07	0.35
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	15	0.34	0.11	0.36
(1,794)	1:144:A:LEU:HD13	1:143:A:LEU:H	15	0.34	0.11	0.36
(1,794)	1:144:A:LEU:HD11	1:143:A:LEU:H	15	0.34	0.11	0.36
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	15	0.34	0.01	0.34
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	15	0.29	0.06	0.32
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	15	0.27	0.04	0.28
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	15	0.27	0.01	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	15	0.26	0.01	0.26
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	15	0.22	0.01	0.22
(1,1389)	1:198:A:VAL:HG11	1:144:A:LEU:HD13	14	1.36	0.5	1.37
(1,1389)	1:198:A:VAL:HG13	1:144:A:LEU:HD13	14	1.36	0.5	1.37
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD13	14	1.36	0.5	1.37
(1,1389)	1:198:A:VAL:HG13	1:144:A:LEU:HD12	14	1.36	0.5	1.37
(1,1389)	1:198:A:VAL:HG11	1:144:A:LEU:HD12	14	1.36	0.5	1.37
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD12	14	1.36	0.5	1.37
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD11	14	1.36	0.5	1.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1114)	1:143:A:LEU:HD13	1:140:A:ARG:HB3	14	1.31	0.99	1.1
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	14	1.31	0.99	1.1
(1,1114)	1:143:A:LEU:HD11	1:140:A:ARG:HB3	14	1.31	0.99	1.1
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	14	0.99	0.42	1.02
(1,1578)	1:203:A:ALA:HB1	1:206:A:ARG:HD3	14	0.99	0.42	1.02
(1,1578)	1:203:A:ALA:HB3	1:206:A:ARG:HD3	14	0.99	0.42	1.02
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	14	0.81	0.22	0.73
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	14	0.81	0.27	0.86
(1,1782)	1:143:A:LEU:HD13	1:194:A:TRP:HZ3	14	0.73	0.78	0.42
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	14	0.73	0.78	0.42
(1,1782)	1:143:A:LEU:HD11	1:194:A:TRP:HZ3	14	0.73	0.78	0.42
(1,967)	1:111:A:MET:HE3	1:148:A:TRP:HA	14	0.68	0.3	0.84
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	14	0.68	0.3	0.84
(1,967)	1:111:A:MET:HE2	1:148:A:TRP:HA	14	0.68	0.3	0.84
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	14	0.6	0.18	0.66
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD11	14	0.48	0.19	0.5
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD12	14	0.48	0.19	0.5
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD12	14	0.48	0.19	0.5
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD13	14	0.48	0.19	0.5
(1,1375)	1:144:A:LEU:HD23	1:153:A:LEU:HD11	14	0.48	0.19	0.5
(1,1375)	1:144:A:LEU:HD23	1:153:A:LEU:HD13	14	0.48	0.19	0.5
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD11	14	0.48	0.19	0.5
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	14	0.48	0.02	0.48
(1,1682)	1:168:A:LEU:HD22	1:165:A:VAL:HB	14	0.43	0.21	0.4
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	14	0.43	0.21	0.4
(1,1682)	1:168:A:LEU:HD23	1:165:A:VAL:HB	14	0.43	0.21	0.4
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG21	14	0.41	0.1	0.42
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	14	0.41	0.1	0.42
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG22	14	0.41	0.1	0.42
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	14	0.41	0.08	0.38
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE1	14	0.41	0.08	0.38
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE3	14	0.41	0.08	0.38
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	14	0.41	0.16	0.39
(1,353)	1:157:A:VAL:HG13	1:154:A:SER:H	14	0.41	0.16	0.39
(1,353)	1:157:A:VAL:HG11	1:154:A:SER:H	14	0.41	0.16	0.39
(1,759)	1:137:A:ILE:HD12	1:138:A:SER:H	14	0.34	0.12	0.32
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	14	0.34	0.12	0.32
(1,759)	1:137:A:ILE:HD13	1:138:A:SER:H	14	0.34	0.12	0.32
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	14	0.29	0.21	0.17
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	14	0.22	0.06	0.24
(1,71)	1:142:A:ALA:HB2	1:144:A:LEU:H	14	0.22	0.06	0.24
(1,71)	1:142:A:ALA:HB1	1:144:A:LEU:H	14	0.22	0.06	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	14	0.22	0.04	0.23
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	14	0.21	0.06	0.23
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB3	14	0.21	0.06	0.23
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB1	14	0.21	0.06	0.23
(1,1087)	1:122:A:LEU:HD12	1:126:A:ARG:HB3	13	1.36	0.58	1.69
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	13	1.36	0.58	1.69
(1,1087)	1:122:A:LEU:HD11	1:126:A:ARG:HB3	13	1.36	0.58	1.69
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	13	0.91	0.23	0.98
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	13	0.86	0.24	0.83
(1,43)	1:165:A:VAL:HG21	1:117:A:PRO:HB3	13	0.84	0.4	0.83
(1,43)	1:165:A:VAL:HG22	1:117:A:PRO:HB3	13	0.84	0.4	0.83
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	13	0.84	0.4	0.83
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	13	0.75	0.3	0.73
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	13	0.75	0.3	0.73
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	13	0.69	0.41	0.57
(1,991)	1:155:A:ILE:HD12	1:154:A:SER:HB2	13	0.69	0.41	0.57
(1,991)	1:155:A:ILE:HD13	1:154:A:SER:HB2	13	0.69	0.41	0.57
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG13	13	0.65	0.18	0.59
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG11	13	0.65	0.18	0.59
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG12	13	0.65	0.18	0.59
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	13	0.6	0.15	0.62
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	13	0.54	0.11	0.58
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	13	0.48	0.04	0.49
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	13	0.42	0.16	0.4
(1,349)	1:191:A:VAL:HG23	1:184:A:MET:H	13	0.4	0.15	0.33
(1,349)	1:191:A:VAL:HG22	1:184:A:MET:H	13	0.4	0.15	0.33
(1,349)	1:191:A:VAL:HG21	1:184:A:MET:H	13	0.4	0.15	0.33
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	13	0.36	0.14	0.33
(1,373)	1:179:A:ILE:HG23	1:182:A:SER:H	13	0.36	0.14	0.33
(1,373)	1:179:A:ILE:HG22	1:182:A:SER:H	13	0.36	0.14	0.33
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	13	0.3	0.09	0.31
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	13	0.22	0.08	0.22
(1,570)	1:162:A:ALA:HB2	1:164:A:LEU:H	13	0.22	0.08	0.22
(1,570)	1:162:A:ALA:HB3	1:164:A:LEU:H	13	0.22	0.08	0.22
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	13	0.19	0.06	0.17
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	12	0.9	0.6	0.56
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG11	12	0.9	0.6	0.56
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	12	0.62	0.11	0.54
(1,641)	1:179:A:ILE:HD13	1:178:A:ASP:H	12	0.55	0.19	0.57
(1,641)	1:179:A:ILE:HD12	1:178:A:ASP:H	12	0.55	0.19	0.57
(1,641)	1:179:A:ILE:HD11	1:178:A:ASP:H	12	0.55	0.19	0.57
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG22	12	0.44	0.21	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG21	12	0.44	0.21	0.44
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG23	12	0.44	0.21	0.44
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	12	0.43	0.14	0.43
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	12	0.39	0.05	0.4
(1,108)	1:157:A:VAL:HG21	1:160:A:ARG:H	12	0.32	0.12	0.32
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	12	0.32	0.12	0.32
(1,108)	1:157:A:VAL:HG22	1:160:A:ARG:H	12	0.32	0.12	0.32
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	12	0.32	0.17	0.25
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD13	12	0.32	0.17	0.25
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD11	12	0.32	0.17	0.25
(1,901)	1:202:A:ILE:HD11	1:203:A:ALA:H	12	0.29	0.09	0.29
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	12	0.29	0.09	0.29
(1,901)	1:202:A:ILE:HD12	1:203:A:ALA:H	12	0.29	0.09	0.29
(1,199)	1:175:A:ALA:HB3	1:178:A:ASP:H	12	0.21	0.07	0.2
(1,199)	1:175:A:ALA:HB1	1:178:A:ASP:H	12	0.21	0.07	0.2
(1,199)	1:175:A:ALA:HB2	1:178:A:ASP:H	12	0.21	0.07	0.2
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	12	0.21	0.13	0.17
(1,667)	1:144:A:LEU:HD23	1:144:A:LEU:H	12	0.15	0.04	0.13
(1,667)	1:144:A:LEU:HD22	1:144:A:LEU:H	12	0.15	0.04	0.13
(1,667)	1:144:A:LEU:HD21	1:144:A:LEU:H	12	0.15	0.04	0.13
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	12	0.14	0.01	0.14
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	11	2.06	0.73	2.07
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	11	1.34	1.42	0.64
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD11	11	1.34	1.42	0.64
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD12	11	1.34	1.42	0.64
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD12	11	1.26	0.84	1.41
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD13	11	1.26	0.84	1.41
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD11	11	1.26	0.84	1.41
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	11	1.22	0.37	1.37
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	11	0.81	0.33	0.94
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD21	11	0.79	0.35	0.94
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD22	11	0.79	0.35	0.94
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD23	11	0.79	0.35	0.94
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	11	0.68	0.49	0.61
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD22	11	0.68	0.49	0.61
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD23	11	0.68	0.49	0.61
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG22	11	0.63	0.33	0.54
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG21	11	0.63	0.33	0.54
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG23	11	0.63	0.33	0.54
(1,1743)	1:161:A:MET:HE2	1:114:A:VAL:HG23	11	0.63	0.33	0.54
(1,1743)	1:161:A:MET:HE3	1:114:A:VAL:HG21	11	0.63	0.33	0.54
(1,1743)	1:161:A:MET:HE3	1:114:A:VAL:HG22	11	0.63	0.33	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1743)	1:161:A:MET:HE2	1:114:A:VAL:HG21	11	0.63	0.33	0.54
(1,1743)	1:161:A:MET:HE2	1:114:A:VAL:HG22	11	0.63	0.33	0.54
(1,1024)	1:122:A:LEU:HD12	1:134:A:CYS:HA	11	0.53	0.42	0.49
(1,1024)	1:122:A:LEU:HD13	1:134:A:CYS:HA	11	0.53	0.42	0.49
(1,1024)	1:122:A:LEU:HD11	1:134:A:CYS:HA	11	0.53	0.42	0.49
(1,1571)	1:137:A:ILE:HG23	1:141:A:LEU:HB3	11	0.38	0.2	0.34
(1,1571)	1:137:A:ILE:HG21	1:141:A:LEU:HB3	11	0.38	0.2	0.34
(1,1571)	1:137:A:ILE:HG22	1:141:A:LEU:HB3	11	0.38	0.2	0.34
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	11	0.34	0.02	0.35
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD13	11	0.32	0.09	0.33
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD11	11	0.32	0.09	0.33
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD12	11	0.32	0.09	0.33
(1,872)	1:176:A:ALA:HB2	1:173:A:TRP:H	11	0.31	0.17	0.29
(1,872)	1:176:A:ALA:HB1	1:173:A:TRP:H	11	0.31	0.17	0.29
(1,872)	1:176:A:ALA:HB3	1:173:A:TRP:H	11	0.31	0.17	0.29
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	11	0.3	0.08	0.33
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	11	0.3	0.06	0.32
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	11	0.29	0.24	0.22
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	11	0.25	0.07	0.27
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	11	0.15	0.03	0.16
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	10	0.93	0.49	1.14
(1,468)	1:122:A:LEU:HD12	1:125:A:CYS:H	10	0.62	0.86	0.37
(1,468)	1:122:A:LEU:HD13	1:125:A:CYS:H	10	0.62	0.86	0.37
(1,468)	1:122:A:LEU:HD11	1:125:A:CYS:H	10	0.62	0.86	0.37
(1,1234)	1:208:A:LEU:HD12	1:205:A:LYS:HE2	10	0.61	0.59	0.4
(1,1234)	1:208:A:LEU:HD11	1:205:A:LYS:HE2	10	0.61	0.59	0.4
(1,1234)	1:208:A:LEU:HD13	1:205:A:LYS:HE2	10	0.61	0.59	0.4
(1,1394)	1:122:A:LEU:HD11	1:134:A:CYS:HB3	10	0.58	0.22	0.55
(1,1394)	1:122:A:LEU:HD12	1:134:A:CYS:HB3	10	0.58	0.22	0.55
(1,1394)	1:122:A:LEU:HD13	1:134:A:CYS:HB3	10	0.58	0.22	0.55
(1,1619)	1:122:A:LEU:HD11	1:134:A:CYS:HB2	10	0.58	0.22	0.59
(1,1619)	1:122:A:LEU:HD12	1:134:A:CYS:HB2	10	0.58	0.22	0.59
(1,1619)	1:122:A:LEU:HD13	1:134:A:CYS:HB2	10	0.58	0.22	0.59
(1,352)	1:115:A:LEU:HD11	1:114:A:VAL:H	10	0.56	0.07	0.57
(1,352)	1:115:A:LEU:HD13	1:114:A:VAL:H	10	0.56	0.07	0.57
(1,352)	1:115:A:LEU:HD12	1:114:A:VAL:H	10	0.56	0.07	0.57
(1,1215)	1:202:A:ILE:HD12	1:177:A:ASP:HB3	10	0.54	0.18	0.49
(1,1215)	1:202:A:ILE:HD11	1:177:A:ASP:HB3	10	0.54	0.18	0.49
(1,1215)	1:202:A:ILE:HD13	1:177:A:ASP:HB3	10	0.54	0.18	0.49
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	10	0.48	0.14	0.48
(1,369)	1:214:A:ALA:HB3	1:215:A:ASN:H	10	0.48	0.14	0.48
(1,369)	1:214:A:ALA:HB1	1:215:A:ASN:H	10	0.48	0.14	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	10	0.41	0.04	0.42
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	10	0.37	0.22	0.26
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	10	0.25	0.08	0.24
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	10	0.23	0.07	0.24
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	10	0.21	0.03	0.22
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	10	0.13	0.02	0.12
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG12	9	2.02	0.46	2.0
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG13	9	2.02	0.46	2.0
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG11	9	2.02	0.46	2.0
(1,1475)	1:183:A:LEU:HD21	1:179:A:ILE:HB	9	0.94	0.83	0.53
(1,1475)	1:183:A:LEU:HD22	1:179:A:ILE:HB	9	0.94	0.83	0.53
(1,1475)	1:183:A:LEU:HD23	1:179:A:ILE:HB	9	0.94	0.83	0.53
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	9	0.94	0.52	0.87
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	9	0.9	0.25	0.84
(1,868)	1:133:A:VAL:HG11	1:133:A:VAL:H	9	0.82	0.01	0.82
(1,868)	1:133:A:VAL:HG12	1:133:A:VAL:H	9	0.82	0.01	0.82
(1,868)	1:133:A:VAL:HG13	1:133:A:VAL:H	9	0.82	0.01	0.82
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	9	0.82	0.42	0.66
(1,1722)	1:133:A:VAL:HG22	1:134:A:CYS:HB3	9	0.82	0.42	0.66
(1,1722)	1:133:A:VAL:HG21	1:134:A:CYS:HB3	9	0.82	0.42	0.66
(1,1534)	1:162:A:ALA:HB3	1:113:A:ASP:HB3	9	0.64	0.21	0.78
(1,1534)	1:162:A:ALA:HB1	1:113:A:ASP:HB3	9	0.64	0.21	0.78
(1,1534)	1:162:A:ALA:HB2	1:113:A:ASP:HB3	9	0.64	0.21	0.78
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD23	9	0.59	0.44	0.43
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD22	9	0.59	0.44	0.43
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	9	0.52	0.16	0.55
(1,485)	1:153:A:LEU:HD11	1:194:A:TRP:HE1	9	0.52	0.16	0.55
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	9	0.49	0.33	0.39
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	9	0.45	0.11	0.42
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	9	0.42	0.22	0.36
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	9	0.38	0.08	0.35
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	9	0.37	0.31	0.24
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	9	0.35	0.05	0.36
(1,1641)	1:153:A:LEU:HD11	1:145:A:GLN:HA	9	0.31	0.14	0.35
(1,1641)	1:153:A:LEU:HD12	1:145:A:GLN:HA	9	0.31	0.14	0.35
(1,1641)	1:153:A:LEU:HD13	1:145:A:GLN:HA	9	0.31	0.14	0.35
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	9	0.23	0.06	0.23
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	9	0.16	0.04	0.15
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	8	1.27	0.56	1.5
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD22	8	0.65	0.25	0.76
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD23	8	0.65	0.25	0.76
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD21	8	0.65	0.25	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	8	0.64	0.02	0.65
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	8	0.56	0.02	0.56
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD13	8	0.46	0.16	0.45
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD12	8	0.46	0.16	0.45
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD11	8	0.46	0.16	0.45
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	8	0.44	0.26	0.34
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	8	0.42	0.04	0.39
(1,358)	1:110:A:VAL:HG23	1:111:A:MET:H	8	0.42	0.04	0.39
(1,358)	1:110:A:VAL:HG21	1:111:A:MET:H	8	0.42	0.04	0.39
(1,1758)	1:191:A:VAL:HG22	1:184:A:MET:HA	8	0.38	0.14	0.34
(1,1758)	1:191:A:VAL:HG21	1:184:A:MET:HA	8	0.38	0.14	0.34
(1,1758)	1:191:A:VAL:HG23	1:184:A:MET:HA	8	0.38	0.14	0.34
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	8	0.34	0.17	0.34
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	8	0.3	0.02	0.3
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	8	0.27	0.1	0.26
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD12	8	0.26	0.11	0.24
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD11	8	0.26	0.11	0.24
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	8	0.25	0.07	0.26
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	8	0.23	0.12	0.18
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	8	0.21	0.03	0.21
(1,693)	1:162:A:ALA:HB1	1:161:A:MET:H	8	0.17	0.03	0.18
(1,693)	1:162:A:ALA:HB3	1:161:A:MET:H	8	0.17	0.03	0.18
(1,693)	1:162:A:ALA:HB2	1:161:A:MET:H	8	0.17	0.03	0.18
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	8	0.16	0.01	0.16
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	8	0.13	0.02	0.12
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	7	1.25	0.05	1.26
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	7	1.13	0.09	1.13
(1,1318)	1:111:A:MET:HE1	1:115:A:LEU:HD13	7	0.98	0.37	1.12
(1,1318)	1:111:A:MET:HE1	1:115:A:LEU:HD11	7	0.98	0.37	1.12
(1,1318)	1:111:A:MET:HE3	1:115:A:LEU:HD13	7	0.98	0.37	1.12
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD12	7	0.98	0.37	1.12
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD11	7	0.98	0.37	1.12
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD13	7	0.98	0.37	1.12
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD11	7	0.72	0.62	0.59
(1,1429)	1:141:A:LEU:HD22	1:144:A:LEU:HD11	7	0.72	0.62	0.59
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD13	7	0.72	0.62	0.59
(1,1429)	1:141:A:LEU:HD22	1:144:A:LEU:HD12	7	0.72	0.62	0.59
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD12	7	0.72	0.62	0.59
(1,154)	1:208:A:LEU:HD12	1:205:A:LYS:H	7	0.71	0.59	0.48
(1,154)	1:208:A:LEU:HD11	1:205:A:LYS:H	7	0.71	0.59	0.48
(1,154)	1:208:A:LEU:HD13	1:205:A:LYS:H	7	0.71	0.59	0.48
(1,488)	1:141:A:LEU:HD22	1:142:A:ALA:H	7	0.59	0.19	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,488)	1:141:A:LEU:HD23	1:142:A:ALA:H	7	0.59	0.19	0.62
(1,488)	1:141:A:LEU:HD21	1:142:A:ALA:H	7	0.59	0.19	0.62
(1,41)	1:204:A:GLU:HG3	1:208:A:LEU:HB3	7	0.57	0.29	0.62
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	7	0.57	0.29	0.62
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG13	7	0.39	0.12	0.42
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG12	7	0.39	0.12	0.42
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG11	7	0.39	0.12	0.42
(1,48)	1:208:A:LEU:HD23	1:208:A:LEU:H	7	0.38	0.07	0.37
(1,48)	1:208:A:LEU:HD12	1:208:A:LEU:H	7	0.38	0.07	0.37
(1,48)	1:208:A:LEU:HD13	1:208:A:LEU:H	7	0.38	0.07	0.37
(1,341)	1:191:A:VAL:HG22	1:188:A:VAL:H	7	0.37	0.11	0.39
(1,341)	1:191:A:VAL:HG21	1:188:A:VAL:H	7	0.37	0.11	0.39
(1,341)	1:191:A:VAL:HG23	1:188:A:VAL:H	7	0.37	0.11	0.39
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	7	0.37	0.16	0.35
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG11	7	0.3	0.06	0.3
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG12	7	0.3	0.06	0.3
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG13	7	0.3	0.06	0.3
(1,81)	1:203:A:ALA:HB3	1:200:A:ARG:H	7	0.27	0.15	0.19
(1,81)	1:203:A:ALA:HB2	1:200:A:ARG:H	7	0.27	0.15	0.19
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	7	0.25	0.06	0.24
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG21	7	0.24	0.08	0.28
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG23	7	0.24	0.08	0.28
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	7	0.21	0.05	0.22
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	7	0.21	0.06	0.21
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	7	0.21	0.03	0.21
(1,834)	1:115:A:LEU:HD11	1:116:A:ARG:H	7	0.2	0.04	0.2
(1,834)	1:115:A:LEU:HD13	1:116:A:ARG:H	7	0.2	0.04	0.2
(1,834)	1:115:A:LEU:HD12	1:116:A:ARG:H	7	0.2	0.04	0.2
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG12	7	0.19	0.08	0.17
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG11	7	0.19	0.08	0.17
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG13	7	0.19	0.08	0.17
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG21	6	1.2	0.25	1.16
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG23	6	1.2	0.25	1.16
(1,1425)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	6	1.01	0.83	0.78
(1,1425)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	6	1.01	0.83	0.78
(1,1425)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	6	1.01	0.83	0.78
(1,1425)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	6	1.01	0.83	0.78
(1,1425)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	6	1.01	0.83	0.78
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	6	0.86	0.25	0.98
(1,1018)	1:114:A:VAL:HG12	1:115:A:LEU:HD11	6	0.76	0.62	0.5
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD11	6	0.76	0.62	0.5
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD13	6	0.76	0.62	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD12	6	0.76	0.62	0.5
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD11	6	0.69	0.45	0.57
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD12	6	0.69	0.45	0.57
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD13	6	0.69	0.45	0.57
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	6	0.68	0.16	0.74
(1,1616)	1:208:A:LEU:HD11	1:125:A:CYS:HB2	6	0.66	0.27	0.71
(1,1616)	1:208:A:LEU:HD12	1:125:A:CYS:HB2	6	0.66	0.27	0.71
(1,1166)	1:111:A:MET:HE1	1:111:A:MET:HB2	6	0.66	0.48	0.64
(1,1166)	1:111:A:MET:HE3	1:111:A:MET:HB2	6	0.66	0.48	0.64
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD12	6	0.63	0.41	0.55
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD11	6	0.63	0.41	0.55
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD13	6	0.63	0.41	0.55
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	6	0.62	0.13	0.68
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	6	0.55	0.19	0.61
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	6	0.39	0.27	0.32
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	6	0.33	0.04	0.34
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	6	0.32	0.14	0.38
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	6	0.31	0.11	0.32
(1,455)	1:168:A:LEU:HD21	1:169:A:SER:H	6	0.27	0.05	0.28
(1,455)	1:168:A:LEU:HD23	1:169:A:SER:H	6	0.27	0.05	0.28
(1,455)	1:168:A:LEU:HD22	1:169:A:SER:H	6	0.27	0.05	0.28
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD13	6	0.25	0.09	0.29
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD11	6	0.25	0.09	0.29
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD12	6	0.25	0.09	0.29
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	6	0.19	0.03	0.18
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	6	0.16	0.06	0.13
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	6	0.16	0.02	0.16
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	6	0.14	0.01	0.14
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	6	0.12	0.01	0.12
(1,1670)	1:152:A:LYS:HA	1:152:A:LYS:HD3	5	1.19	0.08	1.19
(1,1107)	1:134:A:CYS:HB2	1:138:A:SER:HB2	5	1.17	0.65	1.23
(1,304)	1:226:A:ASN:H	1:226:A:ASN:HB2	5	1.02	0.45	1.21
(1,367)	1:181:A:ARG:HB2	1:180:A:HIS:H	5	0.91	0.07	0.91
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB3	5	0.8	0.12	0.84
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB2	5	0.8	0.12	0.84
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB1	5	0.8	0.12	0.84
(1,969)	1:139:A:ARG:HD2	1:140:A:ARG:HA	5	0.69	0.41	0.89
(1,1456)	1:111:A:MET:HB3	1:148:A:TRP:HD1	5	0.64	0.17	0.69
(1,18)	1:229:A:ILE:H	1:228:A:THR:H	5	0.6	0.25	0.62
(1,1089)	1:212:A:GLU:HG2	1:212:A:GLU:HA	5	0.54	0.31	0.74
(1,1489)	1:137:A:ILE:HD12	1:134:A:CYS:HB2	5	0.44	0.18	0.48
(1,1489)	1:137:A:ILE:HD13	1:134:A:CYS:HB2	5	0.44	0.18	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1489)	1:137:A:ILE:HD11	1:134:A:CYS:HB2	5	0.44	0.18	0.48
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG22	5	0.41	0.15	0.35
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG21	5	0.41	0.15	0.35
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG23	5	0.41	0.15	0.35
(1,493)	1:218:A:LYS:HD3	1:218:A:LYS:H	5	0.4	0.21	0.48
(1,633)	1:199:A:LYS:HG2	1:199:A:LYS:H	5	0.33	0.09	0.34
(1,1132)	1:179:A:ILE:HG23	1:161:A:MET:HA	5	0.31	0.05	0.3
(1,1132)	1:179:A:ILE:HG22	1:161:A:MET:HA	5	0.31	0.05	0.3
(1,1597)	1:181:A:ARG:HB2	1:181:A:ARG:HA	5	0.29	0.04	0.28
(1,174)	1:212:A:GLU:HB3	1:212:A:GLU:H	5	0.27	0.02	0.28
(1,1808)	1:158:A:LYS:HB2	1:148:A:TRP:HZ2	5	0.26	0.06	0.24
(1,1700)	1:116:A:ARG:HG2	1:116:A:ARG:HB2	5	0.25	0.06	0.25
(1,608)	1:200:A:ARG:H	1:199:A:LYS:HB2	5	0.23	0.07	0.19
(1,1428)	1:205:A:LYS:HG3	1:173:A:TRP:HZ3	5	0.23	0.19	0.15
(1,1583)	1:201:A:LEU:HD22	1:201:A:LEU:HA	5	0.23	0.01	0.23
(1,1583)	1:201:A:LEU:HD21	1:201:A:LEU:HA	5	0.23	0.01	0.23
(1,741)	1:191:A:VAL:HG23	1:195:A:MET:H	5	0.22	0.12	0.17
(1,741)	1:191:A:VAL:HG22	1:195:A:MET:H	5	0.22	0.12	0.17
(1,741)	1:191:A:VAL:HG21	1:195:A:MET:H	5	0.22	0.12	0.17
(1,443)	1:181:A:ARG:HB2	1:182:A:SER:H	5	0.2	0.03	0.2
(1,552)	1:108:A:GLU:HB3	1:108:A:GLU:H	5	0.2	0.04	0.22
(1,1256)	1:190:A:GLU:HB3	1:187:A:HIS:HA	5	0.2	0.09	0.19
(1,1532)	1:158:A:LYS:HB2	1:155:A:ILE:HA	5	0.19	0.08	0.18
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD12	5	0.17	0.06	0.16
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD13	5	0.17	0.06	0.16
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD11	5	0.17	0.06	0.16
(1,1652)	1:131:A:LYS:HD3	1:131:A:LYS:HB3	5	0.16	0.04	0.15
(1,1842)	1:194:A:TRP:HZ3	1:191:A:VAL:HB	5	0.15	0.02	0.14
(1,540)	1:129:A:THR:HG1	1:133:A:VAL:H	5	0.15	0.04	0.16
(1,975)	1:194:A:TRP:HA	1:143:A:LEU:HB2	5	0.15	0.05	0.13
(1,298)	1:181:A:ARG:H	1:178:A:ASP:H	5	0.15	0.04	0.14
(1,1739)	1:145:A:GLN:HG2	1:145:A:GLN:HE22	5	0.14	0.01	0.15
(1,1681)	1:152:A:LYS:HG2	1:152:A:LYS:HB2	5	0.14	0.01	0.14
(1,998)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	5	0.13	0.02	0.14
(1,1441)	1:148:A:TRP:HB3	1:145:A:GLN:HA	5	0.13	0.02	0.13
(1,460)	1:192:A:SER:H	1:193:A:GLN:H	5	0.12	0.02	0.12
(1,1112)	1:143:A:LEU:HD11	1:194:A:TRP:HB2	4	1.57	0.7	1.86
(1,1112)	1:143:A:LEU:HD12	1:194:A:TRP:HB2	4	1.57	0.7	1.86
(1,1453)	1:183:A:LEU:HD23	1:180:A:HIS:HD1	4	1.52	0.77	1.41
(1,1453)	1:183:A:LEU:HD22	1:180:A:HIS:HD1	4	1.52	0.77	1.41
(1,1341)	1:204:A:GLU:HB2	1:205:A:LYS:HG3	4	1.22	0.46	1.27
(1,1698)	1:183:A:LEU:HD23	1:180:A:HIS:HA	4	1.14	0.56	1.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1698)	1:183:A:LEU:HD22	1:180:A:HIS:HA	4	1.14	0.56	1.36
(1,962)	1:225:A:LYS:HG2	1:226:A:ASN:HB3	4	1.14	0.59	1.1
(1,867)	1:186:A:ASP:HB3	1:185:A:VAL:H	4	1.12	0.04	1.12
(1,1346)	1:225:A:LYS:HB3	1:225:A:LYS:HE2	4	1.1	0.04	1.11
(1,1542)	1:129:A:THR:HG1	1:133:A:VAL:HG21	4	0.84	0.27	0.94
(1,1542)	1:129:A:THR:HG1	1:133:A:VAL:HG22	4	0.84	0.27	0.94
(1,1283)	1:200:A:ARG:H	1:199:A:LYS:HB2	4	0.81	0.37	1.0
(1,1387)	1:117:A:PRO:HD3	1:116:A:ARG:HB3	4	0.74	0.06	0.74
(1,38)	1:157:A:VAL:HG13	1:161:A:MET:HG3	4	0.64	0.4	0.62
(1,38)	1:183:A:LEU:HD23	1:161:A:MET:HG3	4	0.64	0.4	0.62
(1,38)	1:157:A:VAL:HG11	1:161:A:MET:HG3	4	0.64	0.4	0.62
(1,1423)	1:212:A:GLU:HG2	1:212:A:GLU:HB2	4	0.58	0.07	0.61
(1,1644)	1:206:A:ARG:HB3	1:206:A:ARG:HD2	4	0.53	0.03	0.54
(1,1294)	1:116:A:ARG:HD2	1:116:A:ARG:HA	4	0.53	0.23	0.65
(1,966)	1:199:A:LYS:HE2	1:199:A:LYS:HA	4	0.52	0.27	0.37
(1,1225)	1:208:A:LEU:HD13	1:211:A:GLU:HG2	4	0.52	0.13	0.51
(1,1225)	1:208:A:LEU:HD12	1:211:A:GLU:HG2	4	0.52	0.13	0.51
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG22	4	0.49	0.38	0.37
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG23	4	0.49	0.38	0.37
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG21	4	0.49	0.38	0.37
(1,1260)	1:203:A:ALA:HB1	1:206:A:ARG:HD2	4	0.48	0.06	0.46
(1,1260)	1:203:A:ALA:HB2	1:206:A:ARG:HD2	4	0.48	0.06	0.46
(1,1260)	1:203:A:ALA:HB3	1:206:A:ARG:HD2	4	0.48	0.06	0.46
(1,1313)	1:194:A:TRP:HA	1:143:A:LEU:HD23	4	0.48	0.18	0.4
(1,1313)	1:194:A:TRP:HA	1:143:A:LEU:HD22	4	0.48	0.18	0.4
(1,1351)	1:189:A:THR:HG1	1:188:A:VAL:HG11	4	0.46	0.04	0.47
(1,1351)	1:189:A:THR:HG1	1:188:A:VAL:HG13	4	0.46	0.04	0.47
(1,1305)	1:143:A:LEU:HD23	1:193:A:GLN:HB3	4	0.42	0.15	0.4
(1,1305)	1:143:A:LEU:HD22	1:193:A:GLN:HB3	4	0.42	0.15	0.4
(1,1378)	1:116:A:ARG:HA	1:116:A:ARG:HB2	4	0.41	0.08	0.44
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD11	4	0.41	0.12	0.46
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD12	4	0.41	0.12	0.46
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD13	4	0.41	0.12	0.46
(1,718)	1:229:A:ILE:H	1:228:A:THR:H	4	0.4	0.17	0.43
(1,1217)	1:130:A:ARG:HA	1:130:A:ARG:HD3	4	0.38	0.23	0.32
(1,1402)	1:136:A:ASP:HB3	1:132:A:GLN:HG2	4	0.36	0.25	0.25
(1,1744)	1:205:A:LYS:HB2	1:205:A:LYS:HE2	4	0.32	0.01	0.31
(1,1392)	1:158:A:LYS:HE2	1:148:A:TRP:HA	4	0.31	0.24	0.2
(1,1525)	1:155:A:ILE:HB	1:156:A:PRO:HD2	4	0.29	0.06	0.32
(1,637)	1:125:A:CYS:H	1:124:A:ASP:HB3	4	0.27	0.13	0.24
(1,1640)	1:202:A:ILE:HG22	1:206:A:ARG:HD2	4	0.24	0.07	0.24
(1,1640)	1:202:A:ILE:HG21	1:206:A:ARG:HD2	4	0.24	0.07	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1435)	1:153:A:LEU:HA	1:190:A:GLU:HB2	4	0.23	0.11	0.18
(1,320)	1:193:A:GLN:HB2	1:194:A:TRP:H	4	0.22	0.02	0.22
(1,856)	1:158:A:LYS:HE2	1:158:A:LYS:H	4	0.22	0.04	0.2
(1,214)	1:227:A:HIS:H	1:227:A:HIS:HB2	4	0.2	0.07	0.2
(1,1397)	1:163:A:LEU:HA	1:163:A:LEU:HD21	4	0.2	0.06	0.2
(1,1397)	1:163:A:LEU:HA	1:163:A:LEU:HD23	4	0.2	0.06	0.2
(1,660)	1:212:A:GLU:H	1:211:A:GLU:HB3	4	0.18	0.06	0.17
(1,922)	1:218:A:LYS:HG2	1:218:A:LYS:HB3	4	0.18	0.04	0.18
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD13	4	0.16	0.03	0.16
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD12	4	0.16	0.03	0.16
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD11	4	0.16	0.03	0.16
(1,1347)	1:122:A:LEU:HB3	1:122:A:LEU:HG	4	0.16	0.03	0.18
(1,73)	1:148:A:TRP:H	1:149:A:ALA:HB2	4	0.14	0.03	0.14
(1,73)	1:148:A:TRP:H	1:149:A:ALA:HB1	4	0.14	0.03	0.14
(1,1683)	1:141:A:LEU:HA	1:144:A:LEU:HB3	4	0.13	0.03	0.12
(1,329)	1:193:A:GLN:H	1:194:A:TRP:HE1	4	0.12	0.01	0.12
(1,1501)	1:158:A:LYS:HB3	1:148:A:TRP:HZ3	4	0.12	0.02	0.12
(1,1355)	1:206:A:ARG:HD2	1:209:A:PHE:HD1	4	0.11	0.01	0.11
(1,1355)	1:206:A:ARG:HD2	1:209:A:PHE:HD2	4	0.11	0.01	0.11
(1,1714)	1:122:A:LEU:HD12	1:125:A:CYS:HB2	3	1.58	1.14	0.92
(1,1714)	1:122:A:LEU:HD13	1:125:A:CYS:HB2	3	1.58	1.14	0.92
(1,1466)	1:229:A:ILE:HG12	1:230:A:PRO:HG2	3	1.48	0.09	1.51
(1,571)	1:204:A:GLU:H	1:206:A:ARG:HG2	3	1.26	0.74	1.77
(1,1726)	1:118:A:LEU:HG	1:115:A:LEU:HD11	3	1.02	1.2	0.18
(1,1726)	1:118:A:LEU:HG	1:115:A:LEU:HD13	3	1.02	1.2	0.18
(1,1726)	1:118:A:LEU:HG	1:115:A:LEU:HD12	3	1.02	1.2	0.18
(1,1115)	1:152:A:LYS:HE2	1:152:A:LYS:HB3	3	0.95	0.6	1.29
(1,1047)	1:208:A:LEU:HD21	1:205:A:LYS:HE2	3	0.88	0.46	0.56
(1,1047)	1:208:A:LEU:HD22	1:205:A:LYS:HE2	3	0.88	0.46	0.56
(1,221)	1:134:A:CYS:HB3	1:133:A:VAL:H	3	0.84	0.05	0.86
(1,1208)	1:136:A:ASP:HB3	1:133:A:VAL:HG13	3	0.75	0.11	0.73
(1,1208)	1:136:A:ASP:HB3	1:133:A:VAL:HG11	3	0.75	0.11	0.73
(1,1566)	1:124:A:ASP:HB2	1:208:A:LEU:HD23	3	0.74	0.65	0.32
(1,1566)	1:124:A:ASP:HB2	1:208:A:LEU:HD22	3	0.74	0.65	0.32
(1,75)	1:139:A:ARG:HD2	1:140:A:ARG:H	3	0.74	0.33	0.51
(1,726)	1:158:A:LYS:HE2	1:155:A:ILE:H	3	0.7	0.44	0.88
(1,1106)	1:122:A:LEU:HB3	1:125:A:CYS:HB2	3	0.67	0.04	0.65
(1,1781)	1:148:A:TRP:HE3	1:161:A:MET:HG3	3	0.63	0.45	0.42
(1,1612)	1:123:A:GLU:HG3	1:123:A:GLU:HB3	3	0.59	0.03	0.58
(1,152)	1:121:A:ALA:H	1:120:A:GLN:HG2	3	0.55	0.01	0.55
(1,1763)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	3	0.53	0.41	0.26
(1,587)	1:132:A:GLN:HG2	1:133:A:VAL:H	3	0.51	0.08	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,953)	1:158:A:LYS:HE2	1:153:A:LEU:HB2	3	0.48	0.23	0.57
(1,1359)	1:225:A:LYS:HB2	1:225:A:LYS:HE2	3	0.47	0.26	0.46
(1,1384)	1:145:A:GLN:HG2	1:141:A:LEU:HD21	3	0.47	0.15	0.5
(1,1384)	1:145:A:GLN:HG2	1:141:A:LEU:HD23	3	0.47	0.15	0.5
(1,1482)	1:191:A:VAL:HG21	1:184:A:MET:HG3	3	0.47	0.2	0.45
(1,1482)	1:191:A:VAL:HG23	1:184:A:MET:HG3	3	0.47	0.2	0.45
(1,956)	1:230:A:PRO:HG2	1:232:A:PHE:HB2	3	0.45	0.11	0.4
(1,1216)	1:158:A:LYS:HE2	1:158:A:LYS:HG2	3	0.43	0.16	0.5
(1,1205)	1:132:A:GLN:HG2	1:133:A:VAL:HA	3	0.43	0.17	0.32
(1,1634)	1:161:A:MET:HG3	1:161:A:MET:HA	3	0.42	0.32	0.24
(1,1376)	1:119:A:GLU:HG3	1:119:A:GLU:HB3	3	0.41	0.02	0.39
(1,937)	1:205:A:LYS:HG3	1:205:A:LYS:HE2	3	0.4	0.07	0.38
(1,1200)	1:143:A:LEU:HG	1:143:A:LEU:HB3	3	0.39	0.07	0.44
(1,1038)	1:116:A:ARG:HD2	1:116:A:ARG:HB3	3	0.38	0.12	0.3
(1,1539)	1:202:A:ILE:HG21	1:206:A:ARG:HD3	3	0.37	0.32	0.18
(1,1539)	1:202:A:ILE:HG22	1:206:A:ARG:HD3	3	0.37	0.32	0.18
(1,1635)	1:157:A:VAL:HG13	1:153:A:LEU:HA	3	0.37	0.23	0.35
(1,1635)	1:157:A:VAL:HG12	1:153:A:LEU:HA	3	0.37	0.23	0.35
(1,1320)	1:183:A:LEU:HD23	1:194:A:TRP:HZ2	3	0.36	0.18	0.28
(1,1320)	1:183:A:LEU:HD22	1:194:A:TRP:HZ2	3	0.36	0.18	0.28
(1,1284)	1:188:A:VAL:HB	1:191:A:VAL:HG22	3	0.35	0.1	0.3
(1,1284)	1:188:A:VAL:HB	1:191:A:VAL:HG21	3	0.35	0.1	0.3
(1,1506)	1:204:A:GLU:HB2	1:205:A:LYS:HA	3	0.34	0.09	0.37
(1,1745)	1:179:A:ILE:HG22	1:164:A:LEU:HB3	3	0.33	0.16	0.31
(1,1380)	1:205:A:LYS:HG3	1:173:A:TRP:HH2	3	0.31	0.23	0.16
(1,1664)	1:229:A:ILE:HG12	1:229:A:ILE:HB	3	0.31	0.02	0.32
(1,1006)	1:161:A:MET:HG2	1:161:A:MET:HB3	3	0.3	0.01	0.3
(1,309)	1:181:A:ARG:H	1:181:A:ARG:HG2	3	0.29	0.07	0.34
(1,1182)	1:206:A:ARG:HA	1:209:A:PHE:HB2	3	0.28	0.06	0.32
(1,1643)	1:148:A:TRP:HZ3	1:161:A:MET:HG2	3	0.28	0.03	0.27
(1,1510)	1:164:A:LEU:HA	1:167:A:GLU:HG2	3	0.26	0.16	0.15
(1,771)	1:232:A:PHE:H	1:232:A:PHE:HB2	3	0.24	0.02	0.26
(1,1468)	1:198:A:VAL:HA	1:201:A:LEU:HB2	3	0.22	0.05	0.23
(1,1134)	1:126:A:ARG:HD2	1:126:A:ARG:HB2	3	0.22	0.01	0.22
(1,1410)	1:148:A:TRP:HD1	1:111:A:MET:HG3	3	0.22	0.0	0.22
(1,483)	1:212:A:GLU:HB3	1:213:A:ALA:H	3	0.21	0.11	0.16
(1,1497)	1:117:A:PRO:HD3	1:165:A:VAL:HG21	3	0.21	0.04	0.19
(1,1497)	1:117:A:PRO:HD3	1:165:A:VAL:HG22	3	0.21	0.04	0.19
(1,712)	1:199:A:LYS:HE2	1:199:A:LYS:H	3	0.2	0.06	0.18
(1,752)	1:168:A:LEU:H	1:168:A:LEU:HD11	3	0.19	0.03	0.19
(1,752)	1:168:A:LEU:H	1:168:A:LEU:HD12	3	0.19	0.03	0.19
(1,1076)	1:204:A:GLU:HB2	1:204:A:GLU:HA	3	0.18	0.02	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,457)	1:153:A:LEU:HD12	1:154:A:SER:H	3	0.18	0.06	0.18
(1,457)	1:153:A:LEU:HD11	1:154:A:SER:H	3	0.18	0.06	0.18
(1,915)	1:199:A:LYS:HE2	1:199:A:LYS:HG2	3	0.16	0.03	0.15
(1,656)	1:194:A:TRP:HB3	1:194:A:TRP:H	3	0.16	0.01	0.16
(1,864)	1:152:A:LYS:H	1:152:A:LYS:HG3	3	0.16	0.03	0.17
(1,1608)	1:116:A:ARG:HG2	1:116:A:ARG:HA	3	0.16	0.02	0.16
(1,1163)	1:172:A:ARG:HB3	1:170:A:SER:HB2	3	0.16	0.07	0.11
(1,1227)	1:181:A:ARG:HD3	1:181:A:ARG:HG2	3	0.15	0.04	0.13
(1,1455)	1:148:A:TRP:HE3	1:148:A:TRP:HA	3	0.15	0.04	0.14
(1,1461)	1:183:A:LEU:HA	1:183:A:LEU:HB2	3	0.15	0.05	0.14
(1,1083)	1:135:A:ASP:HA	1:135:A:ASP:HB3	3	0.15	0.02	0.14
(1,575)	1:139:A:ARG:HG2	1:139:A:ARG:H	3	0.14	0.03	0.13
(1,1129)	1:161:A:MET:HG3	1:161:A:MET:HB3	3	0.14	0.03	0.16
(1,1152)	1:206:A:ARG:HB3	1:206:A:ARG:HG2	3	0.14	0.02	0.13
(1,1314)	1:208:A:LEU:HD11	1:125:A:CYS:HA	3	0.14	0.03	0.14
(1,1314)	1:208:A:LEU:HD13	1:125:A:CYS:HA	3	0.14	0.03	0.14
(1,1314)	1:208:A:LEU:HD12	1:125:A:CYS:HA	3	0.14	0.03	0.14
(1,1418)	1:179:A:ILE:HA	1:179:A:ILE:HB	3	0.14	0.02	0.14
(1,1519)	1:184:A:MET:HA	1:184:A:MET:HG2	3	0.14	0.02	0.13
(1,193)	1:234:A:GLN:H	1:234:A:GLN:HA	3	0.13	0.0	0.13
(1,533)	1:181:A:ARG:HB2	1:181:A:ARG:H	3	0.12	0.01	0.13
(1,519)	1:210:A:SER:H	1:211:A:GLU:H	3	0.12	0.02	0.11
(1,1068)	1:158:A:LYS:HD2	1:148:A:TRP:HZ2	3	0.12	0.01	0.12
(1,618)	1:191:A:VAL:H	1:190:A:GLU:HB3	3	0.11	0.0	0.11
(1,941)	1:111:A:MET:HB3	1:111:A:MET:HA	3	0.11	0.01	0.11
(1,931)	1:160:A:ARG:HA	1:163:A:LEU:HD13	2	1.64	0.12	1.64
(1,931)	1:160:A:ARG:HA	1:163:A:LEU:HD12	2	1.64	0.12	1.64
(1,782)	1:108:A:GLU:HG2	1:108:A:GLU:H	2	1.14	0.02	1.14
(1,1007)	1:198:A:VAL:HB	1:201:A:LEU:HB3	2	1.08	0.32	1.08
(1,1126)	1:144:A:LEU:HD23	1:115:A:LEU:HD12	2	0.98	0.29	0.98
(1,1126)	1:144:A:LEU:HD21	1:115:A:LEU:HD11	2	0.98	0.29	0.98
(1,1034)	1:199:A:LYS:HE2	1:195:A:MET:HE1	2	0.94	0.62	0.94
(1,1224)	1:199:A:LYS:HE2	1:199:A:LYS:HB2	2	0.92	0.46	0.92
(1,1746)	1:208:A:LEU:HD23	1:124:A:ASP:HB3	2	0.92	0.34	0.92
(1,1746)	1:208:A:LEU:HD22	1:124:A:ASP:HB3	2	0.92	0.34	0.92
(1,1010)	1:168:A:LEU:HD23	1:165:A:VAL:HG13	2	0.91	0.76	0.91
(1,1010)	1:168:A:LEU:HD22	1:165:A:VAL:HG12	2	0.91	0.76	0.91
(1,1720)	1:172:A:ARG:HD3	1:170:A:SER:HB3	2	0.91	0.25	0.91
(1,1339)	1:136:A:ASP:HB3	1:133:A:VAL:HB	2	0.9	0.78	0.9
(1,1012)	1:164:A:LEU:HD13	1:161:A:MET:HE3	2	0.85	0.5	0.85
(1,1012)	1:164:A:LEU:HD11	1:161:A:MET:HE3	2	0.85	0.5	0.85
(1,1241)	1:183:A:LEU:HB3	1:180:A:HIS:HA	2	0.81	0.23	0.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1311)	1:152:A:LYS:HA	1:152:A:LYS:HE2	2	0.81	0.09	0.81
(1,1609)	1:157:A:VAL:HG13	1:194:A:TRP:HH2	2	0.8	0.5	0.8
(1,1609)	1:157:A:VAL:HG12	1:194:A:TRP:HH2	2	0.8	0.5	0.8
(1,1092)	1:180:A:HIS:HB3	1:195:A:MET:HB2	2	0.77	0.66	0.77
(1,248)	1:152:A:LYS:HE2	1:152:A:LYS:H	2	0.72	0.38	0.72
(1,1693)	1:159:A:LYS:HB2	1:159:A:LYS:HE2	2	0.7	0.05	0.7
(1,1372)	1:158:A:LYS:HG2	1:148:A:TRP:HZ2	2	0.61	0.23	0.61
(1,1016)	1:165:A:VAL:HG22	1:161:A:MET:HE1	2	0.56	0.44	0.56
(1,1044)	1:183:A:LEU:HD21	1:161:A:MET:HA	2	0.49	0.22	0.49
(1,1044)	1:183:A:LEU:HD23	1:161:A:MET:HA	2	0.49	0.22	0.49
(1,858)	1:139:A:ARG:HD2	1:139:A:ARG:H	2	0.44	0.34	0.44
(1,1586)	1:157:A:VAL:HG23	1:190:A:GLU:HB2	2	0.44	0.17	0.44
(1,1586)	1:157:A:VAL:HG22	1:190:A:GLU:HB2	2	0.44	0.17	0.44
(1,1522)	1:218:A:LYS:HG2	1:218:A:LYS:HA	2	0.42	0.08	0.42
(1,609)	1:213:A:ALA:HB3	1:212:A:GLU:H	2	0.42	0.2	0.42
(1,609)	1:213:A:ALA:HB1	1:212:A:GLU:H	2	0.42	0.2	0.42
(1,1159)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	2	0.42	0.3	0.42
(1,873)	1:202:A:ILE:HG22	1:203:A:ALA:H	2	0.4	0.12	0.4
(1,873)	1:202:A:ILE:HG21	1:203:A:ALA:H	2	0.4	0.12	0.4
(1,1209)	1:158:A:LYS:HD2	1:148:A:TRP:HB2	2	0.4	0.06	0.4
(1,1181)	1:153:A:LEU:HB2	1:158:A:LYS:HG2	2	0.38	0.1	0.38
(1,70)	1:158:A:LYS:HG2	1:157:A:VAL:H	2	0.36	0.24	0.36
(1,1536)	1:158:A:LYS:HB3	1:158:A:LYS:HD3	2	0.36	0.0	0.36
(1,1823)	1:205:A:LYS:HB2	1:173:A:TRP:HZ3	2	0.34	0.05	0.34
(1,1478)	1:175:A:ALA:HB1	1:167:A:GLU:HA	2	0.3	0.15	0.3
(1,1043)	1:145:A:GLN:HA	1:111:A:MET:HG3	2	0.3	0.12	0.3
(1,1661)	1:158:A:LYS:HD3	1:148:A:TRP:HZ2	2	0.29	0.01	0.29
(1,1651)	1:206:A:ARG:HA	1:209:A:PHE:HB3	2	0.28	0.01	0.28
(1,102)	1:162:A:ALA:HB3	1:166:A:GLN:HE22	2	0.27	0.13	0.27
(1,102)	1:162:A:ALA:HB2	1:166:A:GLN:HE22	2	0.27	0.13	0.27
(1,1186)	1:159:A:LYS:HB2	1:159:A:LYS:HD3	2	0.27	0.13	0.27
(1,835)	1:158:A:LYS:HE2	1:148:A:TRP:HE1	2	0.26	0.08	0.26
(1,1589)	1:201:A:LEU:HA	1:201:A:LEU:HD11	2	0.26	0.0	0.26
(1,1589)	1:201:A:LEU:HA	1:201:A:LEU:HD12	2	0.26	0.0	0.26
(1,427)	1:154:A:SER:HB2	1:155:A:ILE:H	2	0.26	0.15	0.26
(1,1436)	1:116:A:ARG:HD2	1:116:A:ARG:HB2	2	0.26	0.1	0.26
(1,283)	1:116:A:ARG:HG2	1:116:A:ARG:H	2	0.24	0.08	0.24
(1,1099)	1:206:A:ARG:HB3	1:209:A:PHE:HD2	2	0.24	0.08	0.24
(1,1245)	1:158:A:LYS:HE2	1:158:A:LYS:HD2	2	0.23	0.05	0.23
(1,1719)	1:194:A:TRP:HZ3	1:191:A:VAL:HG12	2	0.23	0.06	0.23
(1,1719)	1:194:A:TRP:HZ3	1:191:A:VAL:HG11	2	0.23	0.06	0.23
(1,1172)	1:171:A:HIS:HB2	1:171:A:HIS:HA	2	0.22	0.01	0.22

Continued on next page...

Continued from previous page...

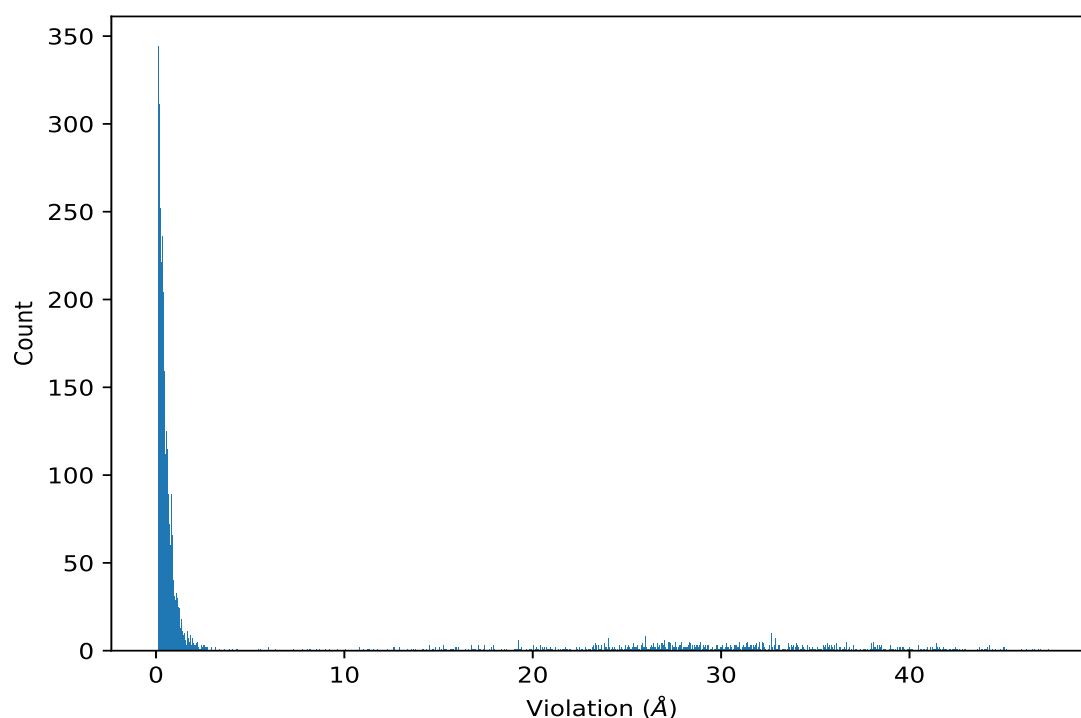
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	1:154:A:SER:H	1:154:A:SER:HB2	2	0.22	0.04	0.22
(1,1601)	1:216:A:GLU:HG2	1:216:A:GLU:HA	2	0.22	0.04	0.22
(1,447)	1:211:A:GLU:H	1:211:A:GLU:HG2	2	0.21	0.01	0.21
(1,813)	1:221:A:ALA:HA	1:221:A:ALA:H	2	0.21	0.0	0.21
(1,372)	1:145:A:GLN:HA	1:145:A:GLN:HE22	2	0.2	0.07	0.2
(1,636)	1:220:A:ALA:H	1:219:A:SER:HA	2	0.2	0.02	0.2
(1,2)	1:155:A:ILE:HG22	1:159:A:LYS:H	2	0.18	0.05	0.18
(1,2)	1:155:A:ILE:HG23	1:159:A:LYS:H	2	0.18	0.05	0.18
(1,215)	1:127:A:GLY:HA2	1:127:A:GLY:H	2	0.18	0.0	0.18
(1,509)	1:179:A:ILE:HG23	1:164:A:LEU:H	2	0.17	0.0	0.17
(1,509)	1:179:A:ILE:HG22	1:164:A:LEU:H	2	0.17	0.0	0.17
(1,1602)	1:206:A:ARG:HA	1:206:A:ARG:HD3	2	0.17	0.06	0.17
(1,833)	1:160:A:ARG:HD2	1:160:A:ARG:H	2	0.17	0.04	0.17
(1,874)	1:158:A:LYS:H	1:154:A:SER:HB2	2	0.16	0.06	0.16
(1,809)	1:108:A:GLU:H	1:107:A:SER:HA	2	0.15	0.02	0.15
(1,1180)	1:181:A:ARG:HB2	1:181:A:ARG:HG2	2	0.15	0.0	0.15
(1,1319)	1:145:A:GLN:HG2	1:145:A:GLN:HA	2	0.15	0.03	0.15
(1,1136)	1:108:A:GLU:HB3	1:108:A:GLU:HA	2	0.14	0.01	0.14
(1,1192)	1:158:A:LYS:HA	1:161:A:MET:HB3	2	0.14	0.01	0.14
(1,1030)	1:156:A:PRO:HD2	1:155:A:ILE:HG13	2	0.14	0.04	0.14
(1,213)	1:219:A:SER:H	1:220:A:ALA:HA	2	0.12	0.02	0.12
(1,799)	1:140:A:ARG:H	1:140:A:ARG:HB2	2	0.12	0.01	0.12
(1,66)	1:174:A:ASP:HB3	1:173:A:TRP:H	2	0.12	0.02	0.12
(1,844)	1:207:A:SER:H	1:207:A:SER:HB3	2	0.12	0.0	0.12
(1,112)	1:140:A:ARG:HB3	1:140:A:ARG:H	2	0.12	0.0	0.12
(1,289)	1:111:A:MET:HB3	1:112:A:GLU:H	2	0.12	0.0	0.12
(1,926)	1:186:A:ASP:HB2	1:186:A:ASP:HA	2	0.11	0.01	0.11
(1,1631)	1:114:A:VAL:HA	1:117:A:PRO:HD2	2	0.11	0.0	0.11
(1,949)	1:155:A:ILE:HA	1:155:A:ILE:HG12	2	0.11	0.0	0.11
(1,1839)	1:114:A:VAL:HB	1:148:A:TRP:HZ2	2	0.11	0.0	0.11
(1,153)	1:168:A:LEU:HA	1:167:A:GLU:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	3	47.36
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	1	46.95
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	14	46.83
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	3	46.63
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	14	46.53
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	14	46.22
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	3	45.9
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	12	45.18
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	14	45.03
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	1	45.01
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	14	44.99
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	3	44.98
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	14	44.84
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	14	44.55
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	12	44.43
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	12	44.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	14	44.24
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	14	44.23
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	12	44.14
(1,1212)	1:110:A:VAL:HG21	1:217:A:GLU:HG3	15	44.13
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	3	44.09
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	3	44.0
(1,595)	1:133:A:VAL:HG21	1:235:A:ALA:H	1	43.95
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	12	43.88
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	1	43.84
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	1	43.74
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	3	43.72
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	5	43.62
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	12	42.98
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	12	42.91
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	12	42.8
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	12	42.67
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	1	42.5
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	3	42.47
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	5	42.43
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	12	42.42
(1,739)	1:133:A:VAL:HG11	1:235:A:ALA:H	12	42.35
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	12	42.3
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	5	42.26
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	1	42.16
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	14	42.14
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	15	41.96
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	3	41.91
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	12	41.85
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	1	41.83
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	12	41.8
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	11	41.77
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	3	41.73
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD12	1	41.61
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	12	41.56
(1,1212)	1:110:A:VAL:HG22	1:217:A:GLU:HG3	7	41.55
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	11	41.54
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	7	41.47
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	5	41.46
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	5	41.43
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	12	41.42
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	12	41.41
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	11	41.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	1	41.39
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	12	41.32
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	5	41.26
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	1	41.24
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	1	41.22
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	1	41.13
(1,595)	1:133:A:VAL:HG22	1:235:A:ALA:H	12	41.1
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	11	40.99
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	14	40.96
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	1	40.9
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	7	40.77
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	11	40.71
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	12	40.61
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	7	40.57
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	12	40.48
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	1	40.47
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	3	40.46
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	1	40.15
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	7	40.1
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	11	40.08
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	1	40.03
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	1	40.03
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	5	39.99
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	12	39.94
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	12	39.88
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	12	39.74
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	9	39.66
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	1	39.66
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	1	39.62
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	1	39.61
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	12	39.54
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	11	39.51
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	5	39.47
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	1	39.45
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	8	39.38
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	12	39.36
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD13	9	39.28
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	12	39.18
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	9	39.12
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	12	39.09
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	12	39.04
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	1	38.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	1	38.96
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	12	38.95
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	12	38.93
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	7	38.71
(1,1460)	1:122:A:LEU:HD11	1:227:A:HIS:HB2	9	38.68
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	1	38.61
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	7	38.54
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	10	38.54
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	1	38.52
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	1	38.47
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	9	38.46
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	5	38.42
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	8	38.41
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	9	38.41
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	12	38.37
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	10	38.32
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	11	38.32
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	10	38.3
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	7	38.21
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	12	38.19
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	1	38.18
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	1	38.13
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	9	38.11
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	12	38.06
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	12	38.06
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	1	38.06
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	12	38.05
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD11	9	38.05
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	15	38.04
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	14	37.99
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	14	37.99
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	1	37.96
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	9	37.95
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	12	37.9
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	10	37.79
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	1	37.69
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	12	37.63
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	1	37.58
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	12	37.42
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	15	37.36
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	10	37.15
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	9	37.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1212)	1:110:A:VAL:HG22	1:217:A:GLU:HG3	8	37.03
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	15	37.03
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	15	37.02
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	2	36.9
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB1	15	36.82
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	15	36.81
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	11	36.75
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	9	36.68
(1,674)	1:110:A:VAL:HG13	1:215:A:ASN:H	15	36.67
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	9	36.66
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	12	36.65
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	1	36.65
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	12	36.62
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	1	36.58
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	6	36.58
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	7	36.51
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	1	36.48
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	5	36.43
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	11	36.33
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	2	36.3
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	7	36.27
(1,674)	1:110:A:VAL:HG13	1:215:A:ASN:H	8	36.27
(1,1212)	1:110:A:VAL:HG21	1:217:A:GLU:HG3	12	36.16
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	6	36.13
(1,739)	1:133:A:VAL:HG13	1:235:A:ALA:H	10	36.12
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	3	36.11
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	3	36.11
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB1	15	36.03
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	7	36.01
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	12	36.01
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	12	35.95
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	1	35.92
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	1	35.9
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	15	35.88
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB1	10	35.88
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	2	35.88
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	6	35.8
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB2	8	35.79
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	1	35.78
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	9	35.76
(1,595)	1:133:A:VAL:HG21	1:235:A:ALA:H	10	35.73
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	8	35.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	15	35.66
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	7	35.65
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	15	35.63
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	5	35.61
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	5	35.61
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	15	35.6
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	15	35.58
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	15	35.54
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	10	35.52
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	10	35.51
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	10	35.49
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB2	8	35.46
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	1	35.44
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	2	35.43
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	2	35.4
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	1	35.31
(1,674)	1:110:A:VAL:HG13	1:215:A:ASN:H	1	35.29
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	9	35.24
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB3	7	35.19
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB1	15	35.14
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	9	35.11
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	9	35.03
(1,1212)	1:110:A:VAL:HG22	1:217:A:GLU:HG3	11	34.99
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB1	2	34.9
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	11	34.84
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	15	34.81
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB1	10	34.77
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	12	34.71
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	15	34.68
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	12	34.65
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD23	7	34.59
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	1	34.59
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	1	34.56
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	7	34.42
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	1	34.39
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	10	34.35
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	7	34.32
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	1	34.32
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB1	10	34.3
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	9	34.29
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	1	34.21
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	12	34.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	9	34.12
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	15	34.08
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB1	15	34.07
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB2	8	34.07
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	10	34.04
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	15	34.03
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB2	8	34.01
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB1	2	34.0
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	7	33.95
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	15	33.95
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	15	33.95
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB1	2	33.93
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	8	33.92
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	6	33.84
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	12	33.82
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	12	33.82
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB2	4	33.79
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	7	33.75
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB2	8	33.72
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD23	5	33.72
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	10	33.71
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	6	33.63
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	1	33.61
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	9	33.58
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	11	33.57
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG13	15	33.56
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG13	15	33.56
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB3	12	33.53
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	13	33.41
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB2	8	33.37
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	10	33.33
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	4	33.25
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB2	11	33.14
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB1	15	33.1
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	9	33.1
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	7	33.04
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	11	33.04
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	11	33.04
(1,1460)	1:122:A:LEU:HD11	1:227:A:HIS:HB2	10	32.99
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB2	8	32.9
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	10	32.88
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	3	32.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	1	32.88
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	1	32.88
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	8	32.87
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	9	32.85
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD12	3	32.85
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG13	8	32.83
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG13	8	32.83
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	5	32.81
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	5	32.73
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD12	5	32.72
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	3	32.69
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	1	32.68
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	12	32.68
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	3	32.67
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	7	32.67
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	9	32.67
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	15	32.66
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB3	1	32.66
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	3	32.66
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	3	32.66
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	7	32.56
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	12	32.55
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	12	32.55
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	12	32.5
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	9	32.37
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB1	10	32.33
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	10	32.31
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	7	32.26
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB2	14	32.25
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	15	32.24
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	11	32.22
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	7	32.21
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	7	32.21
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	14	32.18
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB2	11	32.16
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD23	11	32.16
(1,674)	1:110:A:VAL:HG12	1:215:A:ASN:H	10	32.15
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB2	4	32.15
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	15	32.09
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	7	32.03
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	2	32.03
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	10	32.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB2	11	32.02
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	5	32.0
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	12	31.99
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	13	31.99
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	12	31.92
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	7	31.88
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB1	15	31.87
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	9	31.86
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	6	31.86
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	3	31.84
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	13	31.84
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	10	31.83
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB1	2	31.79
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	5	31.77
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	1	31.73
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	10	31.72
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	3	31.72
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	7	31.67
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	2	31.61
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	8	31.6
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	8	31.6
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG13	1	31.59
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG13	1	31.59
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	3	31.58
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB2	4	31.51
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	5	31.5
(1,1460)	1:122:A:LEU:HD13	1:227:A:HIS:HB2	3	31.45
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	4	31.45
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB2	14	31.42
(1,1460)	1:122:A:LEU:HD13	1:227:A:HIS:HB2	5	31.41
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	7	31.41
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	7	31.41
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	7	31.4
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	3	31.38
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	5	31.36
(1,674)	1:110:A:VAL:HG12	1:215:A:ASN:H	11	31.33
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB1	9	31.33
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	6	31.32
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD11	10	31.32
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	10	31.26
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	10	31.26
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	13	31.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB2	14	31.2
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	5	31.17
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB2	11	31.17
(1,1212)	1:110:A:VAL:HG22	1:217:A:GLU:HG3	9	31.15
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB1	15	31.14
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	7	31.1
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	5	31.0
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	3	30.99
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	10	30.98
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB1	10	30.97
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	9	30.97
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	9	30.96
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	9	30.93
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB1	9	30.92
(1,674)	1:110:A:VAL:HG12	1:215:A:ASN:H	2	30.88
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	15	30.87
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	1	30.84
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	5	30.82
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	5	30.81
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	8	30.78
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	5	30.77
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	9	30.76
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	15	30.74
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	5	30.73
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	3	30.7
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD13	11	30.69
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	5	30.55
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	3	30.53
(1,674)	1:110:A:VAL:HG13	1:215:A:ASN:H	13	30.53
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB2	4	30.47
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	8	30.46
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	7	30.46
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB1	2	30.44
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB1	10	30.35
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	7	30.35
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	5	30.32
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	15	30.3
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	15	30.28
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	11	30.28
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	14	30.27
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	9	30.27
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	3	30.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	5	30.23
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	6	30.18
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	9	30.1
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	11	30.08
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	7	30.08
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	2	30.05
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	11	30.04
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	15	30.01
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	3	29.99
(1,674)	1:110:A:VAL:HG12	1:215:A:ASN:H	14	29.95
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	8	29.91
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	13	29.86
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	4	29.84
(1,739)	1:133:A:VAL:HG13	1:235:A:ALA:H	15	29.82
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB2	14	29.8
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	3	29.79
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	3	29.78
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	8	29.77
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB1	2	29.72
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD11	15	29.65
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	5	29.64
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	3	29.52
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	11	29.51
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	7	29.47
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	4	29.44
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB3	10	29.34
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	1	29.3
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	5	29.3
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	5	29.27
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	9	29.26
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	9	29.26
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	3	29.24
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	15	29.19
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	8	29.18
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	15	29.17
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB1	2	29.12
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	7	29.1
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	14	29.09
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	15	29.08
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	10	29.06
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	15	29.03
(1,739)	1:133:A:VAL:HG11	1:235:A:ALA:H	2	28.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB2	8	28.93
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	5	28.92
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	5	28.9
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB1	9	28.9
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	9	28.89
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	9	28.89
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB1	9	28.89
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	7	28.84
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	15	28.81
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	9	28.76
(1,739)	1:133:A:VAL:HG13	1:235:A:ALA:H	9	28.75
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	14	28.74
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	14	28.74
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	3	28.7
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	14	28.69
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	4	28.67
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	4	28.67
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	8	28.63
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	11	28.61
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB1	15	28.55
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	9	28.55
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	9	28.55
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	11	28.5
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB1	9	28.47
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	14	28.47
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	2	28.47
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD22	4	28.41
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	7	28.36
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	8	28.36
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	5	28.35
(1,595)	1:133:A:VAL:HG21	1:235:A:ALA:H	6	28.35
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	8	28.34
(1,1144)	1:110:A:VAL:HG13	1:214:A:ALA:HB3	13	28.34
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	14	28.33
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG13	13	28.3
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG13	13	28.3
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	12	28.27
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	10	28.27
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	15	28.27
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	14	28.23
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	5	28.21
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB2	14	28.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	8	28.17
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB1	9	28.13
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	7	28.12
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	10	28.05
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	8	28.05
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	6	28.03
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	6	28.03
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	6	27.95
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	11	27.87
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	11	27.86
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	9	27.86
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	10	27.85
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	10	27.85
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	9	27.82
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	4	27.81
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	11	27.8
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	13	27.79
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	9	27.76
(1,1460)	1:122:A:LEU:HD11	1:227:A:HIS:HB2	15	27.75
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	6	27.72
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	11	27.71
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	5	27.62
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB2	11	27.6
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	4	27.59
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	4	27.59
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	5	27.57
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	11	27.56
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	14	27.56
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	9	27.53
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	11	27.53
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB2	11	27.48
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	11	27.46
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB1	9	27.4
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	13	27.4
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD13	4	27.4
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	11	27.33
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	11	27.33
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG12	14	27.31
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG12	14	27.31
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	10	27.29
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	13	27.29
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	13	27.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD12	14	27.28
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	14	27.26
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	8	27.24
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	5	27.24
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	9	27.22
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	13	27.22
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	13	27.21
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	2	27.17
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	9	27.13
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG12	10	27.01
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG12	10	27.01
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	6	26.98
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	15	26.98
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB2	4	26.97
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	11	26.97
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	8	26.96
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	13	26.95
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	3	26.94
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	15	26.91
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	10	26.9
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	14	26.88
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	2	26.88
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	15	26.87
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB2	4	26.86
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	7	26.83
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	5	26.82
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	5	26.82
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	4	26.82
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	8	26.76
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB2	14	26.72
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG12	2	26.7
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG12	2	26.7
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	10	26.67
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	5	26.66
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	11	26.64
(1,595)	1:133:A:VAL:HG22	1:235:A:ALA:H	15	26.64
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	10	26.64
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	5	26.6
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	11	26.59
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	10	26.54
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	10	26.51
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	14	26.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	13	26.45
(1,1460)	1:122:A:LEU:HD13	1:227:A:HIS:HB2	14	26.44
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	10	26.42
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD22	14	26.41
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	3	26.4
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	4	26.36
(1,921)	1:108:A:GLU:HG3	1:214:A:ALA:HB3	6	26.35
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	10	26.33
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	14	26.32
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	7	26.31
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	14	26.25
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	11	26.25
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	14	26.24
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	4	26.19
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	7	26.14
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	7	26.06
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB2	11	26.02
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	11	26.0
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB2	4	25.99
(1,88)	1:110:A:VAL:HA	1:215:A:ASN:H	3	25.98
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	11	25.97
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	15	25.97
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	15	25.96
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	15	25.96
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	2	25.96
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	10	25.95
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	5	25.92
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	8	25.9
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	11	25.89
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	14	25.87
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	11	25.84
(1,674)	1:110:A:VAL:HG12	1:215:A:ASN:H	6	25.84
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG12	11	25.83
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG12	11	25.83
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	3	25.78
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	10	25.77
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	9	25.76
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	15	25.69
(1,1626)	1:108:A:GLU:HB3	1:214:A:ALA:HB3	6	25.63
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	3	25.58
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	13	25.58
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	3	25.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	11	25.52
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	5	25.5
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	8	25.49
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	6	25.46
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	5	25.44
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	5	25.44
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	8	25.36
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	2	25.36
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	2	25.36
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB3	5	25.35
(1,642)	1:109:A:ALA:H	1:214:A:ALA:HB3	6	25.33
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	9	25.32
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB2	14	25.31
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	14	25.31
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	3	25.28
(1,739)	1:133:A:VAL:HG13	1:235:A:ALA:H	4	25.25
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	10	25.2
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	14	25.19
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	7	25.12
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	14	25.11
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	3	25.09
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	6	25.05
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	6	25.05
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	5	25.04
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	15	25.01
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	10	24.98
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	14	24.92
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	2	24.91
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	2	24.91
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	14	24.89
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	14	24.78
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	10	24.7
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	13	24.7
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	7	24.69
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	3	24.64
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	11	24.63
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	10	24.63
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB1	2	24.47
(1,1460)	1:122:A:LEU:HD11	1:227:A:HIS:HB2	8	24.35
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	5	24.33
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	11	24.33
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	11	24.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1212)	1:110:A:VAL:HG21	1:217:A:GLU:HG3	13	24.22
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	5	24.22
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	4	24.15
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	13	24.07
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	4	24.07
(1,595)	1:133:A:VAL:HG21	1:235:A:ALA:H	4	24.03
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	14	24.02
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	7	24.02
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	2	24.01
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	9	24.01
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG12	6	24.0
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG12	6	24.0
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	13	23.98
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	4	23.92
(1,1460)	1:122:A:LEU:HD13	1:227:A:HIS:HB2	4	23.9
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	4	23.88
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	8	23.88
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	10	23.83
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	14	23.82
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	4	23.82
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	13	23.8
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	4	23.69
(1,739)	1:133:A:VAL:HG12	1:235:A:ALA:H	13	23.62
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	14	23.61
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	15	23.6
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB2	11	23.55
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	13	23.5
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	4	23.49
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	5	23.47
(1,595)	1:133:A:VAL:HG23	1:235:A:ALA:H	7	23.47
(1,739)	1:133:A:VAL:HG11	1:235:A:ALA:H	7	23.39
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	4	23.39
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	5	23.38
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	8	23.34
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	4	23.34
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB1	9	23.3
(1,470)	1:148:A:TRP:HZ2	1:215:A:ASN:H	3	23.3
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	3	23.25
(1,1040)	1:109:A:ALA:HA	1:214:A:ALA:HB3	6	23.24
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	9	23.22
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	7	23.22
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	11	23.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB2	4	23.17
(1,674)	1:110:A:VAL:HG11	1:215:A:ASN:H	3	23.07
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	4	23.01
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	13	22.95
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	10	22.86
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	3	22.83
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	5	22.8
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB2	14	22.6
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	10	22.57
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	4	22.49
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	5	22.47
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	4	22.35
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB2	3	22.32
(1,1064)	1:110:A:VAL:HA	1:215:A:ASN:HB3	3	22.32
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	5	22.04
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	8	21.96
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	7	21.92
(1,1123)	1:129:A:THR:HG1	1:234:A:GLN:HA	8	21.8
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	4	21.75
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	4	21.73
(1,1772)	1:148:A:TRP:HZ2	1:214:A:ALA:HB3	6	21.7
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	4	21.69
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	6	21.6
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	8	21.59
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	4	21.45
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	8	21.36
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	6	21.23
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	8	21.21
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	14	21.0
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	6	20.95
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	4	20.9
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	13	20.9
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	8	20.88
(1,595)	1:133:A:VAL:HG21	1:235:A:ALA:H	13	20.83
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	8	20.78
(1,1144)	1:110:A:VAL:HG11	1:214:A:ALA:HB3	3	20.72
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	6	20.71
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	7	20.64
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	2	20.6
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	6	20.59
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	4	20.53
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	3	20.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	7	20.43
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	7	20.43
(1,1015)	1:110:A:VAL:HA	1:214:A:ALA:HB3	6	20.42
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	6	20.31
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	6	20.29
(1,1201)	1:215:A:ASN:HB2	1:110:A:VAL:HG11	3	20.23
(1,1201)	1:215:A:ASN:HB3	1:110:A:VAL:HG11	3	20.23
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	10	20.18
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	7	20.14
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	4	20.04
(1,695)	1:112:A:GLU:H	1:215:A:ASN:H	3	20.03
(1,1212)	1:110:A:VAL:HG23	1:217:A:GLU:HG3	3	20.02
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	14	19.91
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	6	19.87
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	4	19.84
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	14	19.67
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	13	19.43
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	13	19.43
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	4	19.34
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	7	19.29
(1,430)	1:130:A:ARG:HA	1:235:A:ALA:H	8	19.23
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	4	19.22
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	4	19.22
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	6	19.22
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	4	19.22
(1,1144)	1:110:A:VAL:HG12	1:214:A:ALA:HB3	6	19.21
(1,594)	1:112:A:GLU:H	1:217:A:GLU:HG3	6	19.16
(1,1212)	1:110:A:VAL:HG21	1:217:A:GLU:HG3	2	19.12
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	4	19.09
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	4	19.02
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	8	18.61
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	6	18.47
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	4	18.32
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	13	17.96
(1,395)	1:130:A:ARG:HG2	1:235:A:ALA:H	4	17.92
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	4	17.91
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	4	17.9
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	3	17.83
(1,498)	1:134:A:CYS:H	1:235:A:ALA:H	8	17.83
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	4	17.7
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	7	17.42
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	6	17.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	13	17.41
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	14	17.37
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD12	6	17.24
(1,884)	1:130:A:ARG:HB3	1:235:A:ALA:H	8	17.16
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB2	8	17.12
(1,1550)	1:129:A:THR:HG1	1:234:A:GLN:HB3	8	17.12
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	13	17.1
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	6	16.96
(1,1408)	1:113:A:ASP:HB2	1:214:A:ALA:HB3	6	16.9
(1,595)	1:133:A:VAL:HG22	1:235:A:ALA:H	8	16.85
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	13	16.8
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	6	16.73
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	6	16.72
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	13	16.71
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	13	16.57
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	13	16.43
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	13	16.08
(1,325)	1:130:A:ARG:HB2	1:235:A:ALA:H	8	16.08
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD12	13	15.99
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD11	6	15.96
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	6	15.93
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	13	15.86
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	6	15.85
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	13	15.78
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	6	15.72
(1,68)	1:235:A:ALA:H	1:133:A:VAL:H	8	15.66
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	3	15.61
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	7	15.44
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	4	15.35
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	13	15.32
(1,1445)	1:234:A:GLN:HA	1:128:A:HIS:HB2	8	15.28
(1,556)	1:130:A:ARG:HD3	1:235:A:ALA:H	8	15.26
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	13	15.25
(1,94)	1:229:A:ILE:H	1:125:A:CYS:H	2	15.18
(1,1460)	1:122:A:LEU:HD12	1:227:A:HIS:HB2	13	15.04
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	13	15.02
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	2	14.84
(1,739)	1:133:A:VAL:HG11	1:235:A:ALA:H	8	14.83
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	6	14.74
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	6	14.66
(1,886)	1:229:A:ILE:H	1:126:A:ARG:H	2	14.54
(1,688)	1:229:A:ILE:H	1:124:A:ASP:HB3	2	14.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	13	14.54
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	13	14.38
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	6	14.15
(1,551)	1:229:A:ILE:H	1:121:A:ALA:HA	2	14.11
(1,456)	1:229:A:ILE:H	1:124:A:ASP:HA	2	13.75
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	6	13.65
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	13	13.55
(1,1102)	1:115:A:LEU:HB2	1:217:A:GLU:HG3	6	13.39
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	6	12.94
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	13	12.93
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	13	12.66
(1,1118)	1:227:A:HIS:HA	1:125:A:CYS:HB2	2	12.65
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	13	12.64
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	6	12.63
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	13	12.29
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	13	11.78
(1,675)	1:227:A:HIS:H	1:118:A:LEU:HD21	2	11.5
(2,4)	1:227:A:HIS:H	1:118:A:LEU:O	2	11.34
(1,389)	1:121:A:ALA:H	1:229:A:ILE:H	2	11.29
(1,192)	1:228:A:THR:H	1:125:A:CYS:H	2	11.24
(1,267)	1:227:A:HIS:H	1:118:A:LEU:HD13	2	11.04
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	13	10.82
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	13	10.81
(1,486)	1:227:A:HIS:H	1:122:A:LEU:HD13	2	10.06
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	6	9.64
(1,1505)	1:227:A:HIS:HB2	1:122:A:LEU:HG	2	9.2
(1,1161)	1:119:A:GLU:HG2	1:224:A:GLU:HB2	2	9.02
(1,1460)	1:122:A:LEU:HD13	1:227:A:HIS:HB2	2	8.69
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	6	8.52
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	13	8.21
(1,944)	1:227:A:HIS:HA	1:122:A:LEU:HG	2	8.12
(2,5)	1:228:A:THR:H	1:119:A:GLU:O	2	8.02
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	13	7.78
(1,163)	1:228:A:THR:H	1:123:A:GLU:HB2	2	7.25
(1,1196)	1:123:A:GLU:HB3	1:228:A:THR:HA	2	6.3
(1,1204)	1:123:A:GLU:HG2	1:228:A:THR:HA	2	5.99
(1,508)	1:123:A:GLU:HG2	1:228:A:THR:H	2	5.97
(1,1479)	1:123:A:GLU:HG3	1:228:A:THR:HA	2	5.51
(1,1457)	1:227:A:HIS:HB2	1:123:A:GLU:HG2	2	5.44
(1,1292)	1:120:A:GLN:HA	1:227:A:HIS:H	2	4.34
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	2	4.29
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	9	4.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:143:A:LEU:HD11	1:140:A:ARG:HB3	7	3.9
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	7	3.63
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD13	2	3.36
(1,1714)	1:122:A:LEU:HD12	1:125:A:CYS:HB2	2	3.18
(1,468)	1:122:A:LEU:HD12	1:125:A:CYS:H	2	3.17
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG12	13	2.94
(1,1475)	1:183:A:LEU:HD22	1:179:A:ILE:HB	4	2.91
(1,1726)	1:118:A:LEU:HG	1:115:A:LEU:HD12	7	2.71
(1,1782)	1:143:A:LEU:HD13	1:194:A:TRP:HZ3	1	2.7
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	14	2.69
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG13	6	2.67
(1,1453)	1:183:A:LEU:HD22	1:180:A:HIS:HD1	13	2.62
(1,520)	1:164:A:LEU:HD23	1:166:A:GLN:H	14	2.62
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	9	2.59
(1,1782)	1:143:A:LEU:HD11	1:194:A:TRP:HZ3	4	2.58
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	10	2.55
(1,1114)	1:143:A:LEU:HD13	1:140:A:ARG:HB3	9	2.54
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	1	2.54
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG11	10	2.52
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	7	2.48
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	13	2.47
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG13	4	2.42
(1,1114)	1:143:A:LEU:HD11	1:140:A:ARG:HB3	14	2.41
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	11	2.4
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG13	5	2.38
(1,1425)	1:121:A:ALA:HB2	1:122:A:LEU:HD12	1	2.34
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG11	1	2.26
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	13	2.25
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	8	2.24
(1,1107)	1:134:A:CYS:HB2	1:138:A:SER:HB2	8	2.24
(1,1234)	1:208:A:LEU:HD11	1:205:A:LYS:HE2	10	2.21
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG12	11	2.2
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	6	2.2
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG11	12	2.19
(1,1112)	1:143:A:LEU:HD12	1:194:A:TRP:HB2	14	2.18
(1,1429)	1:141:A:LEU:HD22	1:144:A:LEU:HD11	4	2.17
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	5	2.16
(1,154)	1:208:A:LEU:HD11	1:205:A:LYS:H	10	2.14
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD13	14	2.13
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	10	2.13
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD11	7	2.11
(1,1389)	1:198:A:VAL:HG11	1:144:A:LEU:HD12	6	2.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	11	2.07
(1,1389)	1:198:A:VAL:HG13	1:144:A:LEU:HD13	10	2.06
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG13	3	2.03
(1,54)	1:112:A:GLU:H	1:114:A:VAL:HG23	12	2.03
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG13	15	2.0
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	14	1.98
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	5	1.96
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	5	1.95
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	8	1.95
(1,1087)	1:122:A:LEU:HD12	1:126:A:ARG:HB3	11	1.94
(1,1112)	1:143:A:LEU:HD11	1:194:A:TRP:HB2	9	1.93
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	13	1.93
(1,962)	1:225:A:LYS:HG2	1:226:A:ASN:HB3	12	1.93
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	15	1.93
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD23	10	1.93
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG11	15	1.92
(1,482)	1:118:A:LEU:H	1:115:A:LEU:HD13	7	1.89
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG11	9	1.87
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	3	1.85
(1,1600)	1:157:A:VAL:HG12	1:158:A:LYS:HG2	10	1.84
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	12	1.84
(1,1087)	1:122:A:LEU:HD11	1:126:A:ARG:HB3	9	1.84
(1,1453)	1:183:A:LEU:HD23	1:180:A:HIS:HD1	2	1.83
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	1	1.82
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD13	13	1.81
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG12	3	1.8
(1,1341)	1:204:A:GLU:HB2	1:205:A:LYS:HG3	8	1.8
(1,571)	1:204:A:GLU:H	1:206:A:ARG:HG2	14	1.8
(1,1112)	1:143:A:LEU:HD12	1:194:A:TRP:HB2	7	1.79
(1,1425)	1:121:A:ALA:HB1	1:122:A:LEU:HD11	2	1.77
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	9	1.77
(1,571)	1:204:A:GLU:H	1:206:A:ARG:HG2	4	1.77
(1,931)	1:160:A:ARG:HA	1:163:A:LEU:HD12	2	1.76
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	14	1.74
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	13	1.73
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	9	1.73
(1,1024)	1:122:A:LEU:HD12	1:134:A:CYS:HA	2	1.72
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD23	2	1.71
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	3	1.71
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	6	1.7
(1,1475)	1:183:A:LEU:HD21	1:179:A:ILE:HB	2	1.69
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG13	14	1.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1087)	1:122:A:LEU:HD11	1:126:A:ARG:HB3	10	1.69
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD12	8	1.68
(1,1339)	1:136:A:ASP:HB3	1:133:A:VAL:HB	3	1.67
(1,1010)	1:168:A:LEU:HD23	1:165:A:VAL:HG13	10	1.67
(1,43)	1:165:A:VAL:HG21	1:117:A:PRO:HB3	12	1.67
(1,1566)	1:124:A:ASP:HB2	1:208:A:LEU:HD23	10	1.66
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG21	5	1.66
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	1	1.66
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG11	2	1.65
(1,1698)	1:183:A:LEU:HD22	1:180:A:HIS:HA	13	1.63
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD12	7	1.62
(1,1389)	1:198:A:VAL:HG13	1:144:A:LEU:HD12	4	1.6
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	13	1.58
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD13	3	1.58
(1,1466)	1:229:A:ILE:HG12	1:230:A:PRO:HG2	12	1.57
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD11	3	1.56
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD13	5	1.56
(1,1034)	1:199:A:LYS:HE2	1:195:A:MET:HE1	15	1.56
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	14	1.54
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	3	1.53
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG12	1	1.53
(1,1047)	1:208:A:LEU:HD21	1:205:A:LYS:HE2	10	1.53
(1,1578)	1:203:A:ALA:HB3	1:206:A:ARG:HD3	4	1.52
(1,931)	1:160:A:ARG:HA	1:163:A:LEU:HD13	9	1.52
(1,1698)	1:183:A:LEU:HD23	1:180:A:HIS:HA	2	1.51
(1,1466)	1:229:A:ILE:HG12	1:230:A:PRO:HG2	9	1.51
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	2	1.5
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD13	2	1.5
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	11	1.49
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD13	9	1.49
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	2	1.48
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	15	1.48
(1,1578)	1:203:A:ALA:HB3	1:206:A:ARG:HD3	7	1.47
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG11	9	1.47
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD12	10	1.47
(1,1115)	1:152:A:LYS:HE2	1:152:A:LYS:HB3	13	1.46
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD13	6	1.45
(1,962)	1:225:A:LYS:HG2	1:226:A:ASN:HB3	1	1.44
(1,401)	1:165:A:VAL:HG22	1:164:A:LEU:H	10	1.44
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	12	1.43
(1,1092)	1:180:A:HIS:HB3	1:195:A:MET:HB2	1	1.43
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	5	1.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	10	1.42
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD12	11	1.41
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	5	1.41
(1,1107)	1:134:A:CYS:HB2	1:138:A:SER:HB2	12	1.4
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	11	1.4
(1,1007)	1:198:A:VAL:HB	1:201:A:LEU:HB3	12	1.4
(1,1114)	1:143:A:LEU:HD13	1:140:A:ARG:HB3	8	1.39
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	7	1.39
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	7	1.38
(1,1578)	1:203:A:ALA:HB1	1:206:A:ARG:HD3	8	1.38
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	5	1.38
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD12	7	1.38
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD12	9	1.38
(1,1224)	1:199:A:LYS:HE2	1:199:A:LYS:HB2	5	1.38
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	6	1.38
(1,1578)	1:203:A:ALA:HB1	1:206:A:ARG:HD3	5	1.37
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	11	1.37
(1,1153)	1:193:A:GLN:HA	1:196:A:VAL:HG13	5	1.37
(1,1389)	1:198:A:VAL:HG13	1:144:A:LEU:HD13	5	1.36
(1,1466)	1:229:A:ILE:HG12	1:230:A:PRO:HG2	15	1.35
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	4	1.35
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	6	1.35
(1,1012)	1:164:A:LEU:HD11	1:161:A:MET:HE3	14	1.35
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	2	1.35
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	1	1.34
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	13	1.34
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD22	7	1.33
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	4	1.33
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	11	1.33
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	10	1.32
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD21	15	1.32
(1,304)	1:226:A:ASN:H	1:226:A:ASN:HB2	10	1.32
(1,1670)	1:152:A:LYS:HA	1:152:A:LYS:HD3	5	1.31
(1,1553)	1:165:A:VAL:HG22	1:161:A:MET:HA	10	1.31
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	3	1.3
(1,1609)	1:157:A:VAL:HG13	1:194:A:TRP:HH2	10	1.3
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG21	12	1.3
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	10	1.29
(1,1341)	1:204:A:GLU:HB2	1:205:A:LYS:HG3	15	1.29
(1,1115)	1:152:A:LYS:HE2	1:152:A:LYS:HB3	15	1.29
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	14	1.28
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	3	1.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD11	11	1.27
(1,1126)	1:144:A:LEU:HD21	1:115:A:LEU:HD11	7	1.27
(1,1746)	1:208:A:LEU:HD23	1:124:A:ASP:HB3	10	1.26
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	2	1.26
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	7	1.26
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	13	1.26
(1,1341)	1:204:A:GLU:HB2	1:205:A:LYS:HG3	2	1.26
(1,1318)	1:111:A:MET:HE1	1:115:A:LEU:HD13	2	1.26
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG21	1	1.26
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	5	1.26
(1,1781)	1:148:A:TRP:HE3	1:161:A:MET:HG3	11	1.25
(1,1013)	1:164:A:LEU:HD12	1:161:A:MET:HG3	14	1.25
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	10	1.25
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	10	1.25
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	11	1.24
(1,304)	1:226:A:ASN:H	1:226:A:ASN:HB2	12	1.24
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	3	1.23
(1,1670)	1:152:A:LYS:HA	1:152:A:LYS:HD3	4	1.23
(1,1425)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	7	1.23
(1,1318)	1:111:A:MET:HE3	1:115:A:LEU:HD13	4	1.23
(1,1107)	1:134:A:CYS:HB2	1:138:A:SER:HB2	4	1.23
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	3	1.22
(1,1698)	1:183:A:LEU:HD22	1:180:A:HIS:HA	11	1.22
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	3	1.22
(1,399)	1:158:A:LYS:HD3	1:148:A:TRP:HE1	8	1.22
(1,1578)	1:203:A:ALA:HB1	1:206:A:ARG:HD3	2	1.21
(1,1578)	1:203:A:ALA:HB1	1:206:A:ARG:HD3	15	1.21
(1,1166)	1:111:A:MET:HE1	1:111:A:MET:HB2	4	1.21
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	8	1.21
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	2	1.21
(1,304)	1:226:A:ASN:H	1:226:A:ASN:HB2	3	1.21
(1,250)	1:191:A:VAL:HG21	1:185:A:VAL:H	9	1.21
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	3	1.21
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	6	1.21
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	6	1.21
(1,1389)	1:198:A:VAL:HG13	1:144:A:LEU:HD13	2	1.2
(1,991)	1:155:A:ILE:HD12	1:154:A:SER:HB2	2	1.2
(1,75)	1:139:A:ARG:HD2	1:140:A:ARG:H	6	1.2
(1,1783)	1:158:A:LYS:HD3	1:148:A:TRP:HZ2	8	1.19
(1,1670)	1:152:A:LYS:HA	1:152:A:LYS:HD3	11	1.19
(1,1475)	1:183:A:LEU:HD23	1:179:A:ILE:HB	11	1.19
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	4	1.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:186:A:ASP:HB3	1:185:A:VAL:H	7	1.19
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	13	1.19
(1,304)	1:226:A:ASN:H	1:226:A:ASN:HB2	1	1.19
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	14	1.18
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	3	1.18
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	10	1.18
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	8	1.18
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	11	1.17
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	4	1.17
(1,1344)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	10	1.17
(1,1166)	1:111:A:MET:HE3	1:111:A:MET:HB2	10	1.17
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	1	1.16
(1,1720)	1:172:A:ARG:HD3	1:170:A:SER:HB3	11	1.16
(1,1670)	1:152:A:LYS:HA	1:152:A:LYS:HD3	12	1.16
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	1	1.16
(1,782)	1:108:A:GLU:HG2	1:108:A:GLU:H	9	1.16
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	5	1.16
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	8	1.16
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	12	1.15
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD22	4	1.15
(1,250)	1:191:A:VAL:HG23	1:185:A:VAL:H	6	1.15
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	2	1.14
(1,1346)	1:225:A:LYS:HB3	1:225:A:LYS:HE2	4	1.14
(1,1346)	1:225:A:LYS:HB3	1:225:A:LYS:HE2	7	1.14
(1,1114)	1:143:A:LEU:HD11	1:140:A:ARG:HB3	13	1.14
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	3	1.14
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	11	1.14
(1,38)	1:157:A:VAL:HG11	1:161:A:MET:HG3	6	1.14
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	4	1.13
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	8	1.13
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	10	1.13
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	15	1.13
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	15	1.13
(1,1743)	1:161:A:MET:HE2	1:114:A:VAL:HG23	5	1.13
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	8	1.13
(1,1394)	1:122:A:LEU:HD12	1:134:A:CYS:HB3	2	1.13
(1,867)	1:186:A:ASP:HB3	1:185:A:VAL:H	5	1.13
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	7	1.13
(1,1318)	1:111:A:MET:HE1	1:115:A:LEU:HD11	3	1.12
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG23	11	1.12
(1,782)	1:108:A:GLU:HG2	1:108:A:GLU:H	4	1.12
(1,726)	1:158:A:LYS:HE2	1:155:A:ILE:H	1	1.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:164:A:LEU:HD23	1:165:A:VAL:H	14	1.12
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	4	1.11
(1,1763)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	14	1.11
(1,867)	1:186:A:ASP:HB3	1:185:A:VAL:H	12	1.11
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	12	1.1
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	13	1.1
(1,969)	1:139:A:ARG:HD2	1:140:A:ARG:HA	3	1.1
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	2	1.1
(1,248)	1:152:A:LYS:HE2	1:152:A:LYS:H	10	1.1
(1,1542)	1:129:A:THR:HG1	1:133:A:VAL:HG22	15	1.09
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	1	1.09
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG22	3	1.09
(1,1303)	1:138:A:SER:HB2	1:134:A:CYS:HB3	12	1.09
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	14	1.09
(1,250)	1:191:A:VAL:HG23	1:185:A:VAL:H	1	1.09
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	3	1.08
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	15	1.08
(1,1346)	1:225:A:LYS:HB3	1:225:A:LYS:HE2	3	1.08
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	11	1.08
(1,250)	1:191:A:VAL:HG21	1:185:A:VAL:H	10	1.08
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	15	1.07
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	14	1.07
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	6	1.07
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG21	8	1.07
(1,1114)	1:143:A:LEU:HD11	1:140:A:ARG:HB3	6	1.07
(1,867)	1:186:A:ASP:HB3	1:185:A:VAL:H	1	1.07
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG22	15	1.07
(1,1670)	1:152:A:LYS:HA	1:152:A:LYS:HD3	7	1.06
(1,1346)	1:225:A:LYS:HB3	1:225:A:LYS:HE2	5	1.06
(1,1234)	1:208:A:LEU:HD11	1:205:A:LYS:HE2	5	1.06
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD21	1	1.06
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	4	1.06
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	4	1.06
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	4	1.06
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	15	1.05
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG22	6	1.05
(1,1283)	1:200:A:ARG:H	1:199:A:LYS:HB2	9	1.05
(1,1114)	1:143:A:LEU:HD13	1:140:A:ARG:HB3	2	1.05
(1,969)	1:139:A:ARG:HD2	1:140:A:ARG:HA	9	1.05
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	8	1.05
(1,250)	1:191:A:VAL:HG23	1:185:A:VAL:H	5	1.05
(1,250)	1:191:A:VAL:HG21	1:185:A:VAL:H	13	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	1	1.04
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	11	1.04
(1,1241)	1:183:A:LEU:HB3	1:180:A:HIS:HA	3	1.04
(1,1166)	1:111:A:MET:HE1	1:111:A:MET:HB2	11	1.04
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	14	1.04
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	7	1.04
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	11	1.03
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	9	1.03
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	10	1.03
(1,250)	1:191:A:VAL:HG23	1:185:A:VAL:H	12	1.03
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	14	1.02
(1,1743)	1:161:A:MET:HE3	1:114:A:VAL:HG22	13	1.02
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	15	1.02
(1,1542)	1:129:A:THR:HG1	1:133:A:VAL:HG21	2	1.02
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	11	1.02
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG23	6	1.02
(1,1283)	1:200:A:ARG:H	1:199:A:LYS:HB2	8	1.02
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD22	2	1.02
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	3	1.02
(1,41)	1:204:A:GLU:HG3	1:208:A:LEU:HB3	3	1.02
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	15	1.01
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	2	1.0
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	13	1.0
(1,1580)	1:225:A:LYS:HG3	1:120:A:GLN:HA	2	1.0
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	7	1.0
(1,1087)	1:122:A:LEU:HD12	1:126:A:ARG:HB3	12	1.0
(1,1016)	1:165:A:VAL:HG22	1:161:A:MET:HE1	11	1.0
(1,968)	1:110:A:VAL:HA	1:113:A:ASP:HB3	11	1.0
(1,367)	1:181:A:ARG:HB2	1:180:A:HIS:H	9	1.0
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	11	0.99
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	4	0.99
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	1	0.99
(1,1453)	1:183:A:LEU:HD22	1:180:A:HIS:HD1	11	0.99
(1,1283)	1:200:A:ARG:H	1:199:A:LYS:HB2	10	0.99
(1,1157)	1:158:A:LYS:HE2	1:148:A:TRP:HB2	14	0.99
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	1	0.99
(1,966)	1:199:A:LYS:HE2	1:199:A:LYS:HA	15	0.99
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD21	8	0.99
(1,821)	1:157:A:VAL:HG11	1:158:A:LYS:H	10	0.99
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	6	0.99
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	7	0.98
(1,1762)	1:158:A:LYS:HD3	1:158:A:LYS:HA	8	0.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	9	0.98
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	7	0.98
(1,1619)	1:122:A:LEU:HD12	1:134:A:CYS:HB2	2	0.98
(1,1616)	1:208:A:LEU:HD11	1:125:A:CYS:HB2	5	0.98
(1,1513)	1:205:A:LYS:HG3	1:205:A:LYS:HA	9	0.98
(1,367)	1:181:A:ARG:HB2	1:180:A:HIS:H	4	0.98
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	2	0.97
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	8	0.97
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	11	0.97
(1,1286)	1:209:A:PHE:HB2	1:210:A:SER:HB3	9	0.97
(1,1185)	1:208:A:LEU:HB2	1:205:A:LYS:HB2	9	0.97
(1,43)	1:165:A:VAL:HG22	1:117:A:PRO:HB3	6	0.97
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	11	0.96
(1,336)	1:192:A:SER:H	1:193:A:GLN:HB3	4	0.96
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	7	0.96
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	1	0.95
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	5	0.95
(1,330)	1:205:A:LYS:HG3	1:173:A:TRP:HE1	9	0.95
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	10	0.94
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	3	0.94
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	9	0.94
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	11	0.94
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	12	0.94
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	9	0.94
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	4	0.94
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	14	0.94
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	6	0.94
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD21	13	0.94
(1,34)	1:163:A:LEU:HA	1:166:A:GLN:HB2	12	0.94
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	7	0.93
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	10	0.93
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	12	0.93
(1,43)	1:165:A:VAL:HG21	1:117:A:PRO:HB3	2	0.93
(1,1714)	1:122:A:LEU:HD13	1:125:A:CYS:HB2	7	0.92
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	5	0.92
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	13	0.92
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG22	14	0.92
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	14	0.92
(1,353)	1:157:A:VAL:HG13	1:154:A:SER:H	10	0.92
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	5	0.91
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	1	0.91
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	7	0.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	1	0.91
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	2	0.91
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	9	0.91
(1,367)	1:181:A:ARG:HB2	1:180:A:HIS:H	3	0.91
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	9	0.91
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	13	0.91
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	13	0.91
(1,1534)	1:162:A:ALA:HB2	1:113:A:ASP:HB3	13	0.9
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD13	15	0.9
(1,1311)	1:152:A:LYS:HA	1:152:A:LYS:HE2	15	0.9
(1,1289)	1:117:A:PRO:HG3	1:165:A:VAL:HG23	11	0.9
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG11	13	0.9
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG22	10	0.9
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	12	0.9
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	14	0.9
(1,38)	1:183:A:LEU:HD23	1:161:A:MET:HG3	5	0.9
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	4	0.89
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	6	0.89
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	12	0.89
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB3	3	0.89
(1,1208)	1:136:A:ASP:HB3	1:133:A:VAL:HG13	3	0.89
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG12	4	0.89
(1,969)	1:139:A:ARG:HD2	1:140:A:ARG:HA	6	0.89
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	8	0.89
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD22	15	0.89
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	3	0.89
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	8	0.89
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	10	0.89
(1,250)	1:191:A:VAL:HG21	1:185:A:VAL:H	15	0.89
(1,221)	1:134:A:CYS:HB3	1:133:A:VAL:H	7	0.89
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	7	0.88
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG22	1	0.88
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	10	0.88
(1,1578)	1:203:A:ALA:HB1	1:206:A:ARG:HD3	9	0.88
(1,1500)	1:185:A:VAL:HG11	1:187:A:HIS:HA	5	0.88
(1,1137)	1:173:A:TRP:HD1	1:205:A:LYS:HG3	9	0.88
(1,726)	1:158:A:LYS:HE2	1:155:A:ILE:H	3	0.88
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	4	0.88
(1,370)	1:198:A:VAL:HG13	1:198:A:VAL:H	14	0.88
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	4	0.88
(1,18)	1:229:A:ILE:H	1:228:A:THR:H	7	0.88
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	11	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	9	0.87
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	14	0.87
(1,1634)	1:161:A:MET:HG3	1:161:A:MET:HA	11	0.87
(1,1616)	1:208:A:LEU:HD11	1:125:A:CYS:HB2	4	0.87
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	14	0.87
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	15	0.87
(1,1542)	1:129:A:THR:HG1	1:133:A:VAL:HG21	9	0.87
(1,1475)	1:183:A:LEU:HD23	1:179:A:ILE:HB	13	0.87
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	5	0.87
(1,1089)	1:212:A:GLU:HG2	1:212:A:GLU:HA	3	0.87
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG13	1	0.87
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD11	3	0.87
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD23	2	0.87
(1,370)	1:198:A:VAL:HG13	1:198:A:VAL:H	1	0.87
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	6	0.87
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	11	0.87
(1,367)	1:181:A:ARG:HB2	1:180:A:HIS:H	2	0.87
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	8	0.87
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	8	0.87
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	9	0.87
(1,1769)	1:144:A:LEU:HD22	1:194:A:TRP:HZ2	2	0.86
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	13	0.86
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	9	0.86
(1,1389)	1:198:A:VAL:HG11	1:144:A:LEU:HD13	12	0.86
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB3	6	0.86
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	12	0.86
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	7	0.86
(1,370)	1:198:A:VAL:HG12	1:198:A:VAL:H	9	0.86
(1,221)	1:134:A:CYS:HB3	1:133:A:VAL:H	8	0.86
(1,1769)	1:144:A:LEU:HD22	1:194:A:TRP:HZ2	8	0.85
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	6	0.85
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	7	0.85
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	13	0.85
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD13	11	0.85
(1,370)	1:198:A:VAL:HG12	1:198:A:VAL:H	2	0.85
(1,370)	1:198:A:VAL:HG12	1:198:A:VAL:H	5	0.85
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	10	0.85
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	4	0.85
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	14	0.85
(1,18)	1:229:A:ILE:H	1:228:A:THR:H	3	0.85
(1,1769)	1:144:A:LEU:HD23	1:194:A:TRP:HZ2	12	0.84
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	3	0.84

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD21	4	0.84
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	8	0.84
(1,1534)	1:162:A:ALA:HB3	1:113:A:ASP:HB3	14	0.84
(1,1372)	1:158:A:LYS:HG2	1:148:A:TRP:HZ2	10	0.84
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	6	0.84
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB2	5	0.84
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB3	13	0.84
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG12	3	0.84
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	13	0.84
(1,868)	1:133:A:VAL:HG12	1:133:A:VAL:H	10	0.84
(1,868)	1:133:A:VAL:HG12	1:133:A:VAL:H	11	0.84
(1,488)	1:141:A:LEU:HD23	1:142:A:ALA:H	3	0.84
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	8	0.84
(1,370)	1:198:A:VAL:HG11	1:198:A:VAL:H	10	0.84
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	13	0.84
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	2	0.84
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	2	0.84
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	9	0.83
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	9	0.83
(1,1742)	1:158:A:LYS:HA	1:161:A:MET:HB2	14	0.83
(1,1722)	1:133:A:VAL:HG22	1:134:A:CYS:HB3	10	0.83
(1,1616)	1:208:A:LEU:HD12	1:125:A:CYS:HB2	9	0.83
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	4	0.83
(1,1494)	1:183:A:LEU:HD22	1:191:A:VAL:HG22	13	0.83
(1,1456)	1:111:A:MET:HB3	1:148:A:TRP:HD1	11	0.83
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	12	0.83
(1,1288)	1:205:A:LYS:HG3	1:208:A:LEU:HD23	6	0.83
(1,1215)	1:202:A:ILE:HD12	1:177:A:ASP:HB3	11	0.83
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD11	8	0.83
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	1	0.83
(1,868)	1:133:A:VAL:HG13	1:133:A:VAL:H	14	0.83
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	15	0.83
(1,370)	1:198:A:VAL:HG13	1:198:A:VAL:H	3	0.83
(1,370)	1:198:A:VAL:HG13	1:198:A:VAL:H	15	0.83
(1,278)	1:177:A:ASP:HB3	1:176:A:ALA:H	6	0.83
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	15	0.83
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	2	0.83
(1,80)	1:202:A:ILE:HD11	1:201:A:LEU:H	14	0.83
(1,43)	1:165:A:VAL:HG21	1:117:A:PRO:HB3	13	0.83
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	3	0.82
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	5	0.82
(1,1539)	1:202:A:ILE:HG22	1:206:A:ARG:HD3	14	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	1:162:A:ALA:HB2	1:113:A:ASP:HB3	8	0.82
(1,1534)	1:162:A:ALA:HB3	1:113:A:ASP:HB3	15	0.82
(1,1310)	1:165:A:VAL:HA	1:164:A:LEU:HD23	14	0.82
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	15	0.82
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	15	0.82
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	6	0.82
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	15	0.82
(1,868)	1:133:A:VAL:HG11	1:133:A:VAL:H	3	0.82
(1,868)	1:133:A:VAL:HG12	1:133:A:VAL:H	9	0.82
(1,868)	1:133:A:VAL:HG12	1:133:A:VAL:H	12	0.82
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	9	0.81
(1,1731)	1:158:A:LYS:HG2	1:153:A:LEU:HD12	8	0.81
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	3	0.81
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	9	0.81
(1,1500)	1:185:A:VAL:HG11	1:187:A:HIS:HA	10	0.81
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	15	0.81
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD12	4	0.81
(1,868)	1:133:A:VAL:HG11	1:133:A:VAL:H	2	0.81
(1,641)	1:179:A:ILE:HD12	1:178:A:ASP:H	11	0.81
(1,367)	1:181:A:ARG:HB2	1:180:A:HIS:H	12	0.81
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	6	0.81
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	2	0.81
(1,119)	1:183:A:LEU:HD21	1:183:A:LEU:H	4	0.81
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	14	0.81
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	13	0.8
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	2	0.8
(1,1581)	1:194:A:TRP:HB3	1:194:A:TRP:HE3	4	0.8
(1,1570)	1:157:A:VAL:HG13	1:153:A:LEU:HD11	10	0.8
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	2	0.8
(1,1500)	1:185:A:VAL:HG11	1:187:A:HIS:HA	8	0.8
(1,1387)	1:117:A:PRO:HD3	1:116:A:ARG:HB3	8	0.8
(1,1359)	1:225:A:LYS:HB2	1:225:A:LYS:HE2	6	0.8
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	12	0.8
(1,1087)	1:122:A:LEU:HD12	1:126:A:ARG:HB3	2	0.8
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD11	2	0.8
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	11	0.8
(1,868)	1:133:A:VAL:HG12	1:133:A:VAL:H	5	0.8
(1,868)	1:133:A:VAL:HG11	1:133:A:VAL:H	15	0.8
(1,370)	1:198:A:VAL:HG13	1:198:A:VAL:H	12	0.8
(1,273)	1:142:A:ALA:HB1	1:145:A:GLN:H	2	0.8
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	14	0.8
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	1	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	5	0.8
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	8	0.8
(1,119)	1:183:A:LEU:HD21	1:183:A:LEU:H	3	0.8
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	5	0.79
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	5	0.79
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	10	0.79
(1,370)	1:198:A:VAL:HG12	1:198:A:VAL:H	13	0.79
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	1	0.78
(1,1769)	1:144:A:LEU:HD22	1:194:A:TRP:HZ2	7	0.78
(1,1769)	1:144:A:LEU:HD21	1:194:A:TRP:HZ2	10	0.78
(1,1769)	1:144:A:LEU:HD23	1:194:A:TRP:HZ2	15	0.78
(1,1534)	1:162:A:ALA:HB3	1:113:A:ASP:HB3	2	0.78
(1,1402)	1:136:A:ASP:HB3	1:132:A:GLN:HG2	7	0.78
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD11	15	0.78
(1,1215)	1:202:A:ILE:HD12	1:177:A:ASP:HB3	5	0.78
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD11	13	0.78
(1,858)	1:139:A:ARG:HD2	1:139:A:ARG:H	6	0.78
(1,641)	1:179:A:ILE:HD11	1:178:A:ASP:H	5	0.78
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	1	0.78
(1,1571)	1:137:A:ILE:HG22	1:141:A:LEU:HB3	14	0.77
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	1	0.77
(1,1500)	1:185:A:VAL:HG11	1:187:A:HIS:HA	3	0.77
(1,1500)	1:185:A:VAL:HG12	1:187:A:HIS:HA	14	0.77
(1,1456)	1:111:A:MET:HB3	1:148:A:TRP:HD1	3	0.77
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	2	0.77
(1,1387)	1:117:A:PRO:HD3	1:116:A:ARG:HB3	6	0.77
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD12	14	0.77
(1,1313)	1:194:A:TRP:HA	1:143:A:LEU:HD23	2	0.77
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	7	0.77
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	14	0.77
(1,979)	1:117:A:PRO:HA	1:165:A:VAL:HG13	10	0.77
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD12	8	0.77
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	11	0.77
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD23	4	0.77
(1,221)	1:134:A:CYS:HB3	1:133:A:VAL:H	5	0.77
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	11	0.77
(1,1778)	1:158:A:LYS:HB2	1:148:A:TRP:HZ3	6	0.76
(1,1769)	1:144:A:LEU:HD23	1:194:A:TRP:HZ2	13	0.76
(1,1693)	1:159:A:LYS:HB2	1:159:A:LYS:HE2	3	0.76
(1,1682)	1:168:A:LEU:HD22	1:165:A:VAL:HB	8	0.76
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	2	0.76
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD22	5	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1217)	1:130:A:ARG:HA	1:130:A:ARG:HD3	3	0.76
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	6	0.76
(1,1007)	1:198:A:VAL:HB	1:201:A:LEU:HB3	9	0.76
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	3	0.76
(1,962)	1:225:A:LYS:HG2	1:226:A:ASN:HB3	10	0.76
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD13	10	0.76
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD22	9	0.76
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	5	0.76
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD22	1	0.76
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD22	8	0.76
(1,1736)	1:194:A:TRP:HB3	1:198:A:VAL:HG13	13	0.75
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	11	0.75
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	4	0.75
(1,1089)	1:212:A:GLU:HG2	1:212:A:GLU:HA	13	0.75
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	3	0.75
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	2	0.75
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	4	0.75
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	8	0.75
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	11	0.75
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	1	0.75
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD13	10	0.75
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	12	0.74
(1,1769)	1:144:A:LEU:HD23	1:194:A:TRP:HZ2	14	0.74
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD11	14	0.74
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	2	0.74
(1,1215)	1:202:A:ILE:HD13	1:177:A:ASP:HB3	15	0.74
(1,1089)	1:212:A:GLU:HG2	1:212:A:GLU:HA	1	0.74
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD11	1	0.74
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	7	0.74
(1,43)	1:165:A:VAL:HG21	1:117:A:PRO:HB3	1	0.74
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	13	0.73
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	12	0.73
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG21	13	0.73
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	6	0.73
(1,1392)	1:158:A:LYS:HE2	1:148:A:TRP:HA	14	0.73
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD22	6	0.73
(1,1208)	1:136:A:ASP:HB3	1:133:A:VAL:HG13	7	0.73
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	1	0.73
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	10	0.73
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	13	0.73
(1,503)	1:153:A:LEU:HD11	1:149:A:ALA:H	14	0.73
(1,503)	1:153:A:LEU:HD11	1:149:A:ALA:H	15	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:141:A:LEU:HD22	1:142:A:ALA:H	2	0.73
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	8	0.73
(1,250)	1:191:A:VAL:HG22	1:185:A:VAL:H	14	0.73
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	1	0.73
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	1	0.73
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	2	0.72
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	9	0.72
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	12	0.72
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	6	0.72
(1,1619)	1:122:A:LEU:HD13	1:134:A:CYS:HB2	6	0.72
(1,1619)	1:122:A:LEU:HD12	1:134:A:CYS:HB2	10	0.72
(1,1571)	1:137:A:ILE:HG21	1:141:A:LEU:HB3	6	0.72
(1,1482)	1:191:A:VAL:HG21	1:184:A:MET:HG3	6	0.72
(1,1387)	1:117:A:PRO:HD3	1:116:A:ARG:HB3	1	0.72
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	2	0.72
(1,1311)	1:152:A:LYS:HA	1:152:A:LYS:HE2	10	0.72
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	8	0.72
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	10	0.72
(1,1159)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	5	0.72
(1,1106)	1:122:A:LEU:HB3	1:125:A:CYS:HB2	10	0.72
(1,1087)	1:122:A:LEU:HD13	1:126:A:ARG:HB3	4	0.72
(1,1018)	1:114:A:VAL:HG12	1:115:A:LEU:HD11	11	0.72
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	7	0.72
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	9	0.72
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG23	10	0.71
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG22	1	0.71
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG23	8	0.71
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	1	0.71
(1,1682)	1:168:A:LEU:HD22	1:165:A:VAL:HB	14	0.71
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	3	0.71
(1,1225)	1:208:A:LEU:HD13	1:211:A:GLU:HG2	15	0.71
(1,1044)	1:183:A:LEU:HD23	1:161:A:MET:HA	4	0.71
(1,953)	1:158:A:LYS:HE2	1:153:A:LEU:HB2	3	0.71
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD11	9	0.71
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD12	14	0.71
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	3	0.71
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	4	0.71
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	5	0.71
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	14	0.7
(1,1769)	1:144:A:LEU:HD22	1:194:A:TRP:HZ2	11	0.7
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG23	11	0.7
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	15	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	2	0.7
(1,1325)	1:144:A:LEU:HD22	1:141:A:LEU:HD23	4	0.7
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	10	0.7
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	3	0.7
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	10	0.7
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	5	0.7
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	8	0.7
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	11	0.7
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	15	0.7
(1,1679)	1:158:A:LYS:HB3	1:158:A:LYS:HG3	8	0.69
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	9	0.69
(1,1456)	1:111:A:MET:HB3	1:148:A:TRP:HD1	4	0.69
(1,1394)	1:122:A:LEU:HD12	1:134:A:CYS:HB3	9	0.69
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	8	0.69
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	9	0.69
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	12	0.69
(1,1126)	1:144:A:LEU:HD23	1:115:A:LEU:HD12	9	0.69
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	5	0.69
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	11	0.69
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	14	0.69
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD22	13	0.69
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	11	0.69
(1,641)	1:179:A:ILE:HD13	1:178:A:ASP:H	7	0.69
(1,488)	1:141:A:LEU:HD21	1:142:A:ALA:H	8	0.69
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	5	0.68
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	11	0.68
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD22	5	0.68
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	3	0.68
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	10	0.68
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	6	0.68
(1,1394)	1:122:A:LEU:HD11	1:134:A:CYS:HB3	10	0.68
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	3	0.68
(1,1294)	1:116:A:ARG:HD2	1:116:A:ARG:HA	3	0.68
(1,1294)	1:116:A:ARG:HD2	1:116:A:ARG:HA	11	0.68
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG12	11	0.68
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG11	12	0.68
(1,1024)	1:122:A:LEU:HD13	1:134:A:CYS:HA	3	0.68
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	7	0.68
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	14	0.68
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	6	0.68
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG23	4	0.68
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	6	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD12	12	0.68
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	14	0.68
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	3	0.68
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	5	0.67
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	14	0.67
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	4	0.67
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	8	0.67
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	13	0.67
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	9	0.67
(1,1205)	1:132:A:GLN:HG2	1:133:A:VAL:HA	4	0.67
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD11	9	0.67
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	10	0.67
(1,991)	1:155:A:ILE:HD12	1:154:A:SER:HB2	10	0.67
(1,641)	1:179:A:ILE:HD12	1:178:A:ASP:H	13	0.67
(1,566)	1:144:A:LEU:HD23	1:194:A:TRP:HE1	13	0.67
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	1	0.67
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	14	0.67
(1,43)	1:165:A:VAL:HG22	1:117:A:PRO:HB3	15	0.67
(1,1769)	1:144:A:LEU:HD23	1:194:A:TRP:HZ2	4	0.66
(1,1722)	1:133:A:VAL:HG21	1:134:A:CYS:HB3	14	0.66
(1,1720)	1:172:A:ARG:HD3	1:170:A:SER:HB3	1	0.66
(1,1635)	1:157:A:VAL:HG13	1:153:A:LEU:HA	10	0.66
(1,1500)	1:185:A:VAL:HG13	1:187:A:HIS:HA	12	0.66
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	6	0.66
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	12	0.66
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	14	0.66
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	6	0.66
(1,1067)	1:185:A:VAL:HG13	1:183:A:LEU:HA	13	0.66
(1,1024)	1:122:A:LEU:HD12	1:134:A:CYS:HA	10	0.66
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	9	0.66
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	1	0.66
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	5	0.66
(1,872)	1:176:A:ALA:HB3	1:173:A:TRP:H	14	0.66
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	11	0.66
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	1	0.66
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	11	0.66
(1,546)	1:116:A:ARG:HD2	1:116:A:ARG:H	6	0.66
(1,493)	1:218:A:LYS:HD3	1:218:A:LYS:H	6	0.66
(1,352)	1:115:A:LEU:HD11	1:114:A:VAL:H	6	0.66
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	7	0.66
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	4	0.66
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	6	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	5	0.66
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	2	0.65
(1,1693)	1:159:A:LYS:HB2	1:159:A:LYS:HE2	2	0.65
(1,1387)	1:117:A:PRO:HD3	1:116:A:ARG:HB3	14	0.65
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	15	0.65
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	7	0.65
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	5	0.65
(1,1106)	1:122:A:LEU:HB3	1:125:A:CYS:HB2	2	0.65
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	13	0.65
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	9	0.65
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	12	0.65
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	13	0.65
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	3	0.65
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	3	0.65
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	14	0.64
(1,1650)	1:208:A:LEU:HD13	1:211:A:GLU:HG3	6	0.64
(1,1453)	1:183:A:LEU:HD22	1:180:A:HIS:HD1	4	0.64
(1,1429)	1:141:A:LEU:HD22	1:144:A:LEU:HD12	10	0.64
(1,1423)	1:212:A:GLU:HG2	1:212:A:GLU:HB2	15	0.64
(1,1380)	1:205:A:LYS:HG3	1:173:A:TRP:HH2	10	0.64
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	12	0.64
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	14	0.64
(1,1375)	1:144:A:LEU:HD23	1:153:A:LEU:HD13	11	0.64
(1,1305)	1:143:A:LEU:HD23	1:193:A:GLN:HB3	11	0.64
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	14	0.64
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	11	0.64
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	13	0.64
(1,1106)	1:122:A:LEU:HB3	1:125:A:CYS:HB2	3	0.64
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	4	0.64
(1,796)	1:168:A:LEU:HD21	1:168:A:LEU:H	9	0.64
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	15	0.64
(1,503)	1:153:A:LEU:HD11	1:149:A:ALA:H	1	0.64
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	15	0.64
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	10	0.64
(1,349)	1:191:A:VAL:HG21	1:184:A:MET:H	8	0.64
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	7	0.64
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	12	0.64
(1,1714)	1:122:A:LEU:HD12	1:125:A:CYS:HB2	1	0.63
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	14	0.63
(1,1612)	1:123:A:GLU:HG3	1:123:A:GLU:HB3	3	0.63
(1,1384)	1:145:A:GLN:HG2	1:141:A:LEU:HD23	4	0.63
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	5	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	10	0.63
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG11	2	0.63
(1,1208)	1:136:A:ASP:HB3	1:133:A:VAL:HG11	4	0.63
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	6	0.63
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD11	11	0.63
(1,796)	1:168:A:LEU:HD23	1:168:A:LEU:H	3	0.63
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	13	0.63
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	14	0.63
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	2	0.63
(1,154)	1:208:A:LEU:HD11	1:205:A:LYS:H	6	0.63
(1,1758)	1:191:A:VAL:HG21	1:184:A:MET:HA	8	0.62
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	2	0.62
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	9	0.62
(1,1619)	1:122:A:LEU:HD12	1:134:A:CYS:HB2	8	0.62
(1,1489)	1:137:A:ILE:HD12	1:134:A:CYS:HB2	1	0.62
(1,1428)	1:205:A:LYS:HG3	1:173:A:TRP:HZ3	10	0.62
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	11	0.62
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD22	12	0.62
(1,1294)	1:116:A:ARG:HD2	1:116:A:ARG:HA	9	0.62
(1,1234)	1:208:A:LEU:HD13	1:205:A:LYS:HE2	7	0.62
(1,1215)	1:202:A:ILE:HD11	1:177:A:ASP:HB3	7	0.62
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	13	0.62
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	14	0.62
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG22	1	0.62
(1,796)	1:168:A:LEU:HD21	1:168:A:LEU:H	1	0.62
(1,796)	1:168:A:LEU:HD21	1:168:A:LEU:H	2	0.62
(1,796)	1:168:A:LEU:HD23	1:168:A:LEU:H	6	0.62
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	8	0.62
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	13	0.62
(1,641)	1:179:A:ILE:HD13	1:178:A:ASP:H	14	0.62
(1,609)	1:213:A:ALA:HB3	1:212:A:GLU:H	1	0.62
(1,488)	1:141:A:LEU:HD23	1:142:A:ALA:H	13	0.62
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	3	0.62
(1,417)	1:146:A:GLU:HB2	1:146:A:GLU:H	11	0.62
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	7	0.62
(1,352)	1:115:A:LEU:HD12	1:114:A:VAL:H	5	0.62
(1,352)	1:115:A:LEU:HD13	1:114:A:VAL:H	11	0.62
(1,187)	1:170:A:SER:HB2	1:171:A:HIS:H	11	0.62
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	14	0.62
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	14	0.62
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	11	0.62
(1,18)	1:229:A:ILE:H	1:228:A:THR:H	9	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	1:157:A:VAL:HG22	1:190:A:GLU:HB2	7	0.61
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD13	7	0.61
(1,1423)	1:212:A:GLU:HG2	1:212:A:GLU:HB2	10	0.61
(1,1423)	1:212:A:GLU:HG2	1:212:A:GLU:HB2	11	0.61
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	7	0.61
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	4	0.61
(1,1320)	1:183:A:LEU:HD22	1:194:A:TRP:HZ2	13	0.61
(1,1234)	1:208:A:LEU:HD12	1:205:A:LYS:HE2	11	0.61
(1,1059)	1:157:A:VAL:HG13	1:194:A:TRP:HZ2	10	0.61
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	4	0.61
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	7	0.61
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	9	0.61
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD13	9	0.61
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	10	0.61
(1,641)	1:179:A:ILE:HD13	1:178:A:ASP:H	3	0.61
(1,587)	1:132:A:GLN:HG2	1:133:A:VAL:H	4	0.61
(1,485)	1:153:A:LEU:HD11	1:194:A:TRP:HE1	10	0.61
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	1	0.61
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	2	0.61
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	5	0.61
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD23	11	0.61
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	1	0.6
(1,1758)	1:191:A:VAL:HG22	1:184:A:MET:HA	6	0.6
(1,1619)	1:122:A:LEU:HD11	1:134:A:CYS:HB2	5	0.6
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD13	14	0.6
(1,1489)	1:137:A:ILE:HD11	1:134:A:CYS:HB2	14	0.6
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	1	0.6
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	3	0.6
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	13	0.6
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD12	5	0.6
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	8	0.6
(1,1055)	1:176:A:ALA:HA	1:167:A:GLU:HG2	6	0.6
(1,1045)	1:172:A:ARG:HB3	1:170:A:SER:HB3	4	0.6
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	8	0.6
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	1	0.6
(1,956)	1:230:A:PRO:HG2	1:232:A:PHE:HB2	12	0.6
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	10	0.6
(1,796)	1:168:A:LEU:HD23	1:168:A:LEU:H	7	0.6
(1,794)	1:144:A:LEU:HD13	1:143:A:LEU:H	14	0.6
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	9	0.6
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	12	0.6
(1,349)	1:191:A:VAL:HG21	1:184:A:MET:H	12	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:191:A:VAL:HG21	1:188:A:VAL:H	4	0.6
(1,273)	1:142:A:ALA:HB1	1:145:A:GLN:H	7	0.6
(1,70)	1:158:A:LYS:HG2	1:157:A:VAL:H	10	0.6
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD11	11	0.59
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	6	0.59
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD23	6	0.59
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD13	2	0.59
(1,1616)	1:208:A:LEU:HD12	1:125:A:CYS:HB2	12	0.59
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD11	1	0.59
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD12	15	0.59
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	6	0.59
(1,1389)	1:198:A:VAL:HG11	1:144:A:LEU:HD13	1	0.59
(1,1379)	1:194:A:TRP:HD1	1:194:A:TRP:HB2	9	0.59
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	10	0.59
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	2	0.59
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG11	6	0.59
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG13	9	0.59
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	1	0.59
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	3	0.59
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	6	0.59
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	12	0.59
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD11	12	0.59
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	14	0.59
(1,796)	1:168:A:LEU:HD21	1:168:A:LEU:H	5	0.59
(1,796)	1:168:A:LEU:HD23	1:168:A:LEU:H	10	0.59
(1,796)	1:168:A:LEU:HD22	1:168:A:LEU:H	14	0.59
(1,273)	1:142:A:ALA:HB3	1:145:A:GLN:H	4	0.59
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	7	0.58
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG21	9	0.58
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	3	0.58
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	12	0.58
(1,1682)	1:168:A:LEU:HD22	1:165:A:VAL:HB	4	0.58
(1,1619)	1:122:A:LEU:HD11	1:134:A:CYS:HB2	15	0.58
(1,1612)	1:123:A:GLU:HG3	1:123:A:GLU:HB3	9	0.58
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD12	1	0.58
(1,1394)	1:122:A:LEU:HD12	1:134:A:CYS:HB3	12	0.58
(1,1389)	1:198:A:VAL:HG12	1:144:A:LEU:HD13	3	0.58
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD11	1	0.58
(1,1375)	1:144:A:LEU:HD23	1:153:A:LEU:HD11	7	0.58
(1,1260)	1:203:A:ALA:HB2	1:206:A:ARG:HD2	12	0.58
(1,1241)	1:183:A:LEU:HB3	1:180:A:HIS:HA	4	0.58
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	14	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:158:A:LYS:HE2	1:158:A:LYS:HG2	3	0.58
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	12	0.58
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG11	5	0.58
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	11	0.58
(1,352)	1:115:A:LEU:HD12	1:114:A:VAL:H	8	0.58
(1,352)	1:115:A:LEU:HD11	1:114:A:VAL:H	15	0.58
(1,349)	1:191:A:VAL:HG23	1:184:A:MET:H	6	0.58
(1,273)	1:142:A:ALA:HB2	1:145:A:GLN:H	12	0.58
(1,1746)	1:208:A:LEU:HD22	1:124:A:ASP:HB3	5	0.57
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	9	0.57
(1,1641)	1:153:A:LEU:HD11	1:145:A:GLN:HA	15	0.57
(1,1571)	1:137:A:ILE:HG21	1:141:A:LEU:HB3	11	0.57
(1,1547)	1:193:A:GLN:HG3	1:143:A:LEU:HD23	8	0.57
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	2	0.57
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	10	0.57
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	1	0.57
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	1	0.57
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	9	0.57
(1,1024)	1:122:A:LEU:HD12	1:134:A:CYS:HA	12	0.57
(1,991)	1:155:A:ILE:HD13	1:154:A:SER:HB2	4	0.57
(1,991)	1:155:A:ILE:HD12	1:154:A:SER:HB2	7	0.57
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	9	0.57
(1,953)	1:158:A:LYS:HE2	1:153:A:LEU:HB2	1	0.57
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	4	0.57
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	12	0.57
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	7	0.57
(1,718)	1:229:A:ILE:H	1:228:A:THR:H	7	0.57
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	14	0.57
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	3	0.57
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	9	0.57
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	9	0.57
(1,352)	1:115:A:LEU:HD13	1:114:A:VAL:H	13	0.57
(1,81)	1:203:A:ALA:HB3	1:200:A:ARG:H	13	0.57
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	5	0.56
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE3	5	0.56
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	6	0.56
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG23	15	0.56
(1,1722)	1:133:A:VAL:HG23	1:134:A:CYS:HB3	11	0.56
(1,1722)	1:133:A:VAL:HG21	1:134:A:CYS:HB3	15	0.56
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD11	12	0.56
(1,1644)	1:206:A:ARG:HB3	1:206:A:ARG:HD2	12	0.56
(1,1616)	1:208:A:LEU:HD11	1:125:A:CYS:HB2	11	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1596)	1:199:A:LYS:HA	1:202:A:ILE:HD12	9	0.56
(1,1394)	1:122:A:LEU:HD13	1:134:A:CYS:HB3	6	0.56
(1,1312)	1:145:A:GLN:HG2	1:142:A:ALA:HB1	7	0.56
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	4	0.56
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	10	0.56
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	6	0.56
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	7	0.56
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD12	1	0.56
(1,1047)	1:208:A:LEU:HD22	1:205:A:LYS:HE2	6	0.56
(1,1047)	1:208:A:LEU:HD21	1:205:A:LYS:HE2	9	0.56
(1,991)	1:155:A:ILE:HD12	1:154:A:SER:HB2	12	0.56
(1,967)	1:111:A:MET:HE1	1:148:A:TRP:HA	11	0.56
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	3	0.56
(1,759)	1:137:A:ILE:HD12	1:138:A:SER:H	14	0.56
(1,673)	1:172:A:ARG:HB3	1:170:A:SER:H	7	0.56
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	9	0.56
(1,493)	1:218:A:LYS:HD3	1:218:A:LYS:H	3	0.56
(1,468)	1:122:A:LEU:HD12	1:125:A:CYS:H	4	0.56
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	8	0.56
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	10	0.56
(1,369)	1:214:A:ALA:HB3	1:215:A:ASN:H	3	0.56
(1,349)	1:191:A:VAL:HG21	1:184:A:MET:H	11	0.56
(1,152)	1:121:A:ALA:H	1:120:A:GLN:HG2	9	0.56
(1,1644)	1:206:A:ARG:HB3	1:206:A:ARG:HD2	13	0.55
(1,1619)	1:122:A:LEU:HD12	1:134:A:CYS:HB2	12	0.55
(1,1619)	1:122:A:LEU:HD13	1:134:A:CYS:HB2	13	0.55
(1,1612)	1:123:A:GLU:HG3	1:123:A:GLU:HB3	15	0.55
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	3	0.55
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	11	0.55
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	13	0.55
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	14	0.55
(1,1024)	1:122:A:LEU:HD13	1:134:A:CYS:HA	6	0.55
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	4	0.55
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	5	0.55
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	10	0.55
(1,662)	1:109:A:ALA:H	1:108:A:GLU:HG2	8	0.55
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	10	0.55
(1,566)	1:144:A:LEU:HD23	1:194:A:TRP:HE1	14	0.55
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	7	0.55
(1,352)	1:115:A:LEU:HD13	1:114:A:VAL:H	4	0.55
(1,273)	1:142:A:ALA:HB3	1:145:A:GLN:H	3	0.55
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	12	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,152)	1:121:A:ALA:H	1:120:A:GLN:HG2	14	0.55
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	8	0.55
(1,1782)	1:143:A:LEU:HD13	1:194:A:TRP:HZ3	14	0.54
(1,1743)	1:161:A:MET:HE3	1:114:A:VAL:HG21	8	0.54
(1,1394)	1:122:A:LEU:HD13	1:134:A:CYS:HB3	13	0.54
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD13	5	0.54
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG23	4	0.54
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	5	0.54
(1,1087)	1:122:A:LEU:HD11	1:126:A:ARG:HB3	15	0.54
(1,1038)	1:116:A:ARG:HD2	1:116:A:ARG:HB3	4	0.54
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	15	0.54
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	5	0.54
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	1	0.54
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	9	0.54
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	13	0.54
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	14	0.54
(1,796)	1:168:A:LEU:HD23	1:168:A:LEU:H	12	0.54
(1,718)	1:229:A:ILE:H	1:228:A:THR:H	3	0.54
(1,641)	1:179:A:ILE:HD13	1:178:A:ASP:H	1	0.54
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	5	0.54
(1,566)	1:144:A:LEU:HD22	1:194:A:TRP:HE1	8	0.54
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	14	0.54
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	14	0.54
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	11	0.54
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	11	0.54
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD13	5	0.53
(1,1745)	1:179:A:ILE:HG22	1:164:A:LEU:HB3	10	0.53
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	9	0.53
(1,1475)	1:183:A:LEU:HD21	1:179:A:ILE:HB	10	0.53
(1,1225)	1:208:A:LEU:HD13	1:211:A:GLU:HG2	6	0.53
(1,1215)	1:202:A:ILE:HD11	1:177:A:ASP:HB3	9	0.53
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	15	0.53
(1,1107)	1:134:A:CYS:HB2	1:138:A:SER:HB2	7	0.53
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD12	15	0.53
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	6	0.53
(1,872)	1:176:A:ALA:HB2	1:173:A:TRP:H	8	0.53
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	6	0.53
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	3	0.53
(1,641)	1:179:A:ILE:HD13	1:178:A:ASP:H	15	0.53
(1,503)	1:153:A:LEU:HD12	1:149:A:ALA:H	10	0.53
(1,488)	1:141:A:LEU:HD22	1:142:A:ALA:H	9	0.53
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD11	6	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	2	0.53
(1,373)	1:179:A:ILE:HG23	1:182:A:SER:H	2	0.53
(1,152)	1:121:A:ALA:H	1:120:A:GLN:HG2	8	0.53
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	9	0.52
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	15	0.52
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	4	0.52
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	8	0.52
(1,1644)	1:206:A:ARG:HB3	1:206:A:ARG:HD2	10	0.52
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD13	8	0.52
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD12	4	0.52
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG11	6	0.52
(1,1229)	1:236:A:SER:HB3	1:236:A:SER:HA	15	0.52
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	2	0.52
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD23	7	0.52
(1,873)	1:202:A:ILE:HG21	1:203:A:ALA:H	14	0.52
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	15	0.52
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG21	7	0.52
(1,713)	1:165:A:VAL:HG22	1:165:A:VAL:H	10	0.52
(1,503)	1:153:A:LEU:HD12	1:149:A:ALA:H	13	0.52
(1,488)	1:141:A:LEU:HD22	1:142:A:ALA:H	12	0.52
(1,352)	1:115:A:LEU:HD11	1:114:A:VAL:H	9	0.52
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG12	4	0.52
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD13	15	0.51
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	8	0.51
(1,1578)	1:203:A:ALA:HB3	1:206:A:ARG:HD3	14	0.51
(1,1456)	1:111:A:MET:HB3	1:148:A:TRP:HD1	10	0.51
(1,1341)	1:204:A:GLU:HB2	1:205:A:LYS:HG3	14	0.51
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	3	0.51
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	8	0.51
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	15	0.51
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG11	2	0.51
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	6	0.51
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	11	0.51
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	2	0.51
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	7	0.51
(1,485)	1:153:A:LEU:HD11	1:194:A:TRP:HE1	9	0.51
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	10	0.51
(1,352)	1:115:A:LEU:HD11	1:114:A:VAL:H	1	0.51
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD11	9	0.51
(1,273)	1:142:A:ALA:HB3	1:145:A:GLN:H	6	0.51
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	8	0.51
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	6	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	15	0.51
(1,75)	1:139:A:ARG:HD2	1:140:A:ARG:H	9	0.51
(1,1820)	1:148:A:TRP:HE3	1:158:A:LYS:HG3	6	0.5
(1,1743)	1:161:A:MET:HE2	1:114:A:VAL:HG21	14	0.5
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG22	7	0.5
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	1	0.5
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	15	0.5
(1,1522)	1:218:A:LYS:HG2	1:218:A:LYS:HA	12	0.5
(1,1384)	1:145:A:GLN:HG2	1:141:A:LEU:HD21	3	0.5
(1,1351)	1:189:A:THR:HG1	1:188:A:VAL:HG13	10	0.5
(1,1351)	1:189:A:THR:HG1	1:188:A:VAL:HG11	15	0.5
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	11	0.5
(1,1216)	1:158:A:LYS:HE2	1:158:A:LYS:HG2	1	0.5
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	7	0.5
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	5	0.5
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	5	0.5
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	2	0.5
(1,937)	1:205:A:LYS:HG3	1:205:A:LYS:HE2	14	0.5
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD11	8	0.5
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	4	0.5
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	15	0.5
(1,641)	1:179:A:ILE:HD12	1:178:A:ASP:H	2	0.5
(1,587)	1:132:A:GLN:HG2	1:133:A:VAL:H	1	0.5
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	6	0.5
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD11	4	0.5
(1,373)	1:179:A:ILE:HG22	1:182:A:SER:H	6	0.5
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	7	0.5
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	4	0.5
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	5	0.5
(1,75)	1:139:A:ARG:HD2	1:140:A:ARG:H	3	0.5
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	1	0.49
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	11	0.49
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	13	0.49
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD11	7	0.49
(1,1644)	1:206:A:ARG:HB3	1:206:A:ARG:HD2	9	0.49
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	10	0.49
(1,1394)	1:122:A:LEU:HD13	1:134:A:CYS:HB3	4	0.49
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD13	6	0.49
(1,1284)	1:188:A:VAL:HB	1:191:A:VAL:HG21	4	0.49
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	14	0.49
(1,1225)	1:208:A:LEU:HD13	1:211:A:GLU:HG2	3	0.49
(1,1181)	1:153:A:LEU:HB2	1:158:A:LYS:HG2	3	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1024)	1:122:A:LEU:HD11	1:134:A:CYS:HA	14	0.49
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD13	7	0.49
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	4	0.49
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	1	0.49
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	2	0.49
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	6	0.49
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	8	0.49
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	11	0.49
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	14	0.49
(1,830)	1:166:A:GLN:HB2	1:166:A:GLN:HE22	10	0.49
(1,503)	1:153:A:LEU:HD12	1:149:A:ALA:H	3	0.49
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	10	0.49
(1,403)	1:137:A:ILE:HG23	1:137:A:ILE:H	15	0.49
(1,378)	1:149:A:ALA:HB1	1:146:A:GLU:H	3	0.49
(1,378)	1:149:A:ALA:HB1	1:146:A:GLU:H	6	0.49
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	14	0.49
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	4	0.49
(1,154)	1:208:A:LEU:HD12	1:205:A:LYS:H	12	0.49
(1,48)	1:208:A:LEU:HD12	1:208:A:LEU:H	5	0.49
(1,46)	1:157:A:VAL:HG12	1:161:A:MET:HB2	10	0.49
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE3	7	0.48
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	8	0.48
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	2	0.48
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	5	0.48
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	1	0.48
(1,1646)	1:162:A:ALA:HB3	1:148:A:TRP:HZ2	14	0.48
(1,1510)	1:164:A:LEU:HA	1:167:A:GLU:HG2	2	0.48
(1,1489)	1:137:A:ILE:HD11	1:134:A:CYS:HB2	7	0.48
(1,1475)	1:183:A:LEU:HD22	1:179:A:ILE:HB	15	0.48
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	10	0.48
(1,1378)	1:116:A:ARG:HA	1:116:A:ARG:HB2	1	0.48
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD12	10	0.48
(1,1280)	1:176:A:ALA:HA	1:179:A:ILE:HD13	9	0.48
(1,1024)	1:122:A:LEU:HD12	1:134:A:CYS:HA	9	0.48
(1,976)	1:162:A:ALA:HB3	1:148:A:TRP:HZ3	14	0.48
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	9	0.48
(1,637)	1:125:A:CYS:H	1:124:A:ASP:HB3	8	0.48
(1,566)	1:144:A:LEU:HD22	1:194:A:TRP:HE1	2	0.48
(1,503)	1:153:A:LEU:HD12	1:149:A:ALA:H	9	0.48
(1,503)	1:153:A:LEU:HD11	1:149:A:ALA:H	12	0.48
(1,493)	1:218:A:LYS:HD3	1:218:A:LYS:H	11	0.48
(1,468)	1:122:A:LEU:HD13	1:125:A:CYS:H	7	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD12	10	0.48
(1,403)	1:137:A:ILE:HG23	1:137:A:ILE:H	1	0.48
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	2	0.48
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	11	0.48
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	14	0.48
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	1	0.48
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	14	0.48
(1,154)	1:208:A:LEU:HD13	1:205:A:LYS:H	7	0.48
(1,131)	1:185:A:VAL:HG13	1:182:A:SER:H	13	0.48
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG22	4	0.48
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG22	6	0.48
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	9	0.48
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	6	0.48
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	1	0.48
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	7	0.48
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	10	0.48
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	13	0.48
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	14	0.48
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD22	7	0.48
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	15	0.48
(1,18)	1:229:A:ILE:H	1:228:A:THR:H	4	0.48
(1,1641)	1:153:A:LEU:HD13	1:145:A:GLN:HA	6	0.47
(1,1423)	1:212:A:GLU:HG2	1:212:A:GLU:HB2	9	0.47
(1,1378)	1:116:A:ARG:HA	1:116:A:ARG:HB2	6	0.47
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	1	0.47
(1,1313)	1:194:A:TRP:HA	1:143:A:LEU:HD22	5	0.47
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG13	7	0.47
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	15	0.47
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	13	0.47
(1,566)	1:144:A:LEU:HD23	1:194:A:TRP:HE1	15	0.47
(1,503)	1:153:A:LEU:HD13	1:149:A:ALA:H	6	0.47
(1,503)	1:153:A:LEU:HD11	1:149:A:ALA:H	7	0.47
(1,402)	1:139:A:ARG:H	1:140:A:ARG:HB2	9	0.47
(1,378)	1:149:A:ALA:HB3	1:146:A:GLU:H	1	0.47
(1,378)	1:149:A:ALA:HB1	1:146:A:GLU:H	8	0.47
(1,378)	1:149:A:ALA:HB1	1:146:A:GLU:H	15	0.47
(1,369)	1:214:A:ALA:HB2	1:215:A:ASN:H	14	0.47
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	4	0.47
(1,353)	1:157:A:VAL:HG13	1:154:A:SER:H	4	0.47
(1,273)	1:142:A:ALA:HB3	1:145:A:GLN:H	13	0.47
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD12	3	0.47
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	13	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	9	0.47
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG21	12	0.47
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG12	7	0.47
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG11	11	0.47
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	2	0.47
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	3	0.47
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	8	0.47
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	12	0.47
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	3	0.46
(1,1782)	1:143:A:LEU:HD11	1:194:A:TRP:HZ3	10	0.46
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	6	0.46
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	4	0.46
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	5	0.46
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	11	0.46
(1,1534)	1:162:A:ALA:HB3	1:113:A:ASP:HB3	1	0.46
(1,1493)	1:158:A:LYS:HE2	1:153:A:LEU:HA	14	0.46
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	5	0.46
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	7	0.46
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	13	0.46
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG13	15	0.46
(1,1359)	1:225:A:LYS:HB2	1:225:A:LYS:HE2	13	0.46
(1,1305)	1:143:A:LEU:HD23	1:193:A:GLN:HB3	3	0.46
(1,1260)	1:203:A:ALA:HB2	1:206:A:ARG:HD2	10	0.46
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	8	0.46
(1,1234)	1:208:A:LEU:HD11	1:205:A:LYS:HE2	14	0.46
(1,1224)	1:199:A:LYS:HE2	1:199:A:LYS:HB2	11	0.46
(1,1209)	1:158:A:LYS:HD2	1:148:A:TRP:HB2	1	0.46
(1,1107)	1:134:A:CYS:HB2	1:138:A:SER:HB2	5	0.46
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	5	0.46
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD13	8	0.46
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	12	0.46
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	8	0.46
(1,633)	1:199:A:LYS:HG2	1:199:A:LYS:H	3	0.46
(1,566)	1:144:A:LEU:HD23	1:194:A:TRP:HE1	4	0.46
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	15	0.46
(1,403)	1:137:A:ILE:HG22	1:137:A:ILE:H	4	0.46
(1,378)	1:149:A:ALA:HB3	1:146:A:GLU:H	9	0.46
(1,154)	1:208:A:LEU:HD11	1:205:A:LYS:H	5	0.46
(1,154)	1:208:A:LEU:HD12	1:205:A:LYS:H	11	0.46
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	1	0.45
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	1	0.45
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	14	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	7	0.45
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	14	0.45
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	7	0.45
(1,1482)	1:191:A:VAL:HG21	1:184:A:MET:HG3	11	0.45
(1,1478)	1:175:A:ALA:HB1	1:167:A:GLU:HA	6	0.45
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	14	0.45
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	15	0.45
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD11	12	0.45
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	8	0.45
(1,1260)	1:203:A:ALA:HB3	1:206:A:ARG:HD2	14	0.45
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	2	0.45
(1,1215)	1:202:A:ILE:HD12	1:177:A:ASP:HB3	1	0.45
(1,1200)	1:143:A:LEU:HG	1:143:A:LEU:HB3	7	0.45
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	2	0.45
(1,1057)	1:163:A:LEU:HA	1:166:A:GLN:HB2	12	0.45
(1,1018)	1:114:A:VAL:HG12	1:115:A:LEU:HD11	4	0.45
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	6	0.45
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD13	6	0.45
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	15	0.45
(1,76)	1:209:A:PHE:HB3	1:208:A:LEU:H	11	0.45
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	1	0.45
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	12	0.44
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	12	0.44
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	14	0.44
(1,1376)	1:119:A:GLU:HG3	1:119:A:GLU:HB3	10	0.44
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD11	12	0.44
(1,1351)	1:189:A:THR:HG1	1:188:A:VAL:HG11	2	0.44
(1,1260)	1:203:A:ALA:HB1	1:206:A:ARG:HD2	9	0.44
(1,1200)	1:143:A:LEU:HG	1:143:A:LEU:HB3	9	0.44
(1,1193)	1:206:A:ARG:HA	1:206:A:ARG:HB3	4	0.44
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	14	0.44
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	2	0.44
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	4	0.44
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD13	15	0.44
(1,794)	1:144:A:LEU:HD13	1:143:A:LEU:H	3	0.44
(1,794)	1:144:A:LEU:HD11	1:143:A:LEU:H	7	0.44
(1,759)	1:137:A:ILE:HD12	1:138:A:SER:H	8	0.44
(1,741)	1:191:A:VAL:HG23	1:195:A:MET:H	4	0.44
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	1	0.44
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	3	0.44
(1,403)	1:137:A:ILE:HG23	1:137:A:ILE:H	5	0.44
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	7	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	5	0.44
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	13	0.44
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	12	0.44
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	12	0.44
(1,48)	1:208:A:LEU:HD23	1:208:A:LEU:H	14	0.44
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD22	11	0.44
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	4	0.43
(1,1798)	1:148:A:TRP:HZ3	1:158:A:LYS:HG3	6	0.43
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	3	0.43
(1,1682)	1:168:A:LEU:HD23	1:165:A:VAL:HB	11	0.43
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	4	0.43
(1,1534)	1:162:A:ALA:HB3	1:113:A:ASP:HB3	10	0.43
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	11	0.43
(1,1506)	1:204:A:GLU:HB2	1:205:A:LYS:HA	15	0.43
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD23	13	0.43
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	2	0.43
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	10	0.43
(1,1215)	1:202:A:ILE:HD11	1:177:A:ASP:HB3	4	0.43
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	11	0.43
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	6	0.43
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	7	0.43
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	15	0.43
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG13	8	0.43
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	1	0.43
(1,894)	1:121:A:ALA:H	1:122:A:LEU:HD12	3	0.43
(1,759)	1:137:A:ILE:HD13	1:138:A:SER:H	6	0.43
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	8	0.43
(1,485)	1:153:A:LEU:HD13	1:194:A:TRP:HE1	13	0.43
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	11	0.43
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG21	13	0.43
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	4	0.43
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	11	0.43
(1,1781)	1:148:A:TRP:HE3	1:161:A:MET:HG3	6	0.42
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD11	15	0.42
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	7	0.42
(1,1378)	1:116:A:ARG:HA	1:116:A:ARG:HB2	8	0.42
(1,1351)	1:189:A:THR:HG1	1:188:A:VAL:HG11	11	0.42
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	9	0.42
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	7	0.42
(1,1215)	1:202:A:ILE:HD13	1:177:A:ASP:HB3	8	0.42
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	8	0.42
(1,1043)	1:145:A:GLN:HA	1:111:A:MET:HG3	11	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	5	0.42
(1,962)	1:225:A:LYS:HG2	1:226:A:ASN:HB3	2	0.42
(1,872)	1:176:A:ALA:HB1	1:173:A:TRP:H	2	0.42
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	2	0.42
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	14	0.42
(1,641)	1:179:A:ILE:HD11	1:178:A:ASP:H	8	0.42
(1,403)	1:137:A:ILE:HG21	1:137:A:ILE:H	6	0.42
(1,403)	1:137:A:ILE:HG23	1:137:A:ILE:H	7	0.42
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	13	0.42
(1,369)	1:214:A:ALA:HB3	1:215:A:ASN:H	8	0.42
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	2	0.42
(1,349)	1:191:A:VAL:HG22	1:184:A:MET:H	7	0.42
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	10	0.42
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG13	5	0.42
(1,80)	1:202:A:ILE:HD11	1:201:A:LEU:H	1	0.42
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD21	14	0.42
(1,1782)	1:143:A:LEU:HD13	1:194:A:TRP:HZ3	13	0.41
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	13	0.41
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	11	0.41
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD11	13	0.41
(1,1435)	1:153:A:LEU:HA	1:190:A:GLU:HB2	7	0.41
(1,1394)	1:122:A:LEU:HD13	1:134:A:CYS:HB3	14	0.41
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	14	0.41
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	5	0.41
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	2	0.41
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	5	0.41
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	15	0.41
(1,1215)	1:202:A:ILE:HD13	1:177:A:ASP:HB3	6	0.41
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	1	0.41
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	11	0.41
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD12	5	0.41
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	14	0.41
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	2	0.41
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	8	0.41
(1,633)	1:199:A:LYS:HG2	1:199:A:LYS:H	9	0.41
(1,587)	1:132:A:GLN:HG2	1:133:A:VAL:H	11	0.41
(1,403)	1:137:A:ILE:HG22	1:137:A:ILE:H	12	0.41
(1,378)	1:149:A:ALA:HB2	1:146:A:GLU:H	12	0.41
(1,349)	1:191:A:VAL:HG21	1:184:A:MET:H	9	0.41
(1,341)	1:191:A:VAL:HG22	1:188:A:VAL:H	2	0.41
(1,341)	1:191:A:VAL:HG22	1:188:A:VAL:H	11	0.41
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD22	6	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	6	0.41
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	10	0.41
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	7	0.41
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	2	0.41
(1,80)	1:202:A:ILE:HD12	1:201:A:LEU:H	5	0.41
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	9	0.41
(1,80)	1:202:A:ILE:HD12	1:201:A:LEU:H	12	0.41
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	13	0.41
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE3	12	0.4
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	11	0.4
(1,1743)	1:161:A:MET:HE2	1:114:A:VAL:HG22	15	0.4
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	8	0.4
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	15	0.4
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	6	0.4
(1,1682)	1:168:A:LEU:HD23	1:165:A:VAL:HB	12	0.4
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	8	0.4
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	12	0.4
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG11	7	0.4
(1,1542)	1:129:A:THR:HG1	1:133:A:VAL:HG22	13	0.4
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	11	0.4
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	6	0.4
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	13	0.4
(1,1186)	1:159:A:LYS:HB2	1:159:A:LYS:HD3	8	0.4
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	4	0.4
(1,964)	1:164:A:LEU:HD11	1:176:A:ALA:HA	4	0.4
(1,956)	1:230:A:PRO:HG2	1:232:A:PHE:HB2	3	0.4
(1,901)	1:202:A:ILE:HD11	1:203:A:ALA:H	1	0.4
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	13	0.4
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	9	0.4
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	5	0.4
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	7	0.4
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	9	0.4
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	10	0.4
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	11	0.4
(1,566)	1:144:A:LEU:HD22	1:194:A:TRP:HE1	11	0.4
(1,503)	1:153:A:LEU:HD13	1:149:A:ALA:H	11	0.4
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	10	0.4
(1,427)	1:154:A:SER:HB2	1:155:A:ILE:H	11	0.4
(1,403)	1:137:A:ILE:HG23	1:137:A:ILE:H	8	0.4
(1,403)	1:137:A:ILE:HG22	1:137:A:ILE:H	9	0.4
(1,403)	1:137:A:ILE:HG22	1:137:A:ILE:H	13	0.4
(1,373)	1:179:A:ILE:HG22	1:182:A:SER:H	11	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:214:A:ALA:HB1	1:215:A:ASN:H	5	0.4
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	6	0.4
(1,273)	1:142:A:ALA:HB1	1:145:A:GLN:H	9	0.4
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	2	0.4
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	9	0.4
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	12	0.4
(1,102)	1:162:A:ALA:HB3	1:166:A:GLN:HE22	10	0.4
(1,81)	1:203:A:ALA:HB3	1:200:A:ARG:H	1	0.4
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD22	5	0.4
(1,1823)	1:205:A:LYS:HB2	1:173:A:TRP:HZ3	2	0.39
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE1	3	0.39
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	5	0.39
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	2	0.39
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	4	0.39
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	6	0.39
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	13	0.39
(1,1534)	1:162:A:ALA:HB2	1:113:A:ASP:HB3	6	0.39
(1,1533)	1:134:A:CYS:HB2	1:126:A:ARG:HB3	8	0.39
(1,1394)	1:122:A:LEU:HD11	1:134:A:CYS:HB3	1	0.39
(1,1376)	1:119:A:GLU:HG3	1:119:A:GLU:HB3	3	0.39
(1,1376)	1:119:A:GLU:HG3	1:119:A:GLU:HB3	13	0.39
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD12	9	0.39
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	11	0.39
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	1	0.39
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	13	0.39
(1,1132)	1:179:A:ILE:HG23	1:161:A:MET:HA	3	0.39
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD12	12	0.39
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	14	0.39
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	11	0.39
(1,1077)	1:164:A:LEU:HB3	1:179:A:ILE:HD11	6	0.39
(1,794)	1:144:A:LEU:HD13	1:143:A:LEU:H	15	0.39
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	4	0.39
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	5	0.39
(1,570)	1:162:A:ALA:HB2	1:164:A:LEU:H	5	0.39
(1,520)	1:164:A:LEU:HD23	1:166:A:GLN:H	3	0.39
(1,503)	1:153:A:LEU:HD13	1:149:A:ALA:H	5	0.39
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	5	0.39
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	6	0.39
(1,358)	1:110:A:VAL:HG21	1:111:A:MET:H	13	0.39
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	1	0.39
(1,353)	1:157:A:VAL:HG11	1:154:A:SER:H	8	0.39
(1,353)	1:157:A:VAL:HG11	1:154:A:SER:H	12	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:191:A:VAL:HG21	1:188:A:VAL:H	13	0.39
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG21	1	0.39
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	3	0.39
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	6	0.39
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG22	6	0.38
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	9	0.38
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	5	0.38
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	8	0.38
(1,1456)	1:111:A:MET:HB3	1:148:A:TRP:HD1	2	0.38
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	8	0.38
(1,1372)	1:158:A:LYS:HG2	1:148:A:TRP:HZ2	8	0.38
(1,1371)	1:169:A:SER:HB3	1:165:A:VAL:HG11	4	0.38
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	4	0.38
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	7	0.38
(1,1261)	1:185:A:VAL:HG13	1:186:A:ASP:HB3	13	0.38
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	4	0.38
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	9	0.38
(1,1112)	1:143:A:LEU:HD12	1:194:A:TRP:HB2	4	0.38
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	6	0.38
(1,966)	1:199:A:LYS:HE2	1:199:A:LYS:HA	3	0.38
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	13	0.38
(1,937)	1:205:A:LYS:HG3	1:205:A:LYS:HE2	8	0.38
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD21	11	0.38
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	9	0.38
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	12	0.38
(1,759)	1:137:A:ILE:HD13	1:138:A:SER:H	13	0.38
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	1	0.38
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	7	0.38
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	4	0.38
(1,566)	1:144:A:LEU:HD23	1:194:A:TRP:HE1	12	0.38
(1,468)	1:122:A:LEU:HD11	1:125:A:CYS:H	9	0.38
(1,468)	1:122:A:LEU:HD13	1:125:A:CYS:H	13	0.38
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD11	4	0.38
(1,358)	1:110:A:VAL:HG23	1:111:A:MET:H	7	0.38
(1,352)	1:115:A:LEU:HD13	1:114:A:VAL:H	7	0.38
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG21	2	0.38
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG12	15	0.38
(1,108)	1:157:A:VAL:HG21	1:160:A:ARG:H	1	0.38
(1,85)	1:220:A:ALA:H	1:220:A:ALA:HA	5	0.38
(1,48)	1:208:A:LEU:HD23	1:208:A:LEU:H	6	0.38
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	15	0.37
(1,1808)	1:158:A:LYS:HB2	1:148:A:TRP:HZ2	8	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	2	0.37
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE1	8	0.37
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	10	0.37
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE3	15	0.37
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG22	3	0.37
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	8	0.37
(1,1641)	1:153:A:LEU:HD13	1:145:A:GLN:HA	5	0.37
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	9	0.37
(1,1571)	1:137:A:ILE:HG23	1:141:A:LEU:HB3	8	0.37
(1,1506)	1:204:A:GLU:HB2	1:205:A:LYS:HA	2	0.37
(1,1489)	1:137:A:ILE:HD13	1:134:A:CYS:HB2	13	0.37
(1,1475)	1:183:A:LEU:HD21	1:179:A:ILE:HB	3	0.37
(1,1419)	1:140:A:ARG:HB3	1:194:A:TRP:HB2	14	0.37
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	1	0.37
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	10	0.37
(1,892)	1:225:A:LYS:HG3	1:228:A:THR:H	12	0.37
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	15	0.37
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	12	0.37
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	15	0.37
(1,643)	1:161:A:MET:H	1:158:A:LYS:HG2	8	0.37
(1,483)	1:212:A:GLU:HB3	1:213:A:ALA:H	3	0.37
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD12	13	0.37
(1,358)	1:110:A:VAL:HG22	1:111:A:MET:H	10	0.37
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	9	0.37
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	10	0.37
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD11	2	0.37
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	3	0.37
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	2	0.37
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	14	0.37
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	15	0.37
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	8	0.37
(1,48)	1:208:A:LEU:HD13	1:208:A:LEU:H	7	0.37
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	8	0.37
(1,43)	1:165:A:VAL:HG22	1:117:A:PRO:HB3	4	0.37
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE3	9	0.36
(1,1758)	1:191:A:VAL:HG22	1:184:A:MET:HA	1	0.36
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	12	0.36
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	14	0.36
(1,1536)	1:158:A:LYS:HB3	1:158:A:LYS:HD3	1	0.36
(1,1536)	1:158:A:LYS:HB3	1:158:A:LYS:HD3	3	0.36
(1,1436)	1:116:A:ARG:HD2	1:116:A:ARG:HB2	8	0.36
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	1	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1318)	1:111:A:MET:HE2	1:115:A:LEU:HD11	6	0.36
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	6	0.36
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	9	0.36
(1,1256)	1:190:A:GLU:HB3	1:187:A:HIS:HA	2	0.36
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	8	0.36
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	8	0.36
(1,1050)	1:157:A:VAL:HB	1:191:A:VAL:HG13	15	0.36
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	2	0.36
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	3	0.36
(1,991)	1:155:A:ILE:HD11	1:154:A:SER:HB2	1	0.36
(1,966)	1:199:A:LYS:HE2	1:199:A:LYS:HA	12	0.36
(1,966)	1:199:A:LYS:HE2	1:199:A:LYS:HA	13	0.36
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	15	0.36
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD12	8	0.36
(1,901)	1:202:A:ILE:HD12	1:203:A:ALA:H	12	0.36
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	1	0.36
(1,872)	1:176:A:ALA:HB2	1:173:A:TRP:H	7	0.36
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	4	0.36
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	8	0.36
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	3	0.36
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	6	0.36
(1,671)	1:173:A:TRP:HE1	1:173:A:TRP:HB3	13	0.36
(1,566)	1:144:A:LEU:HD21	1:194:A:TRP:HE1	1	0.36
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	6	0.36
(1,520)	1:164:A:LEU:HD23	1:166:A:GLN:H	12	0.36
(1,468)	1:122:A:LEU:HD13	1:125:A:CYS:H	15	0.36
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	9	0.36
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD11	9	0.36
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	14	0.36
(1,199)	1:175:A:ALA:HB2	1:178:A:ASP:H	5	0.36
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	1	0.36
(1,119)	1:183:A:LEU:HD23	1:183:A:LEU:H	14	0.36
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	3	0.36
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	14	0.36
(1,1809)	1:148:A:TRP:HZ2	1:158:A:LYS:HG3	13	0.35
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG21	13	0.35
(1,1782)	1:143:A:LEU:HD11	1:194:A:TRP:HZ3	12	0.35
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	9	0.35
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	12	0.35
(1,1682)	1:168:A:LEU:HD23	1:165:A:VAL:HB	13	0.35
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	14	0.35
(1,1641)	1:153:A:LEU:HD13	1:145:A:GLN:HA	11	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:153:A:LEU:HD12	1:145:A:GLN:HA	14	0.35
(1,1635)	1:157:A:VAL:HG12	1:153:A:LEU:HA	14	0.35
(1,1619)	1:122:A:LEU:HD11	1:134:A:CYS:HB2	1	0.35
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	14	0.35
(1,1597)	1:181:A:ARG:HB2	1:181:A:ARG:HA	3	0.35
(1,1571)	1:137:A:ILE:HG23	1:141:A:LEU:HB3	5	0.35
(1,1534)	1:162:A:ALA:HB1	1:113:A:ASP:HB3	5	0.35
(1,1522)	1:218:A:LYS:HG2	1:218:A:LYS:HA	7	0.35
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	5	0.35
(1,1305)	1:143:A:LEU:HD22	1:193:A:GLN:HB3	5	0.35
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	12	0.35
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	5	0.35
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	6	0.35
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	8	0.35
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	12	0.35
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	15	0.35
(1,1234)	1:208:A:LEU:HD13	1:205:A:LYS:HE2	13	0.35
(1,1225)	1:208:A:LEU:HD12	1:211:A:GLU:HG2	14	0.35
(1,1217)	1:130:A:ARG:HA	1:130:A:ARG:HD3	5	0.35
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	12	0.35
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	15	0.35
(1,1012)	1:164:A:LEU:HD13	1:161:A:MET:HE3	11	0.35
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	13	0.35
(1,956)	1:230:A:PRO:HG2	1:232:A:PHE:HB2	10	0.35
(1,872)	1:176:A:ALA:HB2	1:173:A:TRP:H	1	0.35
(1,818)	1:136:A:ASP:H	1:133:A:VAL:HG23	8	0.35
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	15	0.35
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	2	0.35
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	8	0.35
(1,309)	1:181:A:ARG:H	1:181:A:ARG:HG2	8	0.35
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG21	7	0.35
(1,123)	1:112:A:GLU:HB2	1:114:A:VAL:H	15	0.35
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	6	0.35
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	1	0.35
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	6	0.35
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	9	0.35
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	10	0.35
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	13	0.35
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	15	0.35
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	7	0.35
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	7	0.35
(1,80)	1:202:A:ILE:HD12	1:201:A:LEU:H	7	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG13	11	0.35
(1,48)	1:208:A:LEU:HD13	1:208:A:LEU:H	12	0.35
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	10	0.35
(1,1782)	1:143:A:LEU:HD11	1:194:A:TRP:HZ3	5	0.34
(1,1758)	1:191:A:VAL:HG23	1:184:A:MET:HA	10	0.34
(1,1758)	1:191:A:VAL:HG22	1:184:A:MET:HA	12	0.34
(1,1744)	1:205:A:LYS:HB2	1:205:A:LYS:HE2	12	0.34
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	13	0.34
(1,1700)	1:116:A:ARG:HG2	1:116:A:ARG:HB2	3	0.34
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD13	6	0.34
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	3	0.34
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	10	0.34
(1,1623)	1:156:A:PRO:HD3	1:154:A:SER:HB2	10	0.34
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG11	4	0.34
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG11	9	0.34
(1,1571)	1:137:A:ILE:HG21	1:141:A:LEU:HB3	2	0.34
(1,1525)	1:155:A:ILE:HB	1:156:A:PRO:HD2	12	0.34
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	2	0.34
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	3	0.34
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	4	0.34
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	7	0.34
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	15	0.34
(1,1313)	1:194:A:TRP:HA	1:143:A:LEU:HD22	12	0.34
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	8	0.34
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	1	0.34
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	3	0.34
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	7	0.34
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	10	0.34
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	3	0.34
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	9	0.34
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	2	0.34
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	1	0.34
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	10	0.34
(1,836)	1:166:A:GLN:HG2	1:166:A:GLN:HE21	10	0.34
(1,835)	1:158:A:LYS:HE2	1:148:A:TRP:HE1	5	0.34
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	8	0.34
(1,759)	1:137:A:ILE:HD13	1:138:A:SER:H	5	0.34
(1,633)	1:199:A:LYS:HG2	1:199:A:LYS:H	1	0.34
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	12	0.34
(1,566)	1:144:A:LEU:HD22	1:194:A:TRP:HE1	7	0.34
(1,520)	1:164:A:LEU:HD22	1:166:A:GLN:H	2	0.34
(1,520)	1:164:A:LEU:HD23	1:166:A:GLN:H	8	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	3	0.34
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD13	2	0.34
(1,309)	1:181:A:ARG:H	1:181:A:ARG:HG2	11	0.34
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB3	12	0.34
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	14	0.34
(1,119)	1:183:A:LEU:HD23	1:183:A:LEU:H	1	0.34
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG11	14	0.34
(1,108)	1:157:A:VAL:HG22	1:160:A:ARG:H	15	0.34
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD21	4	0.34
(1,38)	1:157:A:VAL:HG13	1:161:A:MET:HG3	11	0.34
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG21	3	0.33
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE1	13	0.33
(1,1782)	1:143:A:LEU:HD13	1:194:A:TRP:HZ3	6	0.33
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG21	10	0.33
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG22	14	0.33
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	7	0.33
(1,1643)	1:148:A:TRP:HZ3	1:161:A:MET:HG2	6	0.33
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	8	0.33
(1,1532)	1:158:A:LYS:HB2	1:155:A:ILE:HA	5	0.33
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	14	0.33
(1,1425)	1:121:A:ALA:HB1	1:122:A:LEU:HD13	10	0.33
(1,1424)	1:158:A:LYS:HB3	1:148:A:TRP:HZ2	6	0.33
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	8	0.33
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	11	0.33
(1,1313)	1:194:A:TRP:HA	1:143:A:LEU:HD22	6	0.33
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	3	0.33
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	10	0.33
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	9	0.33
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	13	0.33
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	14	0.33
(1,1236)	1:199:A:LYS:HA	1:199:A:LYS:HG2	9	0.33
(1,1209)	1:158:A:LYS:HD2	1:148:A:TRP:HB2	3	0.33
(1,1182)	1:206:A:ARG:HA	1:209:A:PHE:HB2	3	0.33
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	3	0.33
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	8	0.33
(1,967)	1:111:A:MET:HE3	1:148:A:TRP:HA	9	0.33
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD11	7	0.33
(1,916)	1:169:A:SER:HA	1:168:A:LEU:HD13	12	0.33
(1,903)	1:218:A:LYS:HG2	1:218:A:LYS:H	7	0.33
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	9	0.33
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	8	0.33
(1,641)	1:179:A:ILE:HD11	1:178:A:ASP:H	12	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,608)	1:200:A:ARG:H	1:199:A:LYS:HB2	13	0.33
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	4	0.33
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD12	12	0.33
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	4	0.33
(1,373)	1:179:A:ILE:HG22	1:182:A:SER:H	8	0.33
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	13	0.33
(1,349)	1:191:A:VAL:HG21	1:184:A:MET:H	10	0.33
(1,248)	1:152:A:LYS:HE2	1:152:A:LYS:H	11	0.33
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	5	0.33
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG22	15	0.33
(1,119)	1:183:A:LEU:HD23	1:183:A:LEU:H	12	0.33
(1,48)	1:208:A:LEU:HD12	1:208:A:LEU:H	11	0.33
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	13	0.33
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	7	0.33
(1,1677)	1:161:A:MET:HA	1:161:A:MET:HE3	11	0.32
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	1	0.32
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	6	0.32
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	15	0.32
(1,1664)	1:229:A:ILE:HG12	1:229:A:ILE:HB	9	0.32
(1,1664)	1:229:A:ILE:HG12	1:229:A:ILE:HB	15	0.32
(1,1640)	1:202:A:ILE:HG21	1:206:A:ARG:HD2	13	0.32
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	6	0.32
(1,1630)	1:152:A:LYS:HB2	1:152:A:LYS:HG3	1	0.32
(1,1571)	1:137:A:ILE:HG21	1:141:A:LEU:HB3	10	0.32
(1,1566)	1:124:A:ASP:HB2	1:208:A:LEU:HD22	5	0.32
(1,1525)	1:155:A:ILE:HB	1:156:A:PRO:HD2	3	0.32
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	9	0.32
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	13	0.32
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	2	0.32
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	4	0.32
(1,1263)	1:117:A:PRO:HA	1:117:A:PRO:HB3	11	0.32
(1,1205)	1:132:A:GLN:HG2	1:133:A:VAL:HA	11	0.32
(1,1182)	1:206:A:ARG:HA	1:209:A:PHE:HB2	13	0.32
(1,1132)	1:179:A:ILE:HG22	1:161:A:MET:HA	4	0.32
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	6	0.32
(1,1087)	1:122:A:LEU:HD12	1:126:A:ARG:HB3	7	0.32
(1,1085)	1:206:A:ARG:HB3	1:206:A:ARG:HD3	3	0.32
(1,1034)	1:199:A:LYS:HE2	1:195:A:MET:HE1	2	0.32
(1,991)	1:155:A:ILE:HD12	1:154:A:SER:HB2	3	0.32
(1,967)	1:111:A:MET:HE3	1:148:A:TRP:HA	1	0.32
(1,954)	1:145:A:GLN:HB3	1:142:A:ALA:HA	7	0.32
(1,937)	1:205:A:LYS:HG3	1:205:A:LYS:HE2	10	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	3	0.32
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	8	0.32
(1,794)	1:144:A:LEU:HD13	1:143:A:LEU:H	10	0.32
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	13	0.32
(1,455)	1:168:A:LEU:HD21	1:169:A:SER:H	9	0.32
(1,455)	1:168:A:LEU:HD23	1:169:A:SER:H	12	0.32
(1,373)	1:179:A:ILE:HG22	1:182:A:SER:H	15	0.32
(1,281)	1:181:A:ARG:H	1:184:A:MET:HG3	11	0.32
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG23	6	0.32
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	7	0.32
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	2	0.32
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	7	0.32
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	3	0.32
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	4	0.31
(1,1758)	1:191:A:VAL:HG21	1:184:A:MET:HA	7	0.31
(1,1745)	1:179:A:ILE:HG22	1:164:A:LEU:HB3	4	0.31
(1,1744)	1:205:A:LYS:HB2	1:205:A:LYS:HE2	1	0.31
(1,1744)	1:205:A:LYS:HB2	1:205:A:LYS:HE2	2	0.31
(1,1744)	1:205:A:LYS:HB2	1:205:A:LYS:HE2	5	0.31
(1,1710)	1:117:A:PRO:HB3	1:118:A:LEU:HD22	11	0.31
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD12	4	0.31
(1,1682)	1:168:A:LEU:HD23	1:165:A:VAL:HB	15	0.31
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	2	0.31
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	5	0.31
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	10	0.31
(1,1597)	1:181:A:ARG:HB2	1:181:A:ARG:HA	12	0.31
(1,1525)	1:155:A:ILE:HB	1:156:A:PRO:HD2	6	0.31
(1,1514)	1:195:A:MET:HE2	1:184:A:MET:HG2	4	0.31
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	6	0.31
(1,1475)	1:183:A:LEU:HD22	1:179:A:ILE:HB	9	0.31
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	4	0.31
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	12	0.31
(1,1394)	1:122:A:LEU:HD11	1:134:A:CYS:HB3	15	0.31
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD23	3	0.31
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD23	10	0.31
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	3	0.31
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD13	5	0.31
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD11	10	0.31
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	6	0.31
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	15	0.31
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	14	0.31
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	15	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	9	0.31
(1,1155)	1:209:A:PHE:HD2	1:206:A:ARG:HG2	9	0.31
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	10	0.31
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	3	0.31
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	9	0.31
(1,1099)	1:206:A:ARG:HB3	1:209:A:PHE:HD2	14	0.31
(1,1006)	1:161:A:MET:HG2	1:161:A:MET:HB3	5	0.31
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	8	0.31
(1,718)	1:229:A:ILE:H	1:228:A:THR:H	9	0.31
(1,608)	1:200:A:ARG:H	1:199:A:LYS:HB2	12	0.31
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	9	0.31
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	5	0.31
(1,520)	1:164:A:LEU:HD22	1:166:A:GLN:H	7	0.31
(1,520)	1:164:A:LEU:HD22	1:166:A:GLN:H	9	0.31
(1,520)	1:164:A:LEU:HD22	1:166:A:GLN:H	13	0.31
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	15	0.31
(1,503)	1:153:A:LEU:HD13	1:149:A:ALA:H	8	0.31
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	1	0.31
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	10	0.31
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD13	14	0.31
(1,349)	1:191:A:VAL:HG22	1:184:A:MET:H	3	0.31
(1,349)	1:191:A:VAL:HG22	1:184:A:MET:H	15	0.31
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	15	0.31
(1,283)	1:116:A:ARG:HG2	1:116:A:ARG:H	1	0.31
(1,214)	1:227:A:HIS:H	1:227:A:HIS:HB2	7	0.31
(1,108)	1:157:A:VAL:HG21	1:160:A:ARG:H	11	0.31
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	1	0.31
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	6	0.31
(1,1823)	1:205:A:LYS:HB2	1:173:A:TRP:HZ3	9	0.3
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	3	0.3
(1,1700)	1:116:A:ARG:HG2	1:116:A:ARG:HB2	14	0.3
(1,1661)	1:158:A:LYS:HD3	1:148:A:TRP:HZ2	3	0.3
(1,1609)	1:157:A:VAL:HG12	1:194:A:TRP:HH2	6	0.3
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	6	0.3
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	13	0.3
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG12	5	0.3
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	1	0.3
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	9	0.3
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	10	0.3
(1,1284)	1:188:A:VAL:HB	1:191:A:VAL:HG22	2	0.3
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD11	4	0.3
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	11	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1132)	1:179:A:ILE:HG22	1:161:A:MET:HA	12	0.3
(1,1132)	1:179:A:ILE:HG23	1:161:A:MET:HA	15	0.3
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	13	0.3
(1,1038)	1:116:A:ARG:HD2	1:116:A:ARG:HB3	14	0.3
(1,1006)	1:161:A:MET:HG2	1:161:A:MET:HB3	6	0.3
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	12	0.3
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	14	0.3
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD11	9	0.3
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	12	0.3
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	11	0.3
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	4	0.3
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	12	0.3
(1,637)	1:125:A:CYS:H	1:124:A:ASP:HB3	6	0.3
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	3	0.3
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	11	0.3
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	5	0.3
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	15	0.3
(1,334)	1:185:A:VAL:HB	1:185:A:VAL:H	13	0.3
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	5	0.3
(1,154)	1:208:A:LEU:HD12	1:205:A:LYS:H	3	0.3
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	4	0.3
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	14	0.3
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	1	0.3
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	4	0.3
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	7	0.3
(1,101)	1:152:A:LYS:H	1:152:A:LYS:HB3	12	0.3
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	5	0.3
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	9	0.3
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	15	0.3
(1,1808)	1:158:A:LYS:HB2	1:148:A:TRP:HZ2	6	0.29
(1,1793)	1:187:A:HIS:HD1	1:191:A:VAL:HG22	1	0.29
(1,1782)	1:143:A:LEU:HD12	1:194:A:TRP:HZ3	2	0.29
(1,1730)	1:202:A:ILE:HA	1:202:A:ILE:HB	14	0.29
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	11	0.29
(1,1617)	1:180:A:HIS:HA	1:180:A:HIS:HB2	1	0.29
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	4	0.29
(1,1429)	1:141:A:LEU:HD21	1:144:A:LEU:HD11	2	0.29
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	2	0.29
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	12	0.29
(1,1282)	1:160:A:ARG:HB2	1:163:A:LEU:HD12	13	0.29
(1,1217)	1:130:A:ARG:HA	1:130:A:ARG:HD3	7	0.29
(1,1205)	1:132:A:GLN:HG2	1:133:A:VAL:HA	1	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:143:A:LEU:HG	1:143:A:LEU:HB3	14	0.29
(1,1038)	1:116:A:ARG:HD2	1:116:A:ARG:HB3	7	0.29
(1,1018)	1:114:A:VAL:HG11	1:115:A:LEU:HD12	9	0.29
(1,1006)	1:161:A:MET:HG2	1:161:A:MET:HB3	11	0.29
(1,961)	1:184:A:MET:HB2	1:184:A:MET:HG3	9	0.29
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	5	0.29
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD23	12	0.29
(1,873)	1:202:A:ILE:HG22	1:203:A:ALA:H	9	0.29
(1,872)	1:176:A:ALA:HB3	1:173:A:TRP:H	10	0.29
(1,856)	1:158:A:LYS:HE2	1:158:A:LYS:H	4	0.29
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	8	0.29
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	2	0.29
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD22	9	0.29
(1,712)	1:199:A:LYS:HE2	1:199:A:LYS:H	2	0.29
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	15	0.29
(1,503)	1:153:A:LEU:HD13	1:149:A:ALA:H	2	0.29
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	11	0.29
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	4	0.29
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	8	0.29
(1,349)	1:191:A:VAL:HG23	1:184:A:MET:H	1	0.29
(1,349)	1:191:A:VAL:HG22	1:184:A:MET:H	5	0.29
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD12	3	0.29
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD11	13	0.29
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG23	3	0.29
(1,199)	1:175:A:ALA:HB1	1:178:A:ASP:H	15	0.29
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	10	0.29
(1,174)	1:212:A:GLU:HB3	1:212:A:GLU:H	13	0.29
(1,125)	1:112:A:GLU:HG2	1:113:A:ASP:H	7	0.29
(1,81)	1:203:A:ALA:HB3	1:200:A:ARG:H	14	0.29
(1,80)	1:202:A:ILE:HD13	1:201:A:LEU:H	10	0.29
(1,1719)	1:194:A:TRP:HZ3	1:191:A:VAL:HG11	13	0.28
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	5	0.28
(1,1682)	1:168:A:LEU:HD22	1:165:A:VAL:HB	1	0.28
(1,1664)	1:229:A:ILE:HG12	1:229:A:ILE:HB	12	0.28
(1,1651)	1:206:A:ARG:HA	1:209:A:PHE:HB3	5	0.28
(1,1597)	1:181:A:ARG:HB2	1:181:A:ARG:HA	2	0.28
(1,1597)	1:181:A:ARG:HB2	1:181:A:ARG:HA	9	0.28
(1,1468)	1:198:A:VAL:HA	1:201:A:LEU:HB2	10	0.28
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	15	0.28
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	14	0.28
(1,1320)	1:183:A:LEU:HD22	1:194:A:TRP:HZ2	11	0.28
(1,1245)	1:158:A:LYS:HE2	1:158:A:LYS:HD2	8	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	3	0.28
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	7	0.28
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	8	0.28
(1,1181)	1:153:A:LEU:HB2	1:158:A:LYS:HG2	1	0.28
(1,969)	1:139:A:ARG:HD2	1:140:A:ARG:HA	5	0.28
(1,901)	1:202:A:ILE:HD11	1:203:A:ALA:H	6	0.28
(1,660)	1:212:A:GLU:H	1:211:A:GLU:HB3	15	0.28
(1,570)	1:162:A:ALA:HB3	1:164:A:LEU:H	11	0.28
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	10	0.28
(1,455)	1:168:A:LEU:HD21	1:169:A:SER:H	1	0.28
(1,455)	1:168:A:LEU:HD21	1:169:A:SER:H	5	0.28
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	7	0.28
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	13	0.28
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	14	0.28
(1,373)	1:179:A:ILE:HG22	1:182:A:SER:H	3	0.28
(1,341)	1:191:A:VAL:HG21	1:188:A:VAL:H	7	0.28
(1,341)	1:191:A:VAL:HG23	1:188:A:VAL:H	12	0.28
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG23	8	0.28
(1,199)	1:175:A:ALA:HB3	1:178:A:ASP:H	7	0.28
(1,174)	1:212:A:GLU:HB3	1:212:A:GLU:H	1	0.28
(1,174)	1:212:A:GLU:HB3	1:212:A:GLU:H	3	0.28
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	9	0.28
(1,71)	1:142:A:ALA:HB1	1:144:A:LEU:H	13	0.28
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD13	14	0.28
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	2	0.28
(1,47)	1:118:A:LEU:H	1:118:A:LEU:HD23	12	0.28
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	8	0.27
(1,1791)	1:148:A:TRP:HE3	1:161:A:MET:HE2	4	0.27
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	15	0.27
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	3	0.27
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	5	0.27
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	11	0.27
(1,1661)	1:158:A:LYS:HD3	1:148:A:TRP:HZ2	1	0.27
(1,1651)	1:206:A:ARG:HA	1:209:A:PHE:HB3	6	0.27
(1,1643)	1:148:A:TRP:HZ3	1:161:A:MET:HG2	11	0.27
(1,1640)	1:202:A:ILE:HG22	1:206:A:ARG:HD2	10	0.27
(1,1586)	1:157:A:VAL:HG23	1:190:A:GLU:HB2	15	0.27
(1,1556)	1:131:A:LYS:HE2	1:131:A:LYS:HA	9	0.27
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	2	0.27
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	6	0.27
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	8	0.27
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	9	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	10	0.27
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	14	0.27
(1,1497)	1:117:A:PRO:HD3	1:165:A:VAL:HG21	11	0.27
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	9	0.27
(1,1425)	1:121:A:ALA:HB2	1:122:A:LEU:HD13	9	0.27
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	6	0.27
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	13	0.27
(1,1402)	1:136:A:ASP:HB3	1:132:A:GLN:HG2	13	0.27
(1,1397)	1:163:A:LEU:HA	1:163:A:LEU:HD21	8	0.27
(1,1384)	1:145:A:GLN:HG2	1:141:A:LEU:HD21	7	0.27
(1,1378)	1:116:A:ARG:HA	1:116:A:ARG:HB2	14	0.27
(1,1317)	1:218:A:LYS:HE2	1:218:A:LYS:HA	9	0.27
(1,1234)	1:208:A:LEU:HD12	1:205:A:LYS:HE2	8	0.27
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	5	0.27
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	6	0.27
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	15	0.27
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	1	0.27
(1,1044)	1:183:A:LEU:HD21	1:161:A:MET:HA	2	0.27
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD13	4	0.27
(1,872)	1:176:A:ALA:HB1	1:173:A:TRP:H	9	0.27
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	1	0.27
(1,794)	1:144:A:LEU:HD11	1:143:A:LEU:H	13	0.27
(1,570)	1:162:A:ALA:HB3	1:164:A:LEU:H	13	0.27
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	11	0.27
(1,372)	1:145:A:GLN:HA	1:145:A:GLN:HE22	10	0.27
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	5	0.27
(1,71)	1:142:A:ALA:HB2	1:144:A:LEU:H	9	0.27
(1,48)	1:208:A:LEU:HD23	1:208:A:LEU:H	3	0.27
(1,1763)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	10	0.26
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	14	0.26
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	4	0.26
(1,1641)	1:153:A:LEU:HD12	1:145:A:GLN:HA	4	0.26
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	7	0.26
(1,1589)	1:201:A:LEU:HA	1:201:A:LEU:HD11	9	0.26
(1,1589)	1:201:A:LEU:HA	1:201:A:LEU:HD12	12	0.26
(1,1571)	1:137:A:ILE:HG23	1:141:A:LEU:HB3	15	0.26
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	5	0.26
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	8	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	1	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	3	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	4	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	7	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	12	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	13	0.26
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	15	0.26
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	12	0.26
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	6	0.26
(1,1417)	1:131:A:LYS:HE2	1:131:A:LYS:HD2	13	0.26
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	5	0.26
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	1	0.26
(1,1284)	1:188:A:VAL:HB	1:191:A:VAL:HG22	11	0.26
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	3	0.26
(1,1278)	1:173:A:TRP:HE3	1:173:A:TRP:HB3	13	0.26
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	1	0.26
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	2	0.26
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	4	0.26
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	9	0.26
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	13	0.26
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	14	0.26
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	1	0.26
(1,1163)	1:172:A:ARG:HB3	1:170:A:SER:HB2	14	0.26
(1,1128)	1:124:A:ASP:HB2	1:122:A:LEU:HD11	10	0.26
(1,1065)	1:164:A:LEU:HD13	1:177:A:ASP:HA	8	0.26
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	11	0.26
(1,834)	1:115:A:LEU:HD13	1:116:A:ARG:H	13	0.26
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	1	0.26
(1,771)	1:232:A:PHE:H	1:232:A:PHE:HB2	5	0.26
(1,771)	1:232:A:PHE:H	1:232:A:PHE:HB2	8	0.26
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	10	0.26
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	7	0.26
(1,588)	1:145:A:GLN:HG2	1:145:A:GLN:HE21	10	0.26
(1,564)	1:154:A:SER:H	1:154:A:SER:HB2	10	0.26
(1,520)	1:164:A:LEU:HD21	1:166:A:GLN:H	1	0.26
(1,503)	1:153:A:LEU:HD12	1:149:A:ALA:H	4	0.26
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	2	0.26
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	1	0.26
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	2	0.26
(1,353)	1:157:A:VAL:HG11	1:154:A:SER:H	15	0.26
(1,349)	1:191:A:VAL:HG23	1:184:A:MET:H	2	0.26
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD11	8	0.26
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	3	0.26
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB1	9	0.26
(1,119)	1:183:A:LEU:HD21	1:183:A:LEU:H	11	0.26
(1,71)	1:142:A:ALA:HB1	1:144:A:LEU:H	6	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG12	5	0.26
(1,1729)	1:127:A:GLY:HA2	1:126:A:ARG:HD2	5	0.25
(1,1700)	1:116:A:ARG:HG2	1:116:A:ARG:HB2	1	0.25
(1,1687)	1:230:A:PRO:HB3	1:232:A:PHE:HB2	4	0.25
(1,1673)	1:164:A:LEU:HB3	1:161:A:MET:HA	14	0.25
(1,1643)	1:148:A:TRP:HZ3	1:161:A:MET:HG2	5	0.25
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	12	0.25
(1,1601)	1:216:A:GLU:HG2	1:216:A:GLU:HA	7	0.25
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG13	14	0.25
(1,1583)	1:201:A:LEU:HD21	1:201:A:LEU:HA	2	0.25
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	1	0.25
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	2	0.25
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	10	0.25
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	11	0.25
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	13	0.25
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	3	0.25
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	5	0.25
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	7	0.25
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	12	0.25
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	11	0.25
(1,1397)	1:163:A:LEU:HA	1:163:A:LEU:HD23	9	0.25
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	1	0.25
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	12	0.25
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	3	0.25
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	6	0.25
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	3	0.25
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	11	0.25
(1,890)	1:210:A:SER:H	1:208:A:LEU:HD22	5	0.25
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	5	0.25
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	6	0.25
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	9	0.25
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	2	0.25
(1,667)	1:144:A:LEU:HD23	1:144:A:LEU:H	2	0.25
(1,468)	1:122:A:LEU:HD11	1:125:A:CYS:H	8	0.25
(1,457)	1:153:A:LEU:HD12	1:154:A:SER:H	2	0.25
(1,443)	1:181:A:ARG:HB2	1:182:A:SER:H	3	0.25
(1,353)	1:157:A:VAL:HG11	1:154:A:SER:H	11	0.25
(1,320)	1:193:A:GLN:HB2	1:194:A:TRP:H	14	0.25
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	2	0.25
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	8	0.25
(1,1808)	1:158:A:LYS:HB2	1:148:A:TRP:HZ2	14	0.24
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	14	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:191:A:VAL:HG21	1:184:A:MET:HA	11	0.24
(1,1634)	1:161:A:MET:HG3	1:161:A:MET:HA	5	0.24
(1,1597)	1:181:A:ARG:HB2	1:181:A:ARG:HA	4	0.24
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG11	1	0.24
(1,1583)	1:201:A:LEU:HD22	1:201:A:LEU:HA	1	0.24
(1,1566)	1:124:A:ASP:HB2	1:208:A:LEU:HD22	7	0.24
(1,1529)	1:156:A:PRO:HB3	1:156:A:PRO:HA	5	0.24
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	6	0.24
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	5	0.24
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	13	0.24
(1,1435)	1:153:A:LEU:HA	1:190:A:GLU:HB2	15	0.24
(1,1356)	1:198:A:VAL:HA	1:201:A:LEU:HB3	12	0.24
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD22	8	0.24
(1,1349)	1:194:A:TRP:HB2	1:143:A:LEU:HD23	11	0.24
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	13	0.24
(1,1243)	1:124:A:ASP:HB2	1:121:A:ALA:HB2	3	0.24
(1,1239)	1:225:A:LYS:HD3	1:225:A:LYS:HE2	10	0.24
(1,1234)	1:208:A:LEU:HD12	1:205:A:LYS:HE2	4	0.24
(1,1197)	1:230:A:PRO:HB2	1:230:A:PRO:HG2	10	0.24
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	7	0.24
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	12	0.24
(1,1134)	1:126:A:ARG:HD2	1:126:A:ARG:HB2	11	0.24
(1,1132)	1:179:A:ILE:HG22	1:161:A:MET:HA	10	0.24
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	8	0.24
(1,1009)	1:124:A:ASP:HB2	1:124:A:ASP:HA	7	0.24
(1,975)	1:194:A:TRP:HA	1:143:A:LEU:HB2	7	0.24
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	12	0.24
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	7	0.24
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	14	0.24
(1,759)	1:137:A:ILE:HD12	1:138:A:SER:H	1	0.24
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	2	0.24
(1,759)	1:137:A:ILE:HD13	1:138:A:SER:H	4	0.24
(1,741)	1:191:A:VAL:HG22	1:195:A:MET:H	15	0.24
(1,633)	1:199:A:LYS:HG2	1:199:A:LYS:H	12	0.24
(1,552)	1:108:A:GLU:HB3	1:108:A:GLU:H	11	0.24
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	7	0.24
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	3	0.24
(1,208)	1:119:A:GLU:H	1:115:A:LEU:HD13	14	0.24
(1,199)	1:175:A:ALA:HB2	1:178:A:ASP:H	12	0.24
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	1	0.24
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB3	2	0.24
(1,174)	1:212:A:GLU:HB3	1:212:A:GLU:H	10	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:212:A:GLU:HB3	1:212:A:GLU:H	11	0.24
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	15	0.24
(1,71)	1:142:A:ALA:HB2	1:144:A:LEU:H	7	0.24
(1,2)	1:155:A:ILE:HG22	1:159:A:LYS:H	1	0.24
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD11	7	0.23
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	7	0.23
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	2	0.23
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	6	0.23
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	12	0.23
(1,1602)	1:206:A:ARG:HA	1:206:A:ARG:HD3	9	0.23
(1,1583)	1:201:A:LEU:HD21	1:201:A:LEU:HA	6	0.23
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	3	0.23
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	6	0.23
(1,1482)	1:191:A:VAL:HG23	1:184:A:MET:HG3	3	0.23
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	1	0.23
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	2	0.23
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	15	0.23
(1,1468)	1:198:A:VAL:HA	1:201:A:LEU:HB2	9	0.23
(1,1402)	1:136:A:ASP:HB3	1:132:A:GLN:HG2	4	0.23
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	9	0.23
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	11	0.23
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	15	0.23
(1,1305)	1:143:A:LEU:HD23	1:193:A:GLN:HB3	2	0.23
(1,1249)	1:187:A:HIS:HD1	1:157:A:VAL:HG13	14	0.23
(1,1172)	1:171:A:HIS:HB2	1:171:A:HIS:HA	9	0.23
(1,1166)	1:111:A:MET:HE1	1:111:A:MET:HB2	3	0.23
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	12	0.23
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	3	0.23
(1,834)	1:115:A:LEU:HD11	1:116:A:ARG:H	9	0.23
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	12	0.23
(1,752)	1:168:A:LEU:H	1:168:A:LEU:HD12	5	0.23
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	11	0.23
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	10	0.23
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	3	0.23
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	12	0.23
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD13	5	0.23
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD11	8	0.23
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD11	11	0.23
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	5	0.23
(1,341)	1:191:A:VAL:HG23	1:188:A:VAL:H	5	0.23
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	3	0.23
(1,320)	1:193:A:GLN:HB2	1:194:A:TRP:H	3	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	9	0.23
(1,214)	1:227:A:HIS:H	1:227:A:HIS:HB2	6	0.23
(1,199)	1:175:A:ALA:HB3	1:178:A:ASP:H	1	0.23
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB3	4	0.23
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	15	0.23
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	12	0.23
(1,119)	1:183:A:LEU:HD21	1:183:A:LEU:H	13	0.23
(1,87)	1:234:A:GLN:HB2	1:235:A:ALA:H	15	0.23
(1,87)	1:234:A:GLN:HB3	1:235:A:ALA:H	15	0.23
(1,80)	1:202:A:ILE:HD12	1:201:A:LEU:H	4	0.23
(1,71)	1:142:A:ALA:HB1	1:144:A:LEU:H	3	0.23
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	7	0.22
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	13	0.22
(1,1758)	1:191:A:VAL:HG23	1:184:A:MET:HA	9	0.22
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG23	4	0.22
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG21	11	0.22
(1,1723)	1:148:A:TRP:HE3	1:114:A:VAL:HG22	15	0.22
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	1	0.22
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	3	0.22
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	9	0.22
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	12	0.22
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	12	0.22
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	3	0.22
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	5	0.22
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	8	0.22
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	10	0.22
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	14	0.22
(1,1652)	1:131:A:LYS:HD3	1:131:A:LYS:HB3	12	0.22
(1,1587)	1:184:A:MET:HB2	1:185:A:VAL:HG12	8	0.22
(1,1583)	1:201:A:LEU:HD21	1:201:A:LEU:HA	4	0.22
(1,1506)	1:204:A:GLU:HB2	1:205:A:LYS:HA	8	0.22
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	13	0.22
(1,1410)	1:148:A:TRP:HD1	1:111:A:MET:HG3	6	0.22
(1,1410)	1:148:A:TRP:HD1	1:111:A:MET:HG3	7	0.22
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	7	0.22
(1,1215)	1:202:A:ILE:HD13	1:177:A:ASP:HB3	12	0.22
(1,1172)	1:171:A:HIS:HB2	1:171:A:HIS:HA	12	0.22
(1,1166)	1:111:A:MET:HE1	1:111:A:MET:HB2	2	0.22
(1,1134)	1:126:A:ARG:HD2	1:126:A:ARG:HB2	14	0.22
(1,922)	1:218:A:LYS:HG2	1:218:A:LYS:HB3	3	0.22
(1,901)	1:202:A:ILE:HD12	1:203:A:ALA:H	7	0.22
(1,874)	1:158:A:LYS:H	1:154:A:SER:HB2	10	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,834)	1:115:A:LEU:HD13	1:116:A:ARG:H	4	0.22
(1,794)	1:144:A:LEU:HD12	1:143:A:LEU:H	5	0.22
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	15	0.22
(1,759)	1:137:A:ILE:HD11	1:138:A:SER:H	3	0.22
(1,636)	1:220:A:ALA:H	1:219:A:SER:HA	9	0.22
(1,633)	1:199:A:LYS:HG2	1:199:A:LYS:H	13	0.22
(1,571)	1:204:A:GLU:H	1:206:A:ARG:HG2	13	0.22
(1,570)	1:162:A:ALA:HB2	1:164:A:LEU:H	9	0.22
(1,552)	1:108:A:GLU:HB3	1:108:A:GLU:H	5	0.22
(1,552)	1:108:A:GLU:HB3	1:108:A:GLU:H	14	0.22
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	15	0.22
(1,455)	1:168:A:LEU:HD22	1:169:A:SER:H	13	0.22
(1,447)	1:211:A:GLU:H	1:211:A:GLU:HG2	9	0.22
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	6	0.22
(1,385)	1:119:A:GLU:H	1:118:A:LEU:HD12	10	0.22
(1,353)	1:157:A:VAL:HG12	1:154:A:SER:H	7	0.22
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD12	10	0.22
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	5	0.22
(1,199)	1:175:A:ALA:HB2	1:178:A:ASP:H	11	0.22
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	15	0.22
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	6	0.22
(1,1808)	1:158:A:LYS:HB2	1:148:A:TRP:HZ2	5	0.21
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	1	0.21
(1,1781)	1:148:A:TRP:HE3	1:161:A:MET:HG3	5	0.21
(1,1763)	1:158:A:LYS:HB2	1:158:A:LYS:HE2	5	0.21
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG23	12	0.21
(1,1700)	1:116:A:ARG:HG2	1:116:A:ARG:HB2	11	0.21
(1,1698)	1:183:A:LEU:HD22	1:180:A:HIS:HA	4	0.21
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	14	0.21
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	4	0.21
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	7	0.21
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	9	0.21
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	13	0.21
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	15	0.21
(1,1640)	1:202:A:ILE:HG22	1:206:A:ARG:HD2	3	0.21
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	15	0.21
(1,1583)	1:201:A:LEU:HD22	1:201:A:LEU:HA	5	0.21
(1,1571)	1:137:A:ILE:HG23	1:141:A:LEU:HB3	1	0.21
(1,1492)	1:187:A:HIS:HB3	1:190:A:GLU:HB3	9	0.21
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	9	0.21
(1,1461)	1:183:A:LEU:HA	1:183:A:LEU:HB2	3	0.21
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	14	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	2	0.21
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	7	0.21
(1,1410)	1:148:A:TRP:HD1	1:111:A:MET:HG3	5	0.21
(1,1392)	1:158:A:LYS:HE2	1:148:A:TRP:HA	3	0.21
(1,1323)	1:148:A:TRP:HE3	1:158:A:LYS:HG2	1	0.21
(1,1216)	1:158:A:LYS:HE2	1:158:A:LYS:HG2	11	0.21
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	14	0.21
(1,1134)	1:126:A:ARG:HD2	1:126:A:ARG:HB2	10	0.21
(1,1114)	1:143:A:LEU:HD12	1:140:A:ARG:HB3	4	0.21
(1,1076)	1:204:A:GLU:HB2	1:204:A:GLU:HA	2	0.21
(1,1024)	1:122:A:LEU:HD12	1:134:A:CYS:HA	7	0.21
(1,1024)	1:122:A:LEU:HD13	1:134:A:CYS:HA	11	0.21
(1,971)	1:139:A:ARG:HG2	1:138:A:SER:HB2	10	0.21
(1,922)	1:218:A:LYS:HG2	1:218:A:LYS:HB3	13	0.21
(1,856)	1:158:A:LYS:HE2	1:158:A:LYS:H	2	0.21
(1,833)	1:160:A:ARG:HD2	1:160:A:ARG:H	5	0.21
(1,813)	1:221:A:ALA:HA	1:221:A:ALA:H	1	0.21
(1,813)	1:221:A:ALA:HA	1:221:A:ALA:H	12	0.21
(1,771)	1:232:A:PHE:H	1:232:A:PHE:HB2	12	0.21
(1,705)	1:140:A:ARG:H	1:139:A:ARG:HB2	14	0.21
(1,609)	1:213:A:ALA:HB1	1:212:A:GLU:H	5	0.21
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	1	0.21
(1,540)	1:129:A:THR:HG1	1:133:A:VAL:H	14	0.21
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	4	0.21
(1,468)	1:122:A:LEU:HD12	1:125:A:CYS:H	1	0.21
(1,468)	1:122:A:LEU:HD13	1:125:A:CYS:H	6	0.21
(1,408)	1:155:A:ILE:H	1:155:A:ILE:HG13	5	0.21
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	15	0.21
(1,357)	1:207:A:SER:HB3	1:208:A:LEU:H	7	0.21
(1,328)	1:145:A:GLN:HE22	1:145:A:GLN:H	6	0.21
(1,320)	1:193:A:GLN:HB2	1:194:A:TRP:H	7	0.21
(1,303)	1:158:A:LYS:H	1:158:A:LYS:HG3	8	0.21
(1,298)	1:181:A:ARG:H	1:178:A:ASP:H	9	0.21
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	11	0.21
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	2	0.21
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	1	0.21
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD12	11	0.2
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	11	0.2
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG23	10	0.2
(1,1732)	1:225:A:LYS:HB3	1:225:A:LYS:HG2	10	0.2
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	6	0.2
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	8	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:158:A:LYS:HE2	1:153:A:LEU:HD12	13	0.2
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	10	0.2
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	1	0.2
(1,1662)	1:156:A:PRO:HG3	1:156:A:PRO:HB3	11	0.2
(1,1532)	1:158:A:LYS:HB2	1:155:A:ILE:HA	6	0.2
(1,1455)	1:148:A:TRP:HE3	1:148:A:TRP:HA	1	0.2
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	9	0.2
(1,1375)	1:144:A:LEU:HD23	1:153:A:LEU:HD13	8	0.2
(1,1365)	1:184:A:MET:HG3	1:195:A:MET:HE3	1	0.2
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG21	6	0.2
(1,1320)	1:183:A:LEU:HD23	1:194:A:TRP:HZ2	2	0.2
(1,1256)	1:190:A:GLU:HB3	1:187:A:HIS:HA	11	0.2
(1,1227)	1:181:A:ARG:HD3	1:181:A:ARG:HG2	13	0.2
(1,1182)	1:206:A:ARG:HA	1:209:A:PHE:HB2	12	0.2
(1,915)	1:199:A:LYS:HE2	1:199:A:LYS:HG2	8	0.2
(1,913)	1:177:A:ASP:HA	1:177:A:ASP:HB3	6	0.2
(1,879)	1:208:A:LEU:HB2	1:210:A:SER:H	6	0.2
(1,856)	1:158:A:LYS:HE2	1:158:A:LYS:H	7	0.2
(1,834)	1:115:A:LEU:HD11	1:116:A:ARG:H	15	0.2
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	6	0.2
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	2	0.2
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	10	0.2
(1,693)	1:162:A:ALA:HB1	1:161:A:MET:H	3	0.2
(1,693)	1:162:A:ALA:HB2	1:161:A:MET:H	5	0.2
(1,667)	1:144:A:LEU:HD22	1:144:A:LEU:H	10	0.2
(1,667)	1:144:A:LEU:HD21	1:144:A:LEU:H	15	0.2
(1,541)	1:232:A:PHE:H	1:231:A:GLY:HA3	10	0.2
(1,493)	1:218:A:LYS:HD3	1:218:A:LYS:H	4	0.2
(1,488)	1:141:A:LEU:HD21	1:142:A:ALA:H	4	0.2
(1,459)	1:192:A:SER:H	1:190:A:GLU:HB2	4	0.2
(1,455)	1:168:A:LEU:HD21	1:169:A:SER:H	2	0.2
(1,449)	1:182:A:SER:H	1:179:A:ILE:HD11	8	0.2
(1,447)	1:211:A:GLU:H	1:211:A:GLU:HG2	7	0.2
(1,443)	1:181:A:ARG:HB2	1:182:A:SER:H	9	0.2
(1,443)	1:181:A:ARG:HB2	1:182:A:SER:H	12	0.2
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	14	0.2
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	6	0.2
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	11	0.2
(1,168)	1:229:A:ILE:HB	1:229:A:ILE:H	12	0.2
(1,108)	1:157:A:VAL:HG23	1:160:A:ARG:H	3	0.2
(2,18)	1:163:A:LEU:H	1:159:A:LYS:O	14	0.19
(1,1842)	1:194:A:TRP:HZ3	1:191:A:VAL:HB	12	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1808)	1:158:A:LYS:HB2	1:148:A:TRP:HZ2	10	0.19
(1,1743)	1:161:A:MET:HE1	1:114:A:VAL:HG21	2	0.19
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	7	0.19
(1,1660)	1:194:A:TRP:HB2	1:143:A:LEU:HB2	14	0.19
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	12	0.19
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	3	0.19
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	3	0.19
(1,1497)	1:117:A:PRO:HD3	1:165:A:VAL:HG21	5	0.19
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	8	0.19
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	14	0.19
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	1	0.19
(1,1452)	1:152:A:LYS:HE2	1:152:A:LYS:HG2	4	0.19
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	4	0.19
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	8	0.19
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	10	0.19
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	15	0.19
(1,1256)	1:190:A:GLU:HB3	1:187:A:HIS:HA	8	0.19
(1,1076)	1:204:A:GLU:HB2	1:204:A:GLU:HA	8	0.19
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	15	0.19
(1,948)	1:154:A:SER:HA	1:155:A:ILE:HD13	5	0.19
(1,928)	1:161:A:MET:HG3	1:114:A:VAL:HG23	11	0.19
(1,864)	1:152:A:LYS:H	1:152:A:LYS:HG3	12	0.19
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	15	0.19
(1,835)	1:158:A:LYS:HE2	1:148:A:TRP:HE1	8	0.19
(1,834)	1:115:A:LEU:HD13	1:116:A:ARG:H	5	0.19
(1,762)	1:132:A:GLN:HG2	1:132:A:GLN:H	2	0.19
(1,759)	1:137:A:ILE:HD13	1:138:A:SER:H	12	0.19
(1,752)	1:168:A:LEU:H	1:168:A:LEU:HD12	12	0.19
(1,660)	1:212:A:GLU:H	1:211:A:GLU:HB3	7	0.19
(1,608)	1:200:A:ARG:H	1:199:A:LYS:HB2	6	0.19
(1,575)	1:139:A:ARG:HG2	1:139:A:ARG:H	4	0.19
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	5	0.19
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	12	0.19
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	12	0.19
(1,378)	1:149:A:ALA:HB3	1:146:A:GLU:H	4	0.19
(1,320)	1:193:A:GLN:HB2	1:194:A:TRP:H	4	0.19
(1,309)	1:181:A:ARG:H	1:181:A:ARG:HG2	4	0.19
(1,81)	1:203:A:ALA:HB2	1:200:A:ARG:H	5	0.19
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG11	4	0.19
(1,18)	1:229:A:ILE:H	1:228:A:THR:H	2	0.19
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	3	0.18
(1,1754)	1:143:A:LEU:HA	1:143:A:LEU:HB3	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1726)	1:118:A:LEU:HG	1:115:A:LEU:HD13	14	0.18
(1,1683)	1:141:A:LEU:HA	1:144:A:LEU:HB3	7	0.18
(1,1665)	1:152:A:LYS:HD3	1:152:A:LYS:HB3	7	0.18
(1,1652)	1:131:A:LYS:HD3	1:131:A:LYS:HB3	13	0.18
(1,1641)	1:153:A:LEU:HD11	1:145:A:GLN:HA	7	0.18
(1,1641)	1:153:A:LEU:HD11	1:145:A:GLN:HA	12	0.18
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	13	0.18
(1,1608)	1:116:A:ARG:HG2	1:116:A:ARG:HA	14	0.18
(1,1601)	1:216:A:GLU:HG2	1:216:A:GLU:HA	5	0.18
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	7	0.18
(1,1539)	1:202:A:ILE:HG22	1:206:A:ARG:HD3	5	0.18
(1,1538)	1:211:A:GLU:HB2	1:208:A:LEU:HD11	3	0.18
(1,1532)	1:158:A:LYS:HB2	1:155:A:ILE:HA	10	0.18
(1,1525)	1:155:A:ILE:HB	1:156:A:PRO:HD2	2	0.18
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	1	0.18
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	10	0.18
(1,1392)	1:158:A:LYS:HE2	1:148:A:TRP:HA	1	0.18
(1,1375)	1:144:A:LEU:HD22	1:153:A:LEU:HD12	3	0.18
(1,1375)	1:144:A:LEU:HD21	1:153:A:LEU:HD12	13	0.18
(1,1362)	1:208:A:LEU:HD21	1:125:A:CYS:HA	14	0.18
(1,1347)	1:122:A:LEU:HB3	1:122:A:LEU:HG	4	0.18
(1,1347)	1:122:A:LEU:HB3	1:122:A:LEU:HG	15	0.18
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	10	0.18
(1,1314)	1:208:A:LEU:HD12	1:125:A:CYS:HA	6	0.18
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	2	0.18
(1,1245)	1:158:A:LYS:HE2	1:158:A:LYS:HD2	14	0.18
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	11	0.18
(1,1089)	1:212:A:GLU:HG2	1:212:A:GLU:HA	10	0.18
(1,1083)	1:135:A:ASP:HA	1:135:A:ASP:HB3	14	0.18
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	14	0.18
(1,1043)	1:145:A:GLN:HA	1:111:A:MET:HG3	5	0.18
(1,856)	1:158:A:LYS:HE2	1:158:A:LYS:H	15	0.18
(1,834)	1:115:A:LEU:HD12	1:116:A:ARG:H	8	0.18
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	7	0.18
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	8	0.18
(1,755)	1:209:A:PHE:H	1:208:A:LEU:HD21	6	0.18
(1,712)	1:199:A:LYS:HE2	1:199:A:LYS:H	12	0.18
(1,693)	1:162:A:ALA:HB3	1:161:A:MET:H	4	0.18
(1,693)	1:162:A:ALA:HB3	1:161:A:MET:H	6	0.18
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	9	0.18
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	13	0.18
(1,667)	1:144:A:LEU:HD21	1:144:A:LEU:H	13	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:125:A:CYS:H	1:124:A:ASP:HB3	2	0.18
(1,614)	1:188:A:VAL:H	1:188:A:VAL:HG13	9	0.18
(1,572)	1:230:A:PRO:HA	1:231:A:GLY:H	14	0.18
(1,564)	1:154:A:SER:H	1:154:A:SER:HB2	13	0.18
(1,457)	1:153:A:LEU:HD11	1:154:A:SER:H	4	0.18
(1,443)	1:181:A:ARG:HB2	1:182:A:SER:H	2	0.18
(1,443)	1:181:A:ARG:HB2	1:182:A:SER:H	4	0.18
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	6	0.18
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD12	14	0.18
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG21	1	0.18
(1,215)	1:127:A:GLY:HA2	1:127:A:GLY:H	9	0.18
(1,199)	1:175:A:ALA:HB3	1:178:A:ASP:H	9	0.18
(1,199)	1:175:A:ALA:HB1	1:178:A:ASP:H	13	0.18
(1,108)	1:157:A:VAL:HG21	1:160:A:ARG:H	10	0.18
(1,80)	1:202:A:ILE:HD11	1:201:A:LEU:H	8	0.18
(1,80)	1:202:A:ILE:HD11	1:201:A:LEU:H	15	0.18
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	10	0.18
(1,1842)	1:194:A:TRP:HZ3	1:191:A:VAL:HB	13	0.17
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	9	0.17
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD11	13	0.17
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	3	0.17
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	6	0.17
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	9	0.17
(1,1719)	1:194:A:TRP:HZ3	1:191:A:VAL:HG12	3	0.17
(1,1700)	1:116:A:ARG:HG2	1:116:A:ARG:HB2	9	0.17
(1,1639)	1:140:A:ARG:HB3	1:143:A:LEU:HB2	2	0.17
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	9	0.17
(1,1578)	1:203:A:ALA:HB2	1:206:A:ARG:HD3	10	0.17
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	15	0.17
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	1	0.17
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	12	0.17
(1,1530)	1:199:A:LYS:HA	1:199:A:LYS:HD2	13	0.17
(1,1519)	1:184:A:MET:HA	1:184:A:MET:HG2	1	0.17
(1,1497)	1:117:A:PRO:HD3	1:165:A:VAL:HG22	15	0.17
(1,1440)	1:200:A:ARG:HD2	1:200:A:ARG:HG3	15	0.17
(1,1428)	1:205:A:LYS:HG3	1:173:A:TRP:HZ3	2	0.17
(1,1418)	1:179:A:ILE:HA	1:179:A:ILE:HB	6	0.17
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	8	0.17
(1,1347)	1:122:A:LEU:HB3	1:122:A:LEU:HG	8	0.17
(1,1319)	1:145:A:GLN:HG2	1:145:A:GLN:HA	5	0.17
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	1	0.17
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	6	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	15	0.17
(1,1283)	1:200:A:ARG:H	1:199:A:LYS:HB2	15	0.17
(1,1234)	1:208:A:LEU:HD12	1:205:A:LYS:HE2	12	0.17
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	7	0.17
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	10	0.17
(1,1152)	1:206:A:ARG:HB3	1:206:A:ARG:HG2	14	0.17
(1,1129)	1:161:A:MET:HG3	1:161:A:MET:HB3	6	0.17
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	1	0.17
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	7	0.17
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	8	0.17
(1,1030)	1:156:A:PRO:HD2	1:155:A:ILE:HG13	14	0.17
(1,967)	1:111:A:MET:HE3	1:148:A:TRP:HA	7	0.17
(1,864)	1:152:A:LYS:H	1:152:A:LYS:HG3	7	0.17
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	2	0.17
(1,809)	1:108:A:GLU:H	1:107:A:SER:HA	4	0.17
(1,751)	1:136:A:ASP:HB3	1:136:A:ASP:H	3	0.17
(1,741)	1:191:A:VAL:HG22	1:195:A:MET:H	5	0.17
(1,718)	1:229:A:ILE:H	1:228:A:THR:H	4	0.17
(1,693)	1:162:A:ALA:HB2	1:161:A:MET:H	14	0.17
(1,656)	1:194:A:TRP:HB3	1:194:A:TRP:H	4	0.17
(1,636)	1:220:A:ALA:H	1:219:A:SER:HA	12	0.17
(1,608)	1:200:A:ARG:H	1:199:A:LYS:HB2	1	0.17
(1,608)	1:200:A:ARG:H	1:199:A:LYS:HB2	3	0.17
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	8	0.17
(1,509)	1:179:A:ILE:HG23	1:164:A:LEU:H	11	0.17
(1,509)	1:179:A:ILE:HG22	1:164:A:LEU:H	12	0.17
(1,468)	1:122:A:LEU:HD12	1:125:A:CYS:H	12	0.17
(1,373)	1:179:A:ILE:HG23	1:182:A:SER:H	9	0.17
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	6	0.17
(1,215)	1:127:A:GLY:HA2	1:127:A:GLY:H	7	0.17
(1,214)	1:227:A:HIS:H	1:227:A:HIS:HB2	11	0.17
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	7	0.17
(1,108)	1:157:A:VAL:HG21	1:160:A:ARG:H	5	0.17
(1,81)	1:203:A:ALA:HB2	1:200:A:ARG:H	2	0.17
(1,73)	1:148:A:TRP:H	1:149:A:ALA:HB2	10	0.17
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	12	0.17
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG11	15	0.17
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD12	4	0.17
(1,43)	1:165:A:VAL:HG23	1:117:A:PRO:HB3	11	0.17
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	11	0.17
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	6	0.16
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD13	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	10	0.16
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	13	0.16
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	7	0.16
(1,1739)	1:145:A:GLN:HG2	1:145:A:GLN:HE22	4	0.16
(1,1726)	1:118:A:LEU:HG	1:115:A:LEU:HD11	11	0.16
(1,1706)	1:154:A:SER:HB2	1:156:A:PRO:HD2	5	0.16
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	3	0.16
(1,1681)	1:152:A:LYS:HG2	1:152:A:LYS:HB2	5	0.16
(1,1608)	1:116:A:ARG:HG2	1:116:A:ARG:HA	4	0.16
(1,1571)	1:137:A:ILE:HG21	1:141:A:LEU:HB3	3	0.16
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	8	0.16
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	11	0.16
(1,1478)	1:175:A:ALA:HB1	1:167:A:GLU:HA	9	0.16
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	11	0.16
(1,1468)	1:198:A:VAL:HA	1:201:A:LEU:HB2	7	0.16
(1,1441)	1:148:A:TRP:HB3	1:145:A:GLN:HA	1	0.16
(1,1397)	1:163:A:LEU:HA	1:163:A:LEU:HD23	12	0.16
(1,1386)	1:203:A:ALA:HA	1:206:A:ARG:HG2	7	0.16
(1,1380)	1:205:A:LYS:HG3	1:173:A:TRP:HH2	8	0.16
(1,1359)	1:225:A:LYS:HB2	1:225:A:LYS:HE2	8	0.16
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	4	0.16
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	11	0.16
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	3	0.16
(1,1176)	1:159:A:LYS:HA	1:159:A:LYS:HD3	13	0.16
(1,1174)	1:148:A:TRP:HB3	1:111:A:MET:HG3	11	0.16
(1,1129)	1:161:A:MET:HG3	1:161:A:MET:HB3	5	0.16
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	11	0.16
(1,1099)	1:206:A:ARG:HB3	1:209:A:PHE:HD2	15	0.16
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	9	0.16
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	13	0.16
(1,1033)	1:111:A:MET:HA	1:111:A:MET:HE1	11	0.16
(1,1024)	1:122:A:LEU:HD11	1:134:A:CYS:HA	15	0.16
(1,1010)	1:168:A:LEU:HD22	1:165:A:VAL:HG12	14	0.16
(1,998)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	1	0.16
(1,953)	1:158:A:LYS:HE2	1:153:A:LEU:HB2	8	0.16
(1,947)	1:111:A:MET:HE1	1:148:A:TRP:HB2	3	0.16
(1,922)	1:218:A:LYS:HG2	1:218:A:LYS:HB3	5	0.16
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	3	0.16
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	15	0.16
(1,872)	1:176:A:ALA:HB2	1:173:A:TRP:H	13	0.16
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	10	0.16
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	1	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	2	0.16
(1,656)	1:194:A:TRP:HB3	1:194:A:TRP:H	1	0.16
(1,593)	1:187:A:HIS:HB2	1:188:A:VAL:H	9	0.16
(1,570)	1:162:A:ALA:HB1	1:164:A:LEU:H	7	0.16
(1,552)	1:108:A:GLU:HB3	1:108:A:GLU:H	4	0.16
(1,540)	1:129:A:THR:HG1	1:133:A:VAL:H	6	0.16
(1,540)	1:129:A:THR:HG1	1:133:A:VAL:H	8	0.16
(1,483)	1:212:A:GLU:HB3	1:213:A:ALA:H	7	0.16
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	2	0.16
(1,378)	1:149:A:ALA:HB3	1:146:A:GLU:H	5	0.16
(1,349)	1:191:A:VAL:HG22	1:184:A:MET:H	13	0.16
(1,298)	1:181:A:ARG:H	1:178:A:ASP:H	12	0.16
(1,283)	1:116:A:ARG:HG2	1:116:A:ARG:H	8	0.16
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	4	0.16
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB1	6	0.16
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB2	13	0.16
(1,108)	1:157:A:VAL:HG21	1:160:A:ARG:H	14	0.16
(1,81)	1:203:A:ALA:HB3	1:200:A:ARG:H	12	0.16
(1,71)	1:142:A:ALA:HB2	1:144:A:LEU:H	2	0.16
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD13	5	0.16
(1,38)	1:157:A:VAL:HG13	1:161:A:MET:HG3	3	0.16
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	4	0.16
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	9	0.16
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	14	0.16
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	15	0.16
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD12	4	0.15
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD13	6	0.15
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	8	0.15
(1,1745)	1:179:A:ILE:HG22	1:164:A:LEU:HB3	12	0.15
(1,1739)	1:145:A:GLN:HG2	1:145:A:GLN:HE22	2	0.15
(1,1739)	1:145:A:GLN:HG2	1:145:A:GLN:HE22	8	0.15
(1,1676)	1:206:A:ARG:HD2	1:206:A:ARG:HG2	13	0.15
(1,1652)	1:131:A:LYS:HD3	1:131:A:LYS:HB3	4	0.15
(1,1634)	1:161:A:MET:HG3	1:161:A:MET:HA	6	0.15
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	10	0.15
(1,1616)	1:208:A:LEU:HD12	1:125:A:CYS:HB2	6	0.15
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	5	0.15
(1,1607)	1:158:A:LYS:HB3	1:158:A:LYS:HD2	9	0.15
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	6	0.15
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	11	0.15
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	2	0.15
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	4	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	5	0.15
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	10	0.15
(1,1554)	1:203:A:ALA:HA	1:206:A:ARG:HD2	4	0.15
(1,1510)	1:164:A:LEU:HA	1:167:A:GLU:HG2	11	0.15
(1,1475)	1:183:A:LEU:HD23	1:179:A:ILE:HB	12	0.15
(1,1436)	1:116:A:ARG:HD2	1:116:A:ARG:HB2	4	0.15
(1,1428)	1:205:A:LYS:HG3	1:173:A:TRP:HZ3	6	0.15
(1,1425)	1:121:A:ALA:HB1	1:122:A:LEU:HD12	5	0.15
(1,1322)	1:156:A:PRO:HD3	1:156:A:PRO:HB3	14	0.15
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	8	0.15
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	7	0.15
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	8	0.15
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	13	0.15
(1,1192)	1:158:A:LYS:HA	1:161:A:MET:HB3	6	0.15
(1,1180)	1:181:A:ARG:HB2	1:181:A:ARG:HG2	8	0.15
(1,1180)	1:181:A:ARG:HB2	1:181:A:ARG:HG2	11	0.15
(1,1175)	1:165:A:VAL:HA	1:165:A:VAL:HB	10	0.15
(1,1136)	1:108:A:GLU:HB3	1:108:A:GLU:HA	9	0.15
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	5	0.15
(1,1105)	1:138:A:SER:HB2	1:138:A:SER:HA	14	0.15
(1,1103)	1:194:A:TRP:HE3	1:143:A:LEU:HB3	2	0.15
(1,1076)	1:204:A:GLU:HB2	1:204:A:GLU:HA	15	0.15
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	10	0.15
(1,1008)	1:164:A:LEU:HB3	1:161:A:MET:HE3	11	0.15
(1,975)	1:194:A:TRP:HA	1:143:A:LEU:HB2	9	0.15
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD13	11	0.15
(1,915)	1:199:A:LYS:HE2	1:199:A:LYS:HG2	10	0.15
(1,901)	1:202:A:ILE:HD11	1:203:A:ALA:H	8	0.15
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	4	0.15
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	6	0.15
(1,795)	1:191:A:VAL:HG23	1:194:A:TRP:H	4	0.15
(1,752)	1:168:A:LEU:H	1:168:A:LEU:HD11	9	0.15
(1,693)	1:162:A:ALA:HB1	1:161:A:MET:H	15	0.15
(1,683)	1:140:A:ARG:H	1:137:A:ILE:H	9	0.15
(1,660)	1:212:A:GLU:H	1:211:A:GLU:HB3	6	0.15
(1,656)	1:194:A:TRP:HB3	1:194:A:TRP:H	3	0.15
(1,570)	1:162:A:ALA:HB3	1:164:A:LEU:H	6	0.15
(1,552)	1:108:A:GLU:HB3	1:108:A:GLU:H	13	0.15
(1,519)	1:210:A:SER:H	1:211:A:GLU:H	4	0.15
(1,460)	1:192:A:SER:H	1:193:A:GLN:H	9	0.15
(1,382)	1:193:A:GLN:H	1:193:A:GLN:HG2	9	0.15
(1,299)	1:181:A:ARG:HG3	1:181:A:ARG:H	13	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD11	6	0.15
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	2	0.15
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG21	2	0.15
(1,234)	1:191:A:VAL:HG23	1:192:A:SER:H	3	0.15
(1,213)	1:219:A:SER:H	1:220:A:ALA:HA	15	0.15
(1,199)	1:175:A:ALA:HB1	1:178:A:ASP:H	3	0.15
(1,199)	1:175:A:ALA:HB2	1:178:A:ASP:H	8	0.15
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD22	8	0.15
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB1	11	0.15
(1,129)	1:168:A:LEU:H	1:165:A:VAL:HG23	11	0.15
(1,119)	1:183:A:LEU:HD22	1:183:A:LEU:H	8	0.15
(1,73)	1:148:A:TRP:H	1:149:A:ALA:HB1	15	0.15
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG13	13	0.15
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	1	0.15
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	2	0.15
(1,1842)	1:194:A:TRP:HZ3	1:191:A:VAL:HB	3	0.14
(1,1842)	1:194:A:TRP:HZ3	1:191:A:VAL:HB	9	0.14
(1,1739)	1:145:A:GLN:HG2	1:145:A:GLN:HE22	12	0.14
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	6	0.14
(1,1683)	1:141:A:LEU:HA	1:144:A:LEU:HB3	1	0.14
(1,1681)	1:152:A:LYS:HG2	1:152:A:LYS:HB2	4	0.14
(1,1681)	1:152:A:LYS:HG2	1:152:A:LYS:HB2	12	0.14
(1,1640)	1:202:A:ILE:HG22	1:206:A:ARG:HD2	9	0.14
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	5	0.14
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	7	0.14
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	8	0.14
(1,1571)	1:137:A:ILE:HG23	1:141:A:LEU:HB3	7	0.14
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	7	0.14
(1,1546)	1:179:A:ILE:HG13	1:179:A:ILE:HB	4	0.14
(1,1510)	1:164:A:LEU:HA	1:167:A:GLU:HG2	12	0.14
(1,1501)	1:158:A:LYS:HB3	1:148:A:TRP:HZ3	5	0.14
(1,1501)	1:158:A:LYS:HB3	1:148:A:TRP:HZ3	6	0.14
(1,1461)	1:183:A:LEU:HA	1:183:A:LEU:HB2	4	0.14
(1,1455)	1:148:A:TRP:HE3	1:148:A:TRP:HA	7	0.14
(1,1441)	1:148:A:TRP:HB3	1:145:A:GLN:HA	7	0.14
(1,1418)	1:179:A:ILE:HA	1:179:A:ILE:HB	10	0.14
(1,1402)	1:136:A:ASP:HB3	1:132:A:GLN:HG2	15	0.14
(1,1324)	1:136:A:ASP:HB3	1:133:A:VAL:HG22	1	0.14
(1,1314)	1:208:A:LEU:HD11	1:125:A:CYS:HA	4	0.14
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	5	0.14
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	2	0.14
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	6	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1264)	1:158:A:LYS:HG2	1:153:A:LEU:HB3	8	0.14
(1,1186)	1:159:A:LYS:HB2	1:159:A:LYS:HD3	2	0.14
(1,1184)	1:154:A:SER:HA	1:155:A:ILE:HG13	4	0.14
(1,1089)	1:212:A:GLU:HG2	1:212:A:GLU:HA	11	0.14
(1,1083)	1:135:A:ASP:HA	1:135:A:ASP:HB3	15	0.14
(1,998)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	6	0.14
(1,998)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	8	0.14
(1,970)	1:187:A:HIS:HB3	1:183:A:LEU:HA	4	0.14
(1,915)	1:199:A:LYS:HE2	1:199:A:LYS:HG2	6	0.14
(1,901)	1:202:A:ILE:HD13	1:203:A:ALA:H	10	0.14
(1,878)	1:184:A:MET:HG3	1:182:A:SER:H	13	0.14
(1,872)	1:176:A:ALA:HB1	1:173:A:TRP:H	15	0.14
(1,827)	1:152:A:LYS:HG2	1:151:A:GLY:H	13	0.14
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	9	0.14
(1,712)	1:199:A:LYS:HE2	1:199:A:LYS:H	13	0.14
(1,667)	1:144:A:LEU:HD22	1:144:A:LEU:H	3	0.14
(1,570)	1:162:A:ALA:HB2	1:164:A:LEU:H	14	0.14
(1,354)	1:157:A:VAL:H	1:157:A:VAL:HB	10	0.14
(1,329)	1:193:A:GLN:H	1:194:A:TRP:HE1	10	0.14
(1,298)	1:181:A:ARG:H	1:178:A:ASP:H	6	0.14
(1,276)	1:141:A:LEU:H	1:144:A:LEU:HD11	12	0.14
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	4	0.14
(1,252)	1:161:A:MET:H	1:157:A:VAL:HG21	11	0.14
(1,243)	1:159:A:LYS:HD3	1:159:A:LYS:H	10	0.14
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB3	8	0.14
(1,138)	1:167:A:GLU:H	1:166:A:GLN:HE22	12	0.14
(1,113)	1:194:A:TRP:HE1	1:191:A:VAL:HG13	2	0.14
(1,102)	1:162:A:ALA:HB2	1:166:A:GLN:HE22	13	0.14
(1,81)	1:203:A:ALA:HB3	1:200:A:ARG:H	3	0.14
(1,66)	1:174:A:ASP:HB3	1:173:A:TRP:H	5	0.14
(1,17)	1:132:A:GLN:HA	1:132:A:GLN:H	13	0.14
(1,1842)	1:194:A:TRP:HZ3	1:191:A:VAL:HB	10	0.13
(1,1829)	1:194:A:TRP:HE3	1:144:A:LEU:HD13	3	0.13
(1,1825)	1:187:A:HIS:HD1	1:183:A:LEU:HG	1	0.13
(1,1818)	1:148:A:TRP:HZ3	1:144:A:LEU:HD11	5	0.13
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	5	0.13
(1,1771)	1:193:A:GLN:HB2	1:194:A:TRP:HE3	10	0.13
(1,1717)	1:158:A:LYS:HA	1:161:A:MET:HG3	11	0.13
(1,1691)	1:172:A:ARG:HD2	1:172:A:ARG:HA	12	0.13
(1,1681)	1:152:A:LYS:HG2	1:152:A:LYS:HB2	11	0.13
(1,1652)	1:131:A:LYS:HD3	1:131:A:LYS:HB3	3	0.13
(1,1613)	1:165:A:VAL:HA	1:168:A:LEU:HB3	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1608)	1:116:A:ARG:HG2	1:116:A:ARG:HA	2	0.13
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	1	0.13
(1,1579)	1:187:A:HIS:HB3	1:187:A:HIS:HA	13	0.13
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	3	0.13
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	6	0.13
(1,1532)	1:158:A:LYS:HB2	1:155:A:ILE:HA	4	0.13
(1,1519)	1:184:A:MET:HA	1:184:A:MET:HG2	7	0.13
(1,1489)	1:137:A:ILE:HD13	1:134:A:CYS:HB2	6	0.13
(1,1441)	1:148:A:TRP:HB3	1:145:A:GLN:HA	10	0.13
(1,1435)	1:153:A:LEU:HA	1:190:A:GLU:HB2	9	0.13
(1,1435)	1:153:A:LEU:HA	1:190:A:GLU:HB2	11	0.13
(1,1414)	1:148:A:TRP:HZ3	1:158:A:LYS:HG2	13	0.13
(1,1404)	1:158:A:LYS:HB3	1:158:A:LYS:HA	10	0.13
(1,1397)	1:163:A:LEU:HA	1:163:A:LEU:HD21	14	0.13
(1,1380)	1:205:A:LYS:HG3	1:173:A:TRP:HH2	1	0.13
(1,1364)	1:218:A:LYS:HA	1:218:A:LYS:HG3	2	0.13
(1,1355)	1:206:A:ARG:HD2	1:209:A:PHE:HD2	3	0.13
(1,1294)	1:116:A:ARG:HD2	1:116:A:ARG:HA	1	0.13
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	13	0.13
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	1	0.13
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	3	0.13
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	5	0.13
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	10	0.13
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	14	0.13
(1,1256)	1:190:A:GLU:HB3	1:187:A:HIS:HA	3	0.13
(1,1234)	1:208:A:LEU:HD12	1:205:A:LYS:HE2	3	0.13
(1,1227)	1:181:A:ARG:HD3	1:181:A:ARG:HG2	3	0.13
(1,1217)	1:130:A:ARG:HA	1:130:A:ARG:HD3	12	0.13
(1,1192)	1:158:A:LYS:HA	1:161:A:MET:HB3	5	0.13
(1,1179)	1:141:A:LEU:HA	1:141:A:LEU:HD22	4	0.13
(1,1152)	1:206:A:ARG:HB3	1:206:A:ARG:HG2	3	0.13
(1,1152)	1:206:A:ARG:HB3	1:206:A:ARG:HG2	4	0.13
(1,1150)	1:114:A:VAL:HA	1:114:A:VAL:HB	12	0.13
(1,1136)	1:108:A:GLU:HB3	1:108:A:GLU:HA	4	0.13
(1,1068)	1:158:A:LYS:HD2	1:148:A:TRP:HZ2	14	0.13
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	4	0.13
(1,1002)	1:141:A:LEU:HD21	1:142:A:ALA:HA	3	0.13
(1,998)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	12	0.13
(1,975)	1:194:A:TRP:HA	1:143:A:LEU:HB2	2	0.13
(1,974)	1:181:A:ARG:HB3	1:181:A:ARG:HD2	12	0.13
(1,967)	1:111:A:MET:HE2	1:148:A:TRP:HA	6	0.13
(1,833)	1:160:A:ARG:HD2	1:160:A:ARG:H	8	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	4	0.13
(1,809)	1:108:A:GLU:H	1:107:A:SER:HA	9	0.13
(1,799)	1:140:A:ARG:H	1:140:A:ARG:HB2	5	0.13
(1,741)	1:191:A:VAL:HG21	1:195:A:MET:H	11	0.13
(1,741)	1:191:A:VAL:HG21	1:195:A:MET:H	14	0.13
(1,693)	1:162:A:ALA:HB1	1:161:A:MET:H	2	0.13
(1,693)	1:162:A:ALA:HB2	1:161:A:MET:H	9	0.13
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	6	0.13
(1,667)	1:144:A:LEU:HD22	1:144:A:LEU:H	6	0.13
(1,667)	1:144:A:LEU:HD23	1:144:A:LEU:H	8	0.13
(1,667)	1:144:A:LEU:HD22	1:144:A:LEU:H	9	0.13
(1,637)	1:125:A:CYS:H	1:124:A:ASP:HB3	13	0.13
(1,575)	1:139:A:ARG:HG2	1:139:A:ARG:H	6	0.13
(1,547)	1:236:A:SER:HB3	1:236:A:SER:H	7	0.13
(1,533)	1:181:A:ARG:HB2	1:181:A:ARG:H	2	0.13
(1,533)	1:181:A:ARG:HB2	1:181:A:ARG:H	9	0.13
(1,515)	1:152:A:LYS:HA	1:153:A:LEU:H	15	0.13
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	15	0.13
(1,485)	1:153:A:LEU:HD11	1:194:A:TRP:HE1	3	0.13
(1,373)	1:179:A:ILE:HG21	1:182:A:SER:H	1	0.13
(1,372)	1:145:A:GLN:HA	1:145:A:GLN:HE22	14	0.13
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	11	0.13
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	14	0.13
(1,304)	1:226:A:ASN:H	1:226:A:ASN:HB2	2	0.13
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	3	0.13
(1,193)	1:234:A:GLN:H	1:234:A:GLN:HA	2	0.13
(1,193)	1:234:A:GLN:H	1:234:A:GLN:HA	3	0.13
(1,193)	1:234:A:GLN:H	1:234:A:GLN:HA	6	0.13
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	6	0.13
(1,71)	1:142:A:ALA:HB1	1:144:A:LEU:H	4	0.13
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG13	14	0.13
(1,2)	1:155:A:ILE:HG23	1:159:A:LYS:H	15	0.13
(2,3)	1:121:A:ALA:H	1:117:A:PRO:O	8	0.12
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	2	0.12
(1,1760)	1:204:A:GLU:HG3	1:204:A:GLU:HA	15	0.12
(1,1739)	1:145:A:GLN:HG2	1:145:A:GLN:HE22	9	0.12
(1,1734)	1:159:A:LYS:HA	1:155:A:ILE:HG21	4	0.12
(1,1697)	1:177:A:ASP:HA	1:179:A:ILE:HD13	11	0.12
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	9	0.12
(1,1682)	1:168:A:LEU:HD21	1:165:A:VAL:HB	6	0.12
(1,1681)	1:152:A:LYS:HG2	1:152:A:LYS:HB2	7	0.12
(1,1633)	1:159:A:LYS:HE2	1:155:A:ILE:HB	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	1	0.12
(1,1594)	1:174:A:ASP:HA	1:174:A:ASP:HB3	2	0.12
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	14	0.12
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	14	0.12
(1,1539)	1:202:A:ILE:HG21	1:206:A:ARG:HD3	1	0.12
(1,1532)	1:158:A:LYS:HB2	1:155:A:ILE:HA	11	0.12
(1,1502)	1:158:A:LYS:HD2	1:158:A:LYS:HG2	12	0.12
(1,1441)	1:148:A:TRP:HB3	1:145:A:GLN:HA	15	0.12
(1,1429)	1:141:A:LEU:HD22	1:144:A:LEU:HD12	14	0.12
(1,1428)	1:205:A:LYS:HG3	1:173:A:TRP:HZ3	15	0.12
(1,1418)	1:179:A:ILE:HA	1:179:A:ILE:HB	4	0.12
(1,1392)	1:158:A:LYS:HE2	1:148:A:TRP:HA	11	0.12
(1,1345)	1:199:A:LYS:HD2	1:199:A:LYS:HB2	1	0.12
(1,1343)	1:230:A:PRO:HD2	1:229:A:ILE:HA	3	0.12
(1,1339)	1:136:A:ASP:HB3	1:133:A:VAL:HB	15	0.12
(1,1319)	1:145:A:GLN:HG2	1:145:A:GLN:HA	6	0.12
(1,1271)	1:229:A:ILE:HG13	1:229:A:ILE:HA	11	0.12
(1,1227)	1:181:A:ARG:HD3	1:181:A:ARG:HG2	9	0.12
(1,1083)	1:135:A:ASP:HA	1:135:A:ASP:HB3	11	0.12
(1,1068)	1:158:A:LYS:HD2	1:148:A:TRP:HZ2	6	0.12
(1,1052)	1:154:A:SER:HA	1:156:A:PRO:HD3	11	0.12
(1,1016)	1:165:A:VAL:HG22	1:161:A:MET:HE1	4	0.12
(1,975)	1:194:A:TRP:HA	1:143:A:LEU:HB2	6	0.12
(1,941)	1:111:A:MET:HB3	1:111:A:MET:HA	10	0.12
(1,926)	1:186:A:ASP:HB2	1:186:A:ASP:HA	6	0.12
(1,864)	1:152:A:LYS:H	1:152:A:LYS:HG3	15	0.12
(1,844)	1:207:A:SER:H	1:207:A:SER:HB3	5	0.12
(1,844)	1:207:A:SER:H	1:207:A:SER:HB3	6	0.12
(1,799)	1:140:A:ARG:H	1:140:A:ARG:HB2	11	0.12
(1,730)	1:158:A:LYS:HG2	1:153:A:LEU:H	8	0.12
(1,667)	1:144:A:LEU:HD23	1:144:A:LEU:H	7	0.12
(1,667)	1:144:A:LEU:HD23	1:144:A:LEU:H	11	0.12
(1,660)	1:212:A:GLU:H	1:211:A:GLU:HB3	2	0.12
(1,641)	1:179:A:ILE:HD12	1:178:A:ASP:H	9	0.12
(1,618)	1:191:A:VAL:H	1:190:A:GLU:HB3	7	0.12
(1,512)	1:159:A:LYS:HE2	1:160:A:ARG:H	12	0.12
(1,460)	1:192:A:SER:H	1:193:A:GLN:H	8	0.12
(1,460)	1:192:A:SER:H	1:193:A:GLN:H	12	0.12
(1,369)	1:214:A:ALA:HB1	1:215:A:ASN:H	6	0.12
(1,329)	1:193:A:GLN:H	1:194:A:TRP:HE1	3	0.12
(1,329)	1:193:A:GLN:H	1:194:A:TRP:HE1	6	0.12
(1,329)	1:193:A:GLN:H	1:194:A:TRP:HE1	12	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	7	0.12
(1,289)	1:111:A:MET:HB3	1:112:A:GLU:H	4	0.12
(1,261)	1:151:A:GLY:H	1:152:A:LYS:HB3	5	0.12
(1,150)	1:112:A:GLU:HG2	1:112:A:GLU:H	10	0.12
(1,148)	1:137:A:ILE:HG21	1:141:A:LEU:H	10	0.12
(1,112)	1:140:A:ARG:HB3	1:140:A:ARG:H	4	0.12
(1,86)	1:208:A:LEU:HB3	1:208:A:LEU:H	8	0.12
(1,73)	1:148:A:TRP:H	1:149:A:ALA:HB2	13	0.12
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	11	0.12
(1,71)	1:142:A:ALA:HB3	1:144:A:LEU:H	14	0.12
(1,70)	1:158:A:LYS:HG2	1:157:A:VAL:H	14	0.12
(1,61)	1:147:A:GLN:HE21	1:147:A:GLN:H	2	0.12
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD12	1	0.12
(1,41)	1:208:A:LEU:HB3	1:211:A:GLU:HB3	12	0.12
(2,28)	1:204:A:GLU:H	1:200:A:ARG:O	14	0.11
(1,1839)	1:114:A:VAL:HB	1:148:A:TRP:HZ2	14	0.11
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	12	0.11
(1,1779)	1:111:A:MET:HB3	1:148:A:TRP:HD1	6	0.11
(1,1773)	1:187:A:HIS:HD1	1:190:A:GLU:HB2	13	0.11
(1,1750)	1:211:A:GLU:HA	1:211:A:GLU:HG2	14	0.11
(1,1737)	1:191:A:VAL:HG21	1:188:A:VAL:HA	4	0.11
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	5	0.11
(1,1683)	1:141:A:LEU:HA	1:144:A:LEU:HB3	15	0.11
(1,1631)	1:114:A:VAL:HA	1:117:A:PRO:HD2	5	0.11
(1,1631)	1:114:A:VAL:HA	1:117:A:PRO:HD2	12	0.11
(1,1619)	1:122:A:LEU:HD12	1:134:A:CYS:HB2	9	0.11
(1,1602)	1:206:A:ARG:HA	1:206:A:ARG:HD3	12	0.11
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	7	0.11
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	9	0.11
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	15	0.11
(1,1519)	1:184:A:MET:HA	1:184:A:MET:HG2	15	0.11
(1,1501)	1:158:A:LYS:HB3	1:148:A:TRP:HZ3	3	0.11
(1,1501)	1:158:A:LYS:HB3	1:148:A:TRP:HZ3	9	0.11
(1,1471)	1:155:A:ILE:HB	1:155:A:ILE:HG13	4	0.11
(1,1467)	1:140:A:ARG:HA	1:194:A:TRP:HB3	15	0.11
(1,1455)	1:148:A:TRP:HE3	1:148:A:TRP:HA	10	0.11
(1,1441)	1:148:A:TRP:HB3	1:145:A:GLN:HA	9	0.11
(1,1428)	1:205:A:LYS:HG3	1:173:A:TRP:HZ3	7	0.11
(1,1381)	1:186:A:ASP:HB3	1:186:A:ASP:HA	7	0.11
(1,1367)	1:111:A:MET:HA	1:111:A:MET:HG3	12	0.11
(1,1355)	1:206:A:ARG:HD2	1:209:A:PHE:HD2	4	0.11
(1,1314)	1:208:A:LEU:HD13	1:125:A:CYS:HA	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	7	0.11
(1,1290)	1:206:A:ARG:HA	1:206:A:ARG:HG2	11	0.11
(1,1272)	1:147:A:GLN:HB3	1:144:A:LEU:HA	3	0.11
(1,1269)	1:179:A:ILE:HB	1:161:A:MET:HA	6	0.11
(1,1265)	1:152:A:LYS:HA	1:152:A:LYS:HG2	11	0.11
(1,1163)	1:172:A:ARG:HB3	1:170:A:SER:HB2	6	0.11
(1,1159)	1:158:A:LYS:HE2	1:158:A:LYS:HG3	10	0.11
(1,1115)	1:152:A:LYS:HE2	1:152:A:LYS:HB3	8	0.11
(1,1092)	1:180:A:HIS:HB3	1:195:A:MET:HB2	2	0.11
(1,1024)	1:122:A:LEU:HD11	1:134:A:CYS:HA	5	0.11
(1,975)	1:194:A:TRP:HA	1:143:A:LEU:HB2	10	0.11
(1,969)	1:139:A:ARG:HD2	1:140:A:ARG:HA	14	0.11
(1,949)	1:155:A:ILE:HA	1:155:A:ILE:HG12	5	0.11
(1,941)	1:111:A:MET:HB3	1:111:A:MET:HA	4	0.11
(1,922)	1:218:A:LYS:HG2	1:218:A:LYS:HB3	2	0.11
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	10	0.11
(1,917)	1:181:A:ARG:HB2	1:181:A:ARG:HG3	12	0.11
(1,874)	1:158:A:LYS:H	1:154:A:SER:HB2	4	0.11
(1,872)	1:176:A:ALA:HB1	1:173:A:TRP:H	5	0.11
(1,872)	1:176:A:ALA:HB2	1:173:A:TRP:H	11	0.11
(1,858)	1:139:A:ARG:HD2	1:139:A:ARG:H	13	0.11
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	11	0.11
(1,842)	1:145:A:GLN:HG2	1:145:A:GLN:H	14	0.11
(1,834)	1:115:A:LEU:HD11	1:116:A:ARG:H	1	0.11
(1,831)	1:207:A:SER:H	1:206:A:ARG:HD2	14	0.11
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	7	0.11
(1,822)	1:118:A:LEU:H	1:117:A:PRO:HB3	14	0.11
(1,794)	1:144:A:LEU:HD13	1:143:A:LEU:H	11	0.11
(1,735)	1:193:A:GLN:H	1:194:A:TRP:H	11	0.11
(1,680)	1:166:A:GLN:HG2	1:166:A:GLN:H	1	0.11
(1,652)	1:159:A:LYS:HB2	1:158:A:LYS:H	8	0.11
(1,618)	1:191:A:VAL:H	1:190:A:GLU:HB3	5	0.11
(1,618)	1:191:A:VAL:H	1:190:A:GLU:HB3	11	0.11
(1,575)	1:139:A:ARG:HG2	1:139:A:ARG:H	11	0.11
(1,570)	1:162:A:ALA:HB2	1:164:A:LEU:H	12	0.11
(1,540)	1:129:A:THR:HG1	1:133:A:VAL:H	1	0.11
(1,540)	1:129:A:THR:HG1	1:133:A:VAL:H	7	0.11
(1,533)	1:181:A:ARG:HB2	1:181:A:ARG:H	4	0.11
(1,519)	1:210:A:SER:H	1:211:A:GLU:H	8	0.11
(1,504)	1:157:A:VAL:HG22	1:159:A:LYS:H	8	0.11
(1,483)	1:212:A:GLU:HB3	1:213:A:ALA:H	13	0.11
(1,460)	1:192:A:SER:H	1:193:A:GLN:H	2	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:154:A:SER:HB2	1:155:A:ILE:H	5	0.11
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	5	0.11
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	8	0.11
(1,314)	1:135:A:ASP:HB3	1:135:A:ASP:H	15	0.11
(1,305)	1:142:A:ALA:HB2	1:141:A:LEU:H	2	0.11
(1,298)	1:181:A:ARG:H	1:178:A:ASP:H	3	0.11
(1,298)	1:181:A:ARG:H	1:178:A:ASP:H	15	0.11
(1,289)	1:111:A:MET:HB3	1:112:A:GLU:H	11	0.11
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	5	0.11
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	8	0.11
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	15	0.11
(1,214)	1:227:A:HIS:H	1:227:A:HIS:HB2	13	0.11
(1,199)	1:175:A:ALA:HB3	1:178:A:ASP:H	6	0.11
(1,190)	1:125:A:CYS:H	1:208:A:LEU:HD21	2	0.11
(1,184)	1:174:A:ASP:H	1:175:A:ALA:HB3	5	0.11
(1,119)	1:183:A:LEU:HD21	1:183:A:LEU:H	10	0.11
(1,112)	1:140:A:ARG:HB3	1:140:A:ARG:H	14	0.11
(1,58)	1:144:A:LEU:H	1:144:A:LEU:HD11	11	0.11
(1,1839)	1:114:A:VAL:HB	1:148:A:TRP:HZ2	15	0.1
(1,1806)	1:148:A:TRP:HE3	1:144:A:LEU:HG	11	0.1
(1,1755)	1:156:A:PRO:HB2	1:156:A:PRO:HD2	5	0.1
(1,1696)	1:208:A:LEU:HB2	1:208:A:LEU:HA	7	0.1
(1,1683)	1:141:A:LEU:HA	1:144:A:LEU:HB3	4	0.1
(1,1652)	1:131:A:LYS:HD3	1:131:A:LYS:HB3	15	0.1
(1,1641)	1:153:A:LEU:HD11	1:145:A:GLN:HA	1	0.1
(1,1635)	1:157:A:VAL:HG12	1:153:A:LEU:HA	13	0.1
(1,1567)	1:172:A:ARG:HB3	1:172:A:ARG:HA	10	0.1
(1,1558)	1:201:A:LEU:HA	1:201:A:LEU:HB2	13	0.1
(1,1461)	1:183:A:LEU:HA	1:183:A:LEU:HB2	9	0.1
(1,1355)	1:206:A:ARG:HD2	1:209:A:PHE:HD1	1	0.1
(1,1355)	1:206:A:ARG:HD2	1:209:A:PHE:HD2	6	0.1
(1,1347)	1:122:A:LEU:HB3	1:122:A:LEU:HG	13	0.1
(1,1256)	1:190:A:GLU:HB3	1:187:A:HIS:HA	14	0.1
(1,1166)	1:111:A:MET:HE3	1:111:A:MET:HB2	8	0.1
(1,1163)	1:172:A:ARG:HB3	1:170:A:SER:HB2	15	0.1
(1,1129)	1:161:A:MET:HG3	1:161:A:MET:HB3	14	0.1
(1,1113)	1:122:A:LEU:HG	1:126:A:ARG:HB2	7	0.1
(1,1068)	1:158:A:LYS:HD2	1:148:A:TRP:HZ2	10	0.1
(1,1030)	1:156:A:PRO:HD2	1:155:A:ILE:HG13	12	0.1
(1,1027)	1:191:A:VAL:HB	1:180:A:HIS:HD1	11	0.1
(1,1000)	1:204:A:GLU:HG2	1:204:A:GLU:HA	15	0.1
(1,998)	1:117:A:PRO:HD2	1:117:A:PRO:HB2	5	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:155:A:ILE:HA	1:155:A:ILE:HG12	3	0.1
(1,941)	1:111:A:MET:HB3	1:111:A:MET:HA	11	0.1
(1,930)	1:145:A:GLN:HA	1:115:A:LEU:HD13	12	0.1
(1,926)	1:186:A:ASP:HB2	1:186:A:ASP:HA	14	0.1
(1,919)	1:167:A:GLU:HA	1:167:A:GLU:HG2	14	0.1
(1,891)	1:187:A:HIS:HB3	1:190:A:GLU:H	10	0.1
(1,726)	1:158:A:LYS:HE2	1:155:A:ILE:H	4	0.1
(1,667)	1:144:A:LEU:HD21	1:144:A:LEU:H	4	0.1
(1,667)	1:144:A:LEU:HD21	1:144:A:LEU:H	14	0.1
(1,579)	1:181:A:ARG:HG3	1:182:A:SER:H	2	0.1
(1,519)	1:210:A:SER:H	1:211:A:GLU:H	11	0.1
(1,501)	1:172:A:ARG:H	1:172:A:ARG:HD2	7	0.1
(1,493)	1:218:A:LYS:HD3	1:218:A:LYS:H	15	0.1
(1,460)	1:192:A:SER:H	1:193:A:GLN:H	13	0.1
(1,457)	1:153:A:LEU:HD12	1:154:A:SER:H	5	0.1
(1,253)	1:169:A:SER:H	1:172:A:ARG:H	1	0.1
(1,213)	1:219:A:SER:H	1:220:A:ALA:HA	9	0.1
(1,199)	1:175:A:ALA:HB2	1:178:A:ASP:H	14	0.1
(1,153)	1:168:A:LEU:HA	1:167:A:GLU:H	4	0.1
(1,153)	1:168:A:LEU:HA	1:167:A:GLU:H	5	0.1
(1,73)	1:148:A:TRP:H	1:149:A:ALA:HB2	14	0.1
(1,67)	1:190:A:GLU:H	1:191:A:VAL:HG12	2	0.1
(1,66)	1:174:A:ASP:HB3	1:173:A:TRP:H	2	0.1

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

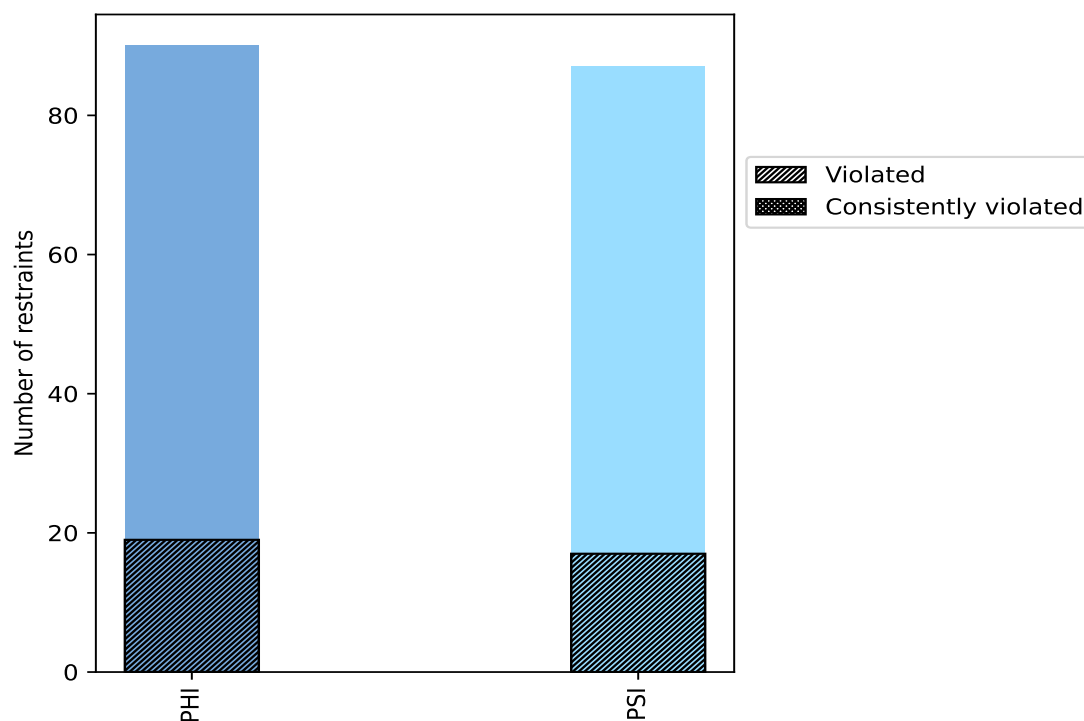
10.1 Summary of dihedral-angle violations [i](#)

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	90	50.8	19	21.1	10.7	0	0.0	0.0
PSI	87	49.2	17	19.5	9.6	0	0.0	0.0
Total	177	100.0	36	20.3	20.3	0	0.0	0.0

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

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



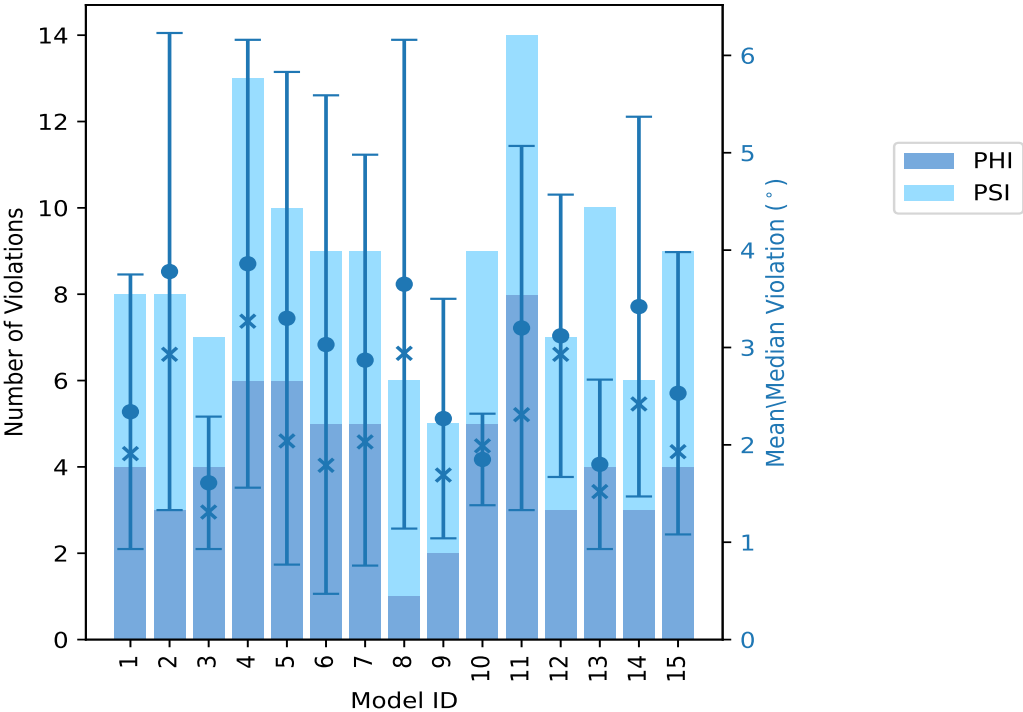
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	4	4	8	2.34	4.8	1.41	1.91
2	3	5	8	3.78	7.85	2.45	2.93
3	4	3	7	1.61	3.11	0.68	1.31
4	6	7	13	3.86	9.3	2.3	3.27
5	6	4	10	3.3	8.85	2.53	2.04
6	5	4	9	3.03	7.88	2.56	1.79
7	5	4	9	2.87	8.1	2.11	2.03
8	1	5	6	3.65	8.31	2.51	2.94
9	2	3	5	2.27	4.47	1.23	1.69
10	5	4	9	1.85	2.63	0.47	1.99
11	8	6	14	3.2	6.85	1.87	2.31
12	3	4	7	3.12	5.28	1.45	2.93
13	4	6	10	1.8	3.83	0.87	1.52
14	3	3	6	3.42	7.25	1.95	2.42
15	4	5	9	2.53	5.59	1.45	1.93

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

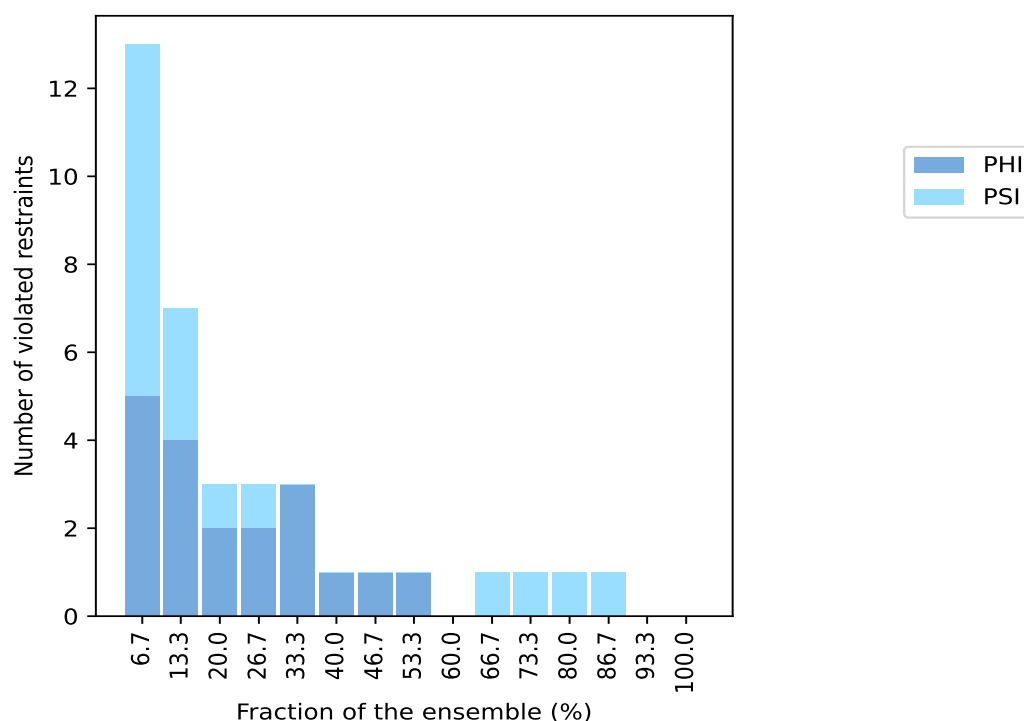
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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	%
5	8	13	1	6.7
4	3	7	2	13.3
2	1	3	3	20.0
2	1	3	4	26.7
3	0	3	5	33.3
1	0	1	6	40.0
1	0	1	7	46.7
1	0	1	8	53.3
0	0	0	9	60.0
0	1	1	10	66.7
0	1	1	11	73.3
0	1	1	12	80.0
0	1	1	13	86.7
0	0	0	14	93.3
0	0	0	15	100.0

¹ Number of models with violations

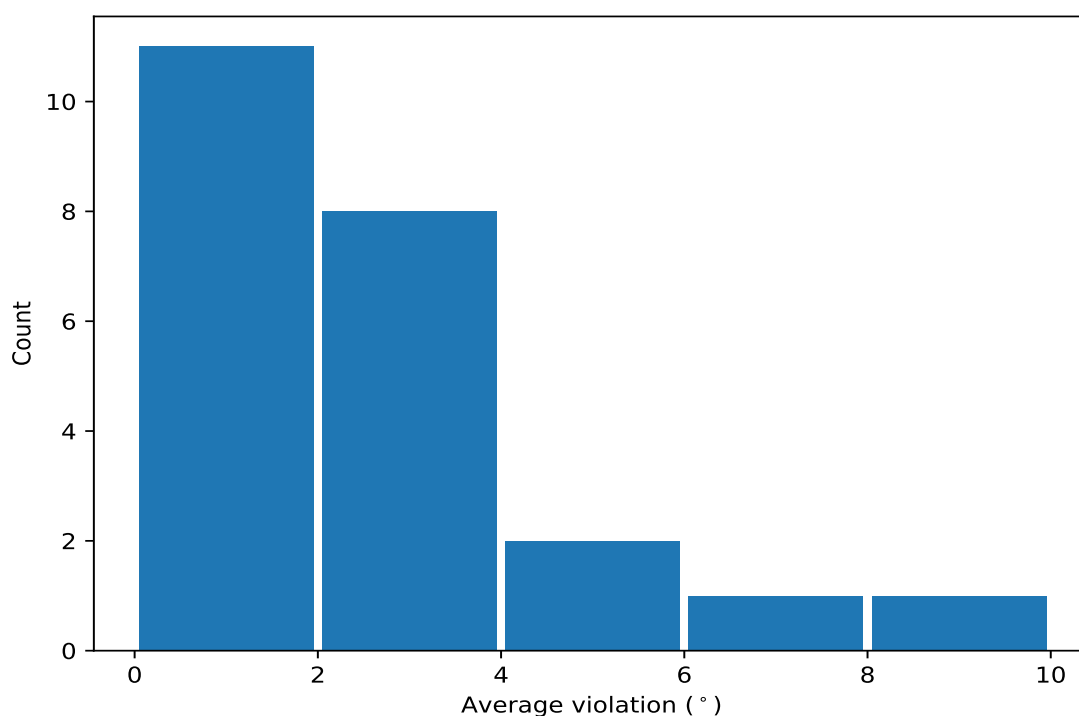
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	13	2.47	1.37	1.92
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	12	3.83	1.5	3.9
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	11	3.58	1.25	3.33
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	10	4.31	2.41	4.31
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	8	4.04	2.66	3.58
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	7	1.85	0.55	1.73
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	6	3.06	1.52	3.2
(1,39)	1:128:A:HIS:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	5	2.46	1.01	2.28
(1,127)	1:176:A:ALA:C	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	5	1.72	0.43	1.93
(1,31)	1:123:A:GLU:C	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	5	1.41	0.38	1.17
(1,79)	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	1:151:A:GLY:N	4	8.21	0.95	8.35
(1,80)	1:150:A:GLY:C	1:151:A:GLY:N	1:151:A:GLY:CA	1:151:A:GLY:C	4	6.26	0.75	6.58
(1,25)	1:120:A:GLN:C	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	4	2.42	0.58	2.33
(1,139)	1:182:A:SER:C	1:183:A:LEU:N	1:183:A:LEU:CA	1:183:A:LEU:C	3	1.34	0.2	1.31
(1,12)	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	1:115:A:LEU:N	3	1.29	0.05	1.26
(1,116)	1:169:A:SER:C	1:170:A:SER:N	1:170:A:SER:CA	1:170:A:SER:C	3	1.15	0.08	1.2
(1,4)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:MET:N	2	2.08	0.72	2.08
(1,34)	1:125:A:CYS:N	1:125:A:CYS:CA	1:125:A:CYS:C	1:126:A:ARG:N	2	2.0	0.26	2.0
(1,37)	1:127:A:GLY:C	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	2	1.78	0.7	1.78
(1,177)	1:211:A:GLU:C	1:212:A:GLU:N	1:212:A:GLU:CA	1:212:A:GLU:C	2	1.55	0.23	1.55
(1,144)	1:194:A:TRP:N	1:194:A:TRP:CA	1:194:A:TRP:C	1:195:A:MET:N	2	1.4	0.28	1.4

Continued on next page...

Continued from previous page...

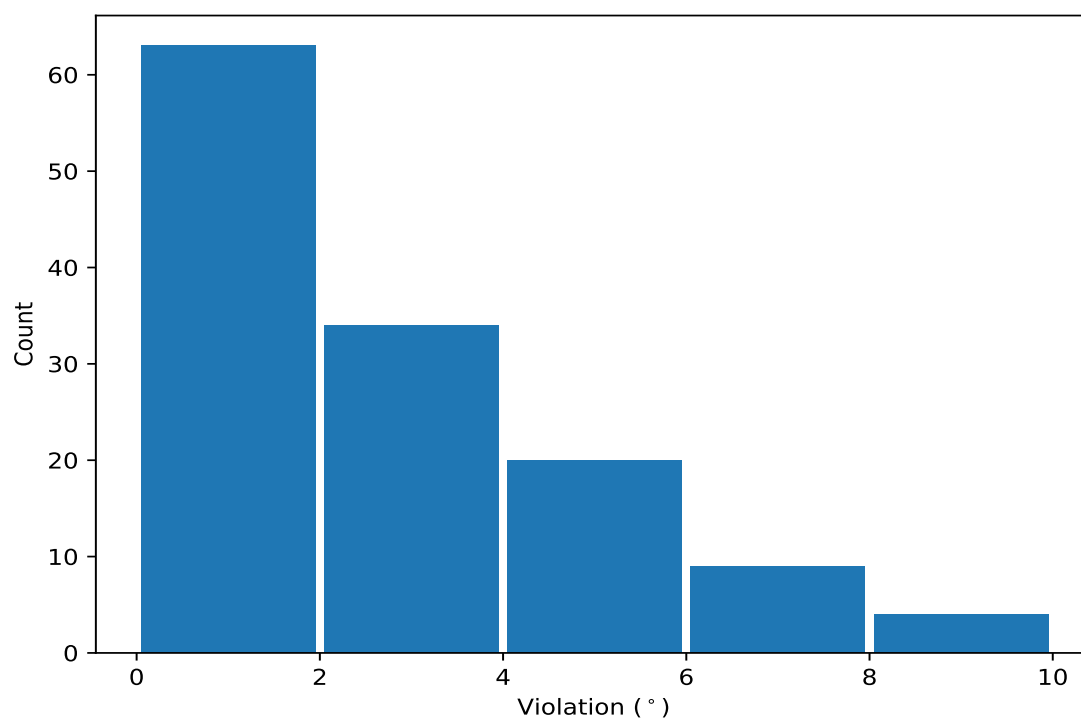
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,33)	1:124:A:ASP:C	1:125:A:CYS:N	1:125:A:CYS:CA	1:125:A:CYS:C	2	1.25	0.1	1.25
(1,143)	1:184:A:MET:C	1:185:A:VAL:N	1:185:A:VAL:CA	1:185:A:VAL:C	2	1.14	0.1	1.14

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 (°)
(1,79)	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	1:151:A:GLY:N	4	9.3
(1,79)	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	1:151:A:GLY:N	5	8.85
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	8	8.31
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	7	8.1
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	6	7.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,79)	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	1:151:A:GLY:N	2	7.85
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	6	7.4
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	14	7.25
(1,80)	1:150:A:GLY:C	1:151:A:GLY:N	1:151:A:GLY:CA	1:151:A:GLY:C	2	6.89
(1,79)	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	1:151:A:GLY:N	11	6.85
(1,80)	1:150:A:GLY:C	1:151:A:GLY:N	1:151:A:GLY:CA	1:151:A:GLY:C	5	6.67
(1,80)	1:150:A:GLY:C	1:151:A:GLY:N	1:151:A:GLY:CA	1:151:A:GLY:C	4	6.5
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	11	6.2
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	15	5.59
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	12	5.28
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	4	5.27
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	2	5.22
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	4	5.18
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	8	5.01
(1,80)	1:150:A:GLY:C	1:151:A:GLY:N	1:151:A:GLY:CA	1:151:A:GLY:C	11	4.98
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	12	4.96
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	4	4.84
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	1	4.8
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	4	4.77
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	11	4.61
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	14	4.59
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	11	4.47
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	9	4.47
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	1	4.39
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	5	4.37
(1,39)	1:128:A:HIS:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	15	4.33
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	7	4.21
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	8	4.07
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	5	3.97
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	11	3.97
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	2	3.84
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	13	3.83
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	7	3.52
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	6	3.33
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	4	3.27
(1,25)	1:120:A:GLN:C	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	12	3.27
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	15	3.12
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	3	3.11
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	13	3.04
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	12	2.93
(1,4)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:MET:N	14	2.81
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	12	2.76
(1,28)	1:122:A:LEU:N	1:122:A:LEU:CA	1:122:A:LEU:C	1:123:A:GLU:N	7	2.72
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	9	2.71
(1,25)	1:120:A:GLN:C	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	10	2.63
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	1	2.59
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	11	2.59
(1,37)	1:127:A:GLY:C	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	4	2.49
(1,39)	1:128:A:HIS:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	4	2.47
(1,176)	1:210:A:SER:N	1:210:A:SER:CA	1:210:A:SER:C	1:211:A:GLU:N	15	2.35
(1,39)	1:128:A:HIS:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	6	2.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:125:A:CYS:N	1:125:A:CYS:CA	1:125:A:CYS:C	1:126:A:ARG:N	5	2.26
(1,127)	1:176:A:ALA:C	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	4	2.23
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	10	2.21
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	10	2.11
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	3	2.07
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	1	2.04
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	14	2.03
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	10	2.03
(1,25)	1:120:A:GLN:C	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	11	2.03
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	7	2.03
(1,81)	1:151:A:GLY:N	1:151:A:GLY:CA	1:151:A:GLY:C	1:152:A:LYS:N	2	2.02
(1,127)	1:176:A:ALA:C	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	10	1.99
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	11	1.99
(1,38)	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	1:129:A:THR:N	10	1.94
(1,127)	1:176:A:ALA:C	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	14	1.93
(1,31)	1:123:A:GLU:C	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	15	1.93
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	14	1.92
(1,171)	1:207:A:SER:C	1:208:A:LEU:N	1:208:A:LEU:CA	1:208:A:LEU:C	11	1.91
(1,39)	1:128:A:HIS:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	2	1.9
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	8	1.81
(1,31)	1:123:A:GLU:C	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	5	1.81
(1,128)	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	1:178:A:ASP:N	6	1.79
(1,177)	1:211:A:GLU:C	1:212:A:GLU:N	1:212:A:GLU:CA	1:212:A:GLU:C	1	1.78
(1,137)	1:181:A:ARG:C	1:182:A:SER:N	1:182:A:SER:CA	1:182:A:SER:C	13	1.78
(1,25)	1:120:A:GLN:C	1:121:A:ALA:N	1:121:A:ALA:CA	1:121:A:ALA:C	13	1.76
(1,34)	1:125:A:CYS:N	1:125:A:CYS:CA	1:125:A:CYS:C	1:126:A:ARG:N	11	1.74
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	15	1.73
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	9	1.69
(1,144)	1:194:A:TRP:N	1:194:A:TRP:CA	1:194:A:TRP:C	1:195:A:MET:N	13	1.68
(1,139)	1:182:A:SER:C	1:183:A:LEU:N	1:183:A:LEU:CA	1:183:A:LEU:C	4	1.6
(1,52)	1:136:A:ASP:C	1:137:A:ILE:N	1:137:A:ILE:CA	1:137:A:ILE:C	7	1.57
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	5	1.42
(1,111)	1:167:A:GLU:N	1:167:A:GLU:CA	1:167:A:GLU:C	1:168:A:LEU:N	6	1.4
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	10	1.4
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	12	1.4
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	3	1.39
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	2	1.37
(1,12)	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	1:115:A:LEU:N	8	1.36
(1,4)	1:110:A:VAL:N	1:110:A:VAL:CA	1:110:A:VAL:C	1:111:A:MET:N	13	1.36
(1,127)	1:176:A:ALA:C	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	9	1.34
(1,33)	1:124:A:ASP:C	1:125:A:CYS:N	1:125:A:CYS:CA	1:125:A:CYS:C	7	1.34
(1,177)	1:211:A:GLU:C	1:212:A:GLU:N	1:212:A:GLU:CA	1:212:A:GLU:C	15	1.32
(1,39)	1:128:A:HIS:C	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	8	1.32
(1,139)	1:182:A:SER:C	1:183:A:LEU:N	1:183:A:LEU:CA	1:183:A:LEU:C	3	1.31
(1,78)	1:149:A:ALA:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	10	1.31
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	5	1.28
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	5	1.26
(1,12)	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	1:115:A:LEU:N	4	1.26
(1,143)	1:184:A:MET:C	1:185:A:VAL:N	1:185:A:VAL:CA	1:185:A:VAL:C	12	1.25
(1,40)	1:129:A:THR:N	1:129:A:THR:CA	1:129:A:THR:C	1:130:A:ARG:N	13	1.25
(1,12)	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	1:115:A:LEU:N	15	1.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,116)	1:169:A:SER:C	1:170:A:SER:N	1:170:A:SER:CA	1:170:A:SER:C	3	1.2
(1,116)	1:169:A:SER:C	1:170:A:SER:N	1:170:A:SER:CA	1:170:A:SER:C	7	1.2
(1,43)	1:132:A:GLN:N	1:132:A:GLN:CA	1:132:A:GLN:C	1:133:A:VAL:N	11	1.18
(1,31)	1:123:A:GLU:C	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	11	1.17
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	15	1.15
(1,33)	1:124:A:ASP:C	1:125:A:CYS:N	1:125:A:CYS:CA	1:125:A:CYS:C	11	1.15
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	3	1.13
(1,77)	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	1:150:A:GLY:N	13	1.13
(1,2)	1:109:A:ALA:N	1:109:A:ALA:CA	1:109:A:ALA:C	1:110:A:VAL:N	9	1.13
(1,144)	1:194:A:TRP:N	1:194:A:TRP:CA	1:194:A:TRP:C	1:195:A:MET:N	2	1.12
(1,139)	1:182:A:SER:C	1:183:A:LEU:N	1:183:A:LEU:CA	1:183:A:LEU:C	7	1.12
(1,127)	1:176:A:ALA:C	1:177:A:ASP:N	1:177:A:ASP:CA	1:177:A:ASP:C	13	1.1
(1,76)	1:148:A:TRP:C	1:149:A:ALA:N	1:149:A:ALA:CA	1:149:A:ALA:C	6	1.09
(1,31)	1:123:A:GLU:C	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	3	1.09
(1,169)	1:206:A:ARG:C	1:207:A:SER:N	1:207:A:SER:CA	1:207:A:SER:C	5	1.08
(1,37)	1:127:A:GLY:C	1:128:A:HIS:N	1:128:A:HIS:CA	1:128:A:HIS:C	13	1.08
(1,132)	1:179:A:ILE:N	1:179:A:ILE:CA	1:179:A:ILE:C	1:180:A:HIS:N	4	1.06
(1,143)	1:184:A:MET:C	1:185:A:VAL:N	1:185:A:VAL:CA	1:185:A:VAL:C	6	1.04
(1,116)	1:169:A:SER:C	1:170:A:SER:N	1:170:A:SER:CA	1:170:A:SER:C	1	1.04
(1,41)	1:129:A:THR:C	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1	1.04
(1,11)	1:113:A:ASP:C	1:114:A:VAL:N	1:114:A:VAL:CA	1:114:A:VAL:C	10	1.04
(1,42)	1:130:A:ARG:N	1:130:A:ARG:CA	1:130:A:ARG:C	1:131:A:LYS:N	1	1.03
(1,31)	1:123:A:GLU:C	1:124:A:ASP:N	1:124:A:ASP:CA	1:124:A:ASP:C	6	1.03